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One-Group Cross Sections for $^{232}_{90}$Th, $^{233}_{92}$U, $^{238}_{92}$U, $^{235}_{92}$U and $^{239}_{94}$Pu Isotopes Averaged over OPAL and TERRA Neutron Spectra

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1. Introduction

Periodically, evaluated nuclear data libraries are updated. However, before being used to check certain values or as an input data for calculation softwares, these nuclear data must be processed. This work aims to present one-group microscopic cross sections for $^{232}_{90}$Th, $^{233}_{92}$U, $^{238}_{92}$U, $^{235}_{92}$U and $^{239}_{94}$Pu isotopes generated from the nuclear data processing codes PREPRO 2019, by the use of OPAL and TERRA's reactor specifics weighting functions. The cross sections obtained were compared with the cross sections weighted by Maxwellian and Fission functions of JEF Report 14 handbook.

2. Methodology

In this paper, LINEAR/RECENT/SIGMA1/GROUPIE codes from ENDF/B Pre-processing codes (PREPRO 2019) [1] were used to process $^{232}_{90}$Th, $^{233}_{92}$U, $^{235}_{92}$U, $^{238}_{92}$U and $^{239}_{94}$Pu nuclear data taken from the ENDF/B-VIII library [2]. LINEAR code linearizes the cross sections to an interpolable form, with accuracy of 0.1%. RECENT code adds the contribution of resonances to the cross sections, with reconstruction accuracy of 0.1%. SIGMA1 code Doppler broads the cross sections up to 300 K. GROUPIE code was used to calculate the one-group averaged microscopic cross sections using two specifics problem dependent weighting functions: i) thermal neutron flux of TG4 neutron guide (TG4 15 Oct, 300kW) of Open-Pool Australian Lightwater reactor (OPAL) [3] and, ii) neutron flux inside the fuel of "TEcnologia de Reatores Rápidos Avançados" (TERRA reactor) [4]. This code calculates the one-group averaged cross sections by

$$\overline{\sigma}^x = \frac{\int_{\mathrm{E_L}}^{\mathrm{E_H}} \sigma^x(\mathrm{E})\mathrm{S}(\mathrm{E})\mathrm{dE}}{\int_{\mathrm{E_L}}^{\mathrm{E_H}} \mathrm{S}(\mathrm{E})\mathrm{dE}}, \tag{1}$$

where $\overline{\sigma}^x$ represents the one-group averaged cross section for x neutron production reaction, σ^x is the pointwise cross section, $\mathrm{E_L}$ is the lower integration limit, $\mathrm{E_H}$ is the upper integration limit and S(E) is the energy dependent weighting function.

OPAL and TERRA weighting functions were recovered by GetData Graph Digitizer [5] software. For OPAL case, it was necessary to convert the measure unit of the abcissa axis, which was in wavelength, to eletron-volt energy, by applying the Broglie's and kinetic energy's equations,

$$\mathrm{E} = \frac{h^2}{2\lambda^2 m_n}, \tag{2}$$

where E denotes neutron energy, h is the Planck's constant, λ is the wavelength and m_n is the neutron mass. For this function, the energy band is from $\mathrm{E_L}$= 3.0E−03 eV to $\mathrm{E_H}$= 80 keV. In TERRA case, the energy band is from $\mathrm{E_L}$= 1 eV to $\mathrm{E_H}$= 20 MeV. Both functions S(E) are presented in Fig.1.

After the one-group microscopic cross sections generation, presented in Table I, the quality of these cross sections needed to be checked. The procedure was to compare the calculated values with those from the JEF Report 14 handbook [6], also showed in Table I.

The calculated values that used OPAL weighting function were compared with tabulated values for Maxwellian Average function, described by $\mathrm{S(E)} = \mathrm{E}\exp\left(-\mathrm{E}/\theta_{\mathrm{t}}\right)$, where $\theta_{\mathrm{t}} = 0.0253$ eV and the integration limits of the one-group averaged cross sections are $\mathrm{E_L}$= 1.0E−05 eV, $\mathrm{E_H}$= 10 eV. The calculated values that used TERRA weighting function were compared with tabulated values for Fission Average function, described by $\mathrm{S(E)} = \sqrt{\mathrm{E}}\exp\left(-\mathrm{E}/\theta_{\mathrm{f}}\right)$, with $\theta_{\mathrm{f}} = 1.35$ MeV, $\mathrm{E_L}$= 1 keV and $\mathrm{E_H}$= 20 MeV. The Maxwellian and Fission functions are also presented in Fig.1.

