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Evaluation of Thermal Neutron Capture Gamma Spectra

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International Atomic Energy Agency, Vienna, Austria

May 2020

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Background

At the CSEWG Meeting at the Brookhaven National Laboratory in November 2019, Marie-Laure Mauborgne showed results of calculations relevant to oil-well logging, where new evaluations showed degraded performance compared to ENDF/B-VI.3, where experimental data for the gamma spectra were used in the evaluation. The case of ^{55}Mn was selected for a more detailed investigation because this is an IAEA evaluation that was adopted for ENDF/B-VII.1 and transferred without change into ENDF/B-VIII.0. The relevant plot from her presentation is shown in Figure 1.

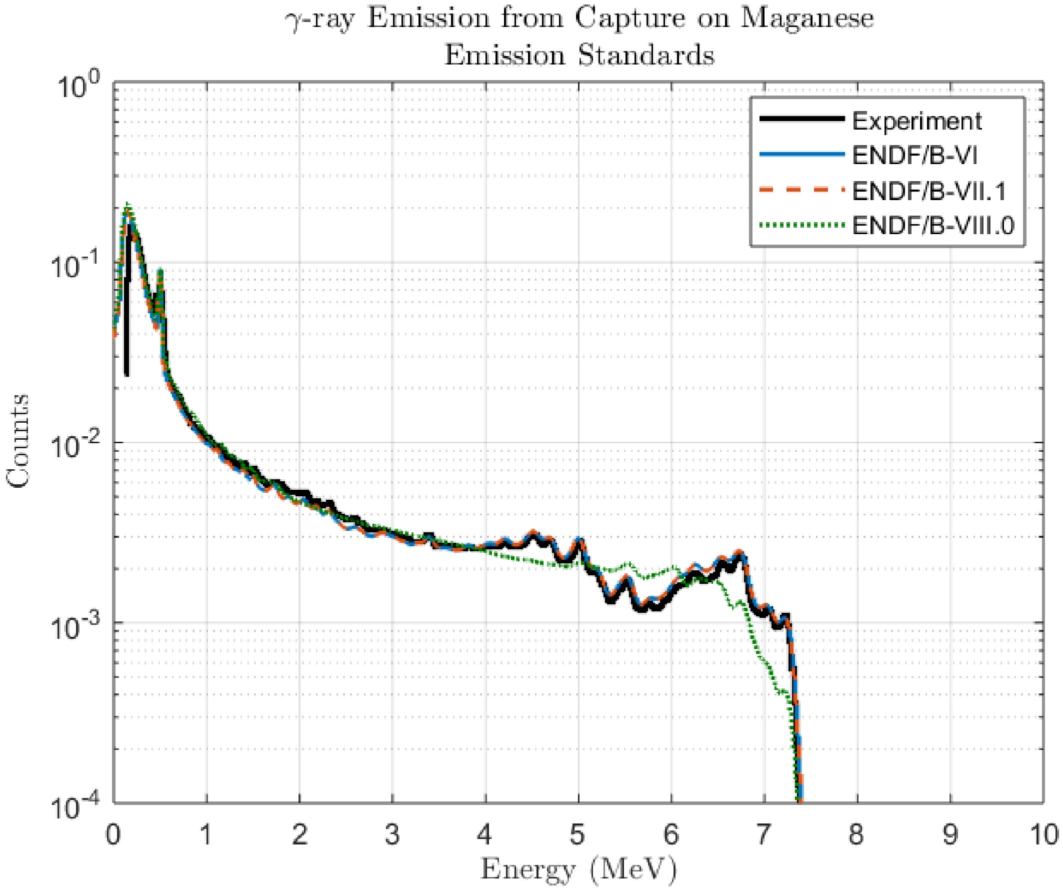

Figure 1 Comparison of calculated gamma spectra with different data libraries to the measured spectrum for a 55Mn Model Standard used at Schlumberger (note: label ENDF/B-VII.1 actually refers to ENDF/B-VII.0).

Assembly of an improved evaluated data file for ^{55}Mn

The original IAEA ^{55}Mn evaluation was based on EMPIRE calculation with level-scheme from the RIPL database. In principle, the low-energy part of the gamma spectrum which contains gammas from transition between well-established excited levels is expected to be highly accurate, reflecting the accuracy of the level scheme. However, the gamma spectra were calculated on a relatively coarse outgoing photon energy grid with resolution as a % of the outgoing energy. That makes the resolution of the high-energy primary gammas too poor for applications, leading to poor performance. Additionally, branching ratio information in the RIPL database is not as good as direct experimental data of photon emission for thermal neutrons contained in the EGAF database. Finally, the probability of emission of high-energy photons (e.g., above high 5 MeV) which are crucial for applications can be accurately derived from EGAF measurements, but not so from calculations. Comparison of the gamma spectra induced by thermal neutrons to the spectrum from the ENDF/B-VI.8 library is shown in Figure 2.