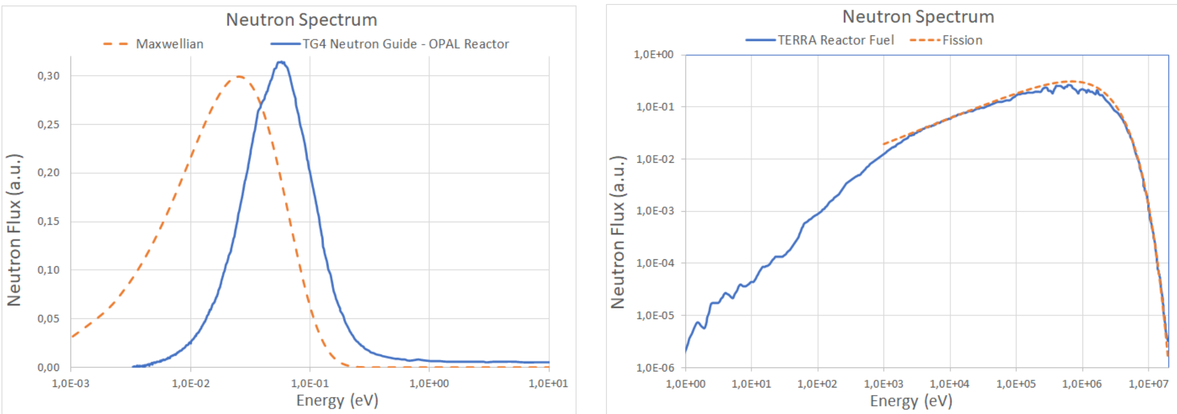

Figure 1: OPAL weighting function vs Maxwellian function (left) and TERRA weighting function vs Fission function (right).

3. Results and Discussion

The results were compared through percentage differences, Difference (%) $= 100\left(\frac{\mathrm{C}}{\mathrm{H}} - 1\right)$, where C and H represent the calculated and handbook cross sections values, respectively.

The results for OPAL function showed greater differences compared to Maxwellian function, mainly for $^{233}_{92}$U, $^{235}_{92}$U, and $^{239}_{94}$Pu isotopes, that have odd mass numbers. The Maxwellian function, as seen in Fig.1, has greater importance in the energy range from 1.0E−03 eV to 1.0E−01 eV, and it is precisely in this interval that the odd mass isotopes have the highest microscopic cross section variations, which contributes a lot to these large values. On the other hand, for even mass number isotopes, the total cross section showed a difference of −25.4% for $^{232}_{90}$Th and 19.3% for $^{233}_{92}$U. These differences are within expectations, since these isotopes's cross sections vary little in the energy range from 1.0E−03 eV a 1 eV, most important range of OPAL and Maxwellian function. Fig.2 presents $^{235}_{92}$U and $^{238}_{92}$U total microscopic cross sections curves, for this energy range.

For comparison purposes between generated cross sections of TERRA and Fission function, in general, the differences do not exceed 6.5%, except for the inelastic reaction of $^{233}_{92}$U, (n,g) reaction of $^{239}_{94}$Pu and (n,2n) and (n,3n) reactions of all the five isotopes. This high difference is due to the change of both the nuclear data library version and the weighting functions used.

Table I: One-group microscopic cross sections from Maxwellian, OPAL, Fission and TERRA functions (barns).