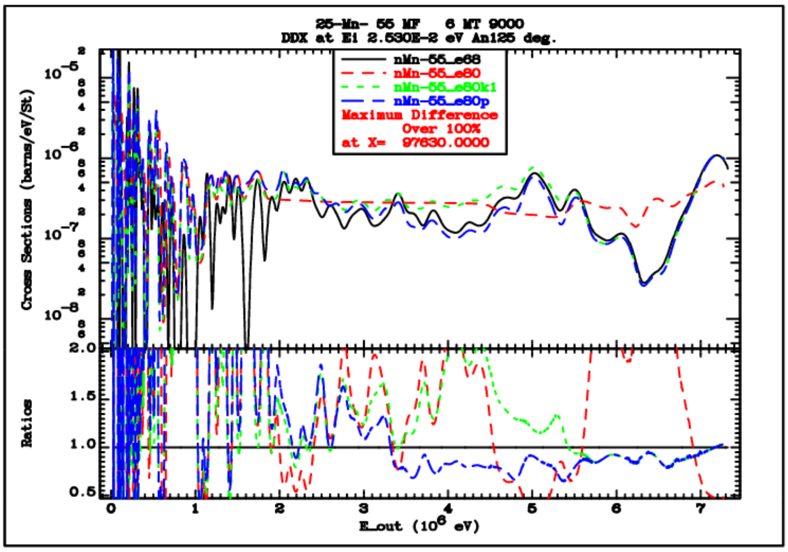

Figure 2: Comparison of the resolution-broadened thermal-neutron-induced gamma spectra from different libraries, namely ENDF/B-VI.8 (label "e68"), ENDF/B-VIII.0 (label "e80") and improved evaluations (suffix "e80k1" and "e80p").

Several differences in the spectra are observed. Below 2 MeV the ENDF/B-VI.8 spectrum is lower because it is based on empirical data and missing the continuum contribution, which cannot be extracted from experimental data. Above 2 MeV the ENDF/B-VIII.0 spectrum is flat because it is based on calculation, that relies on models that involve approximations for the transitions between levels in the continuum region. Improvements to the evaluation were attempted by:

- Explicitly including the gamma lines from the EGAF library, which are based on measured data below 2 MeV.

- Re-calculating the gamma-spectra with EMPIRE on a much denser energy grid using NEX=1000, i.e., thousands outgoing energy points (this is possible at low incident neutron energies where only the elastic and capture reaction channels are open).

- Taking into the account the continuum contribution to the gamma spectrum below 2 MeV, which is missing if only the gamma lines from EGAF are considered.

- Adding the EGAF primary gamma spectra to the continuum contribution calculated with EMPIRE above 2 MeV. The 5.9 MeV gamma line in EGAF was reduced by a factor of 10, because it was considered a typing error.

The spectrum is actually the double-differential cross section that can be decomposed into the cross section σg(E), multiplicity y(E) and the distribution f(E',μ), where the distribution is normalized such that the integral over the outgoing energy E' and the cosine of the scattering angle μ is equal to one:

$$\sigma_g(E,E',\mu) = \sigma(E)y(E)f(E',\mu)$$

At the incident neutron energies under consideration the gamma multiplicities y(E) are very weakly energy-dependent and can be assumed constant. The incident-neutron energy-dependence can be taken out by dividing by the cross section

$$\vartheta(E',\mu) = \sigma_g(E,E',\mu)/\sigma(E)$$

The gamma spectrum is assumed isotropic in EMPIRE, so the angular variable μ drops out. The cross sections calculated by EMPIRE may differ from the true cross sections from resonance analysis, but the ratio $\vartheta(E')$ is believed to be accurate.

The EGAF database gives gamma-production cross sections (in mb) from which the spectrum can be generated by approximating the delta-function in energy by trapezoidal shape functions of arbitrarily chosen width (set at 0.1 % of the energy of the gamma-line) such that the integrals match the individual gamma-production cross sections. Assuming that the gamma lines not present in EGAF do not contribute to the integral, we obtain the spectrum distribution $f(E',\mu)$ by normalizing the spectrum to one. The EGAF library is given for incident thermal neutrons. By scaling the EGAF normalized spectrum distribution with the gamma yield at thermal (from EMPIRE calculation) and dividing by the best-known thermal cross section we obtain $\vartheta_m(E')$ which is comparable to the $\vartheta_c(E')$ calculated with EMPIRE, noting that the shape does not include the continuum contribution to the spectrum.

The EMPIRE code was modified to suppress the addition of the primary gamma contributions to the spectrum. The $\vartheta_x(E')$ was calculated by dividing the calculated distribution with the same cross sections as used in obtaining $\vartheta_m(E')$. Primary gamma contribution from EGAF $\vartheta_m(E')$ was added. With this, all elements for the assembly of the spectra were available.