Nuclide	Reaction	Maxwellian function	OPAL function	Difference (%)	Fission function	TERRA function	Difference (%)
$^{232}_{90}$Th	Total	19.54	14.58	−25.4	7.695	7.775	1.0
	Elastic	12.99	13.91	7.1	4.805	4.951	3.1
	Inelastic	-	-	-	2.703	2.626	−2.9
	n,2n	-	-	-	1.940 10^{-2}	2.545 10^{-2}	31.2
	n,3n	-	-	-	2.293 10^{-4}	2.609 10^{-4}	13.8
	Fiss.	-	-	-	7.428 10^{-2}	7.840 10^{-2}	5.5
	n,g	6.564	6.122 10^{-1}	−90.7	9.333 10^{-2}	9.338 10^{-2}	0.1
$^{233}_{92}$U	Total	522.6	14.39	−97.2	7.672	7.705	0.4
	Elastic	12.46	10.84	−13.0	4.810	4.537	−5.7
	Inelastic	-	-	-	8.882 10^{-1}	1.194	34.4
	n,2n	-	-	-	6.514 10^{-3}	2.724 10^{-3}	−58.2
	n,3n	-	-	-	3.643 10^{-6}	2.897 10^{-6}	−20.5
	Fiss.	468.4	3.14	−99.3	1.911	1.909	−0.1
	n,g	41.78	3.747 10^{-1}	−99.1	5.686 10^{-2}	6.019 10^{-2}	5.9
$^{238}_{92}$U	Total	11.87	14.16	19.3	7.792	7.822	0.4
	Elastic	9.44	13.53	43.3	4.860	4.835	−0.5
	Inelastic	-	-	-	2.544	2.579	1.4
	n,2n	-	-	-	1.763 10^{-2}	2.221 10^{-2}	26.0
	n,3n	-	-	-	1.372 10^{-4}	1.716 10^{-4}	25.1
	Fiss.	1.052 10^{-5}	9.222 10^{-5}	776.6	2.990 10^{-1}	3.174 10^{-1}	6.2
	n,g	2.43	5.405 10^{-1}	−77.8	7.095 10^{-2}	6.885 10^{-2}	−3.0
$^{235}_{92}$U	Total	612.2	14.34	−97.7	7.663	7.769	1.4
	Elastic	15.04	11.02	−26.8	4.418	4.598	4.1
	Inelastic	-	-	-	1.917	1.831	−4.5
	n,2n	-	-	-	1.369 10^{-2}	1.752 10^{-2}	28.0
	n,3n	-	-	-	1.922 10^{-5}	2.286 10^{-5}	19.0
	Fiss.	509.9	2.42	−99.5	1.218	1.230	1.0
	n,g	87.28	8.510 10^{-1}	−99.0	9.557 10^{-2}	9.442 10^{-2}	−1.2
$^{239}_{94}$Pu	Total	987.6	14.44	−98.5	7.790	7.813	0.3
	Elastic	7.78	11.33	45.7	4.421	4.391	−0.7
	Inelastic	-	-	-	1.535	1.576	2.7
	n,2n	-	-	-	7.379 10^{-3}	5.483 10^{-3}	−25.7
	n,3n	-	-	-	1.160 10^{-5}	1.748 10^{-5}	50.7
	Fiss.	703.0	1.92	−99.7	1.784	1.791	0.4
	n,g	276.8	7.987 10^{-1}	−99.7	4.167 10^{-2}	4.748 10^{-2}	14.0

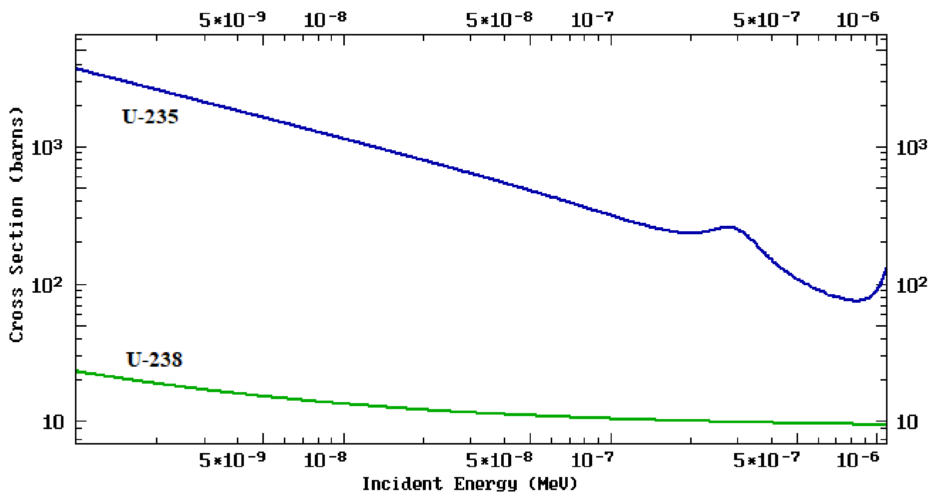

Figure 2: $^{235}_{92}$U and $^{238}_{92}$U total microscopic cross sections curves from 1.0E−03 eV to 1 eV.

4. Conclusions

The paper showed the cross sections results for the $^{232}_{90}$Th, $^{233}_{92}$U, $^{238}_{92}$U, $^{235}_{92}$U, $^{239}_{94}$Pu isotopes obtained from the calculations made by the nuclear data processing codes PREPRO 2019, that used OPAL and TERRA's reactor specifics weighting functions and compared with the cross sections average values from the JEF Report 14 handbook, that used respectively Maxwellian and Fission functions.

The microscopic cross sections calculated with OPAL and TERRA functions presented maximum differences close to 100% and 30%, respectively, when compared to the Maxwellian and Fission functions, indicating that Maxwellian wasn't a good choice to be used as weighting function, while Fission was.

The understanding and careful processing of nuclear data are necessary and it is very important to know the neutron spectrum of the problem, so that an appropriate weighting function can be used for verification.

This work is part of the Master's thesis of the first author and it intends to produce two handbooks, one of that contains pointwise cross sections (0.0253 eV and 14 MeV) and the other one-group cross sections, for all neutron induced reactions from ENDF/B-VIII.0 library, using the same codes, with five problem dependent weighting functions to be available for universities and research institutes.

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