Procedure

EMPIRE calculation cannot be performed at very low incident neutron energies below 10 eV. The incident energy points in the EMPIRE calculation included 10 eV, 1 keV, 2 keV, 4 keV, 7 keV and 10 keV on an outgoing particle and photon energy grid of 1000 points. The calculated differential cross sections were divided by the corresponding calculated cross sections for the full spectrum to obtain $\vartheta_c(E')$. The same was done to obtain the continuum spectrum without the primary gammas $\vartheta_x(E')$. It was observed that the peaks from discrete-level transitions do not extend above outgoing energies of 2 MeV. The $\vartheta_c(E')$ was combined with the continuum contribution $\vartheta_x(E')$ above 2 MeV. To this distribution the EGAF contribution $\vartheta_m(E')$ for E'>2 MeV was added to obtain the final distribution $\vartheta(E')$.

$$\vartheta(E',\mu) = \vartheta_c(E',\mu) + \vartheta_m(E',\mu)\, ; E' < 2\ MeV$$

$$\vartheta(E',\mu) = \vartheta_x(E',\mu) + \vartheta_m(E',\mu)\,;E' > 2\ MeV$$

In the process of formatting the ENDF file the distribution $\vartheta(E')$ was normalized to one. The multiplicity y(E) was adopted from the full original EMPIRE calculation. The cross sections σg(E) were taken from the resonance analysis.

Conclusions

In the improved ^{55}Mn evaluation version "e80p" the spectrum in the energy range 1 MeV – 2 MeV is higher compared to ENDF/B-VI.8, which seems to be favorable, according the results in Figure 1. The evaluation in ENDF format will be available from the IAEA INDEN webpage at https://www-nds.iaea.org/INDEN. From 2 MeV to 5 MeV the spectrum is a bit lower, possibly due to some underestimation of the continuum component. Above this energy the spectrum in "e80p" is very similar to the one in ENDF/B-VI.8, which supports the normalization applied to the EGAF measured spectrum. The current evaluation is likely to enhance the performance for oil-well logging applications as shown in Figure 2, since for this and similar applications the high-energy peaks are more important than the energy region dominated by the continuum contribution.

The established evaluation procedure for the thermal-neutron-induced gamma spectra forms the basis for future improved evaluations of structural materials.

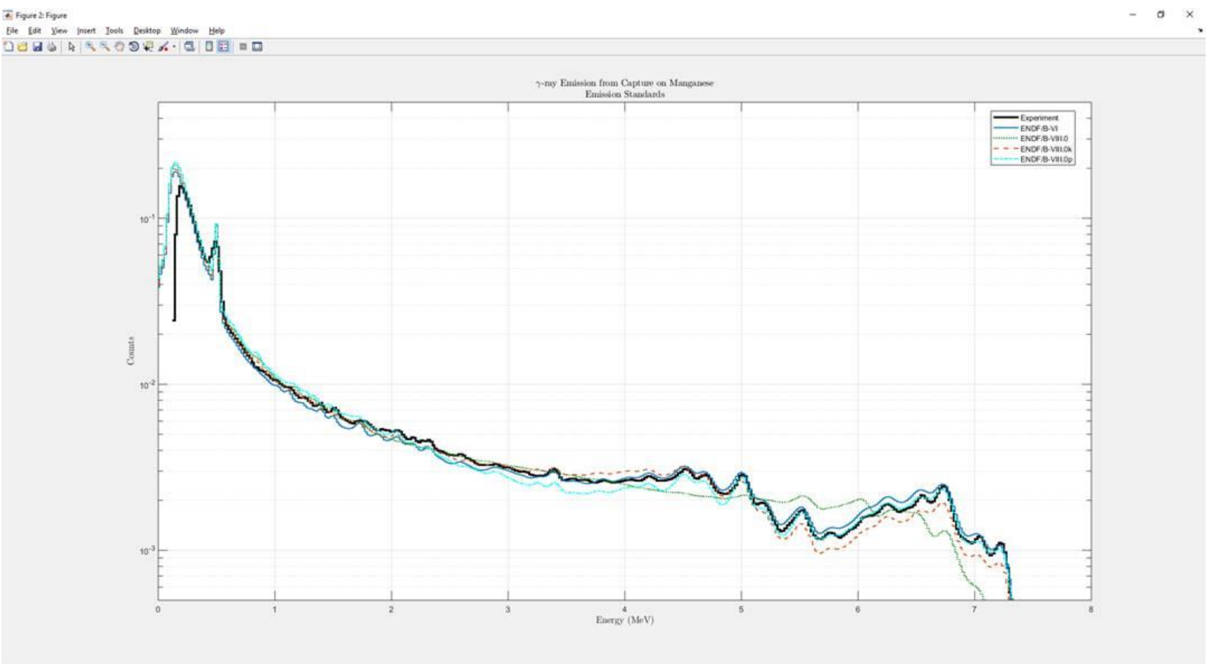

Figure 2 Comparison of calculated gamma spectra with different data libraries to the measured spectrum for a ^{55}Mn Model Standard used at Schlumberger (note: label ENDF/B-VII.1 actually refers to ENDF/B-VII.0). The cyan curve is the updated evaluation that shows an excellent agreement with data above 5 MeV.

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