Analysis constants for database of neutron nuclear data

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Abstract. At present there is a variety of experimental and calculation nuclear data which are rather entirely presented in the following evaluated nuclear data libraries: ENDF (USA), JEFF (Europe), JENDL (Japan), TENDL (Russian Federation), ROSFOND (Russian Federation). Libraries of nuclear data, used for neutron-physics calculations in programs: Scale (Origen-Arp), MCNP, WIMS, MCU, and others. Nevertheless all existing nuclear data bases, including evaluated ones, contain practically no information about threshold neutron reactions on ^{232}Th nuclei; available values of outputs and cross-sections significantly differ by orders. The work shows necessity of nuclear constants corrections which are used in the calculations of grids and thorium storage systems. The results of numerical experiments lattices and storage systems with thorium.

1. Introduction

Accuracy of cross-sections evaluation of neutron interaction in fuel compositions is very important for reliable evaluation of uranium-thorium nuclear fuel cycle (NFC). At present there is a variety of experimental and calculation nuclear data which are rather entirely presented in the following evaluated nuclear data libraries: ENDF (USA), JEFF (Europe), JENDL (Japan), TENDL (Russian Federation), ROSFOND (Russian Federation).

One of the most valuable sources of information is the international library ENDSF (Evaluated Nuclear Structure Data File), which provides recommended data as well as initial experimental data's. It should be noted that the libraries of such nuclear data are used for neutron-physical calculations in such precision programs as Scale (Origen-Arp), MCNP, WIMS, MCU and other.

Nevertheless all existing nuclear data bases, including evaluated ones, contain practically no information about threshold neutron reactions on ^{232}Th nuclei; available values of outputs and cross-sections significantly differ by orders. If we consider nuclear data base JENDL-4.0 as an example, in which during neutron data preparation for thermal and epithermal the energies of ^{232}Th fission cross-sections, were prepared based on simple physical consumptions, which give the dependence of ~1/υ type. There is no sufficient data necessary for calculation of threshold neutron reactions on ^{232}Th nuclei in the nuclear data base ENDF/B-VIII.0, which is recommended by the majority of computing engineers. Thus it is difficult to speak about practical certainty of existing data for threshold reactions on ^{232}Th nuclei in the range of thermal energies and resolved resonances.

Current situation concerning cross-sections of radiation capture is perfectly demonstrated by the researches carried out in Japan (Kyoto university, 2004) [1]. The comparison of the values of cross-sections radiation capture on ^{232}Th nuclei was performed using SRAC system code from evaluated nuclear data libraries (JENDL-3.3, JENDL-4.0, ENDF/B-VIII, JEFF 3.1.1). Result shows that there is significant gap (up to ~40%) between the libraries.

Considering the importance of thorium data and concerning about the accuracy of ^{232}Th cross section libraries, a series of experiments on thorium critical core with different neutron spectra has been implemented at Kyoto University Critical Assembly [2]. Calculations of sensitivity coefficient of ^{232}Th reactivity were conducted and its result shows the more contribution of ^{232}Th cross section uncertainty at the thermal range to the calculation error. It suggests that ^{232}Th capture cross section is needed to be adjusted at thermal energy range to obtain more reliable calculated data.

It is obvious that plurality of information sources, their imperfection and disagreement can influence the results of critical calculations of the fuel-rod arrays and systems with thorium, mainly because in calculation of k_{eff} the required functionals have dependences σ_i(E,r,**Ω**).

In researches carried out for multiplying thorium-containing systems {(m%U,n%Th)O_2, (m%Pu,n%Th)O_2} operating on thermal neutrons the accuracy evaluation of available methods of resonant effects description was made. The calculation values showed that formalism describing the processes of neutrons interaction with nuclei, including absorption and scattering did not provide satisfactory agreement with the experimental data (Germany, Institute ISR-2 of the Forschungszentrum Julich, 1999) [3, 4].

Therefore there is vital necessity have precise nuclear data for calculating resonant absorption parameters in fuel-rod arrays ad systems containing thorium.

During numerical experiments on the study of reactor system physics, the most important is the constant provision state. Constant provision to calculation of slow nuclide kinetics even for uranium-plutonium fuel cycle is far from perfect. In the case of reactor systems with thorium nuclear fuel calculations is necessary to take into account imperfection of constant provision [5, 6].

It should be noted that the purpose of the work is to attract attention to the problem of using thorium in nuclear fuel cycle during execution of the new technology platform of nuclear power industry in Russia.

2. Analytical model of nuclear-physical processes in thorium-containing systems

The neutron interaction mechanism in the region of allowed and not allowed resonances, resonant interaction effects belong to the class of wave processes and can be considered as the product of the effective neutron "size" $\pi(\lambda_n/2\pi)^2$ and the transmissivity p of the phase surface formed by [7, 8]:

$$\sigma_c = \pi\left(\lambda_n / 2\pi\right)^2 \cdot p, \tag{1}$$

where the permeability $p = |\boldsymbol{J}_1| / |\boldsymbol{J}_2| = 4k_1 \cdot k_2/(k_1 + k_2)^2$ can be found from the Schrodinger equation, $|\boldsymbol{J}_1|$ and $|\boldsymbol{J}_2|$ are the probability density vectors of the transmitted and incident waves, and k_1 and k_2 are

the corresponding wave numbers of neutron.

At a stage of calculated estimates, we used the Fermi gas model within which the potential $V_c(r)$ should be presented as

$$V_c(r) = V_r(r) + iV_m(r), \tag{2}$$

where the real and imaginary parts of expression (2) are responsible for elastic and inelastic channels ofnuclear interactions, respectively.

One of such potentials is the Fermi pseudopotential

$$V_c(r) = \frac{2\pi\hbar^2}{\mu} \cdot b \cdot \delta(r) = U \cdot \delta(r), \tag{3}$$

where $\delta(r)$ is the Dirac delta function, b is the scattering length, and the parameter $b = x + iy$ is a complex quantity in the general case.

The parameter b in Eq. (3) was selected so that the calculated potential well depth U would correspond to the data of [7].

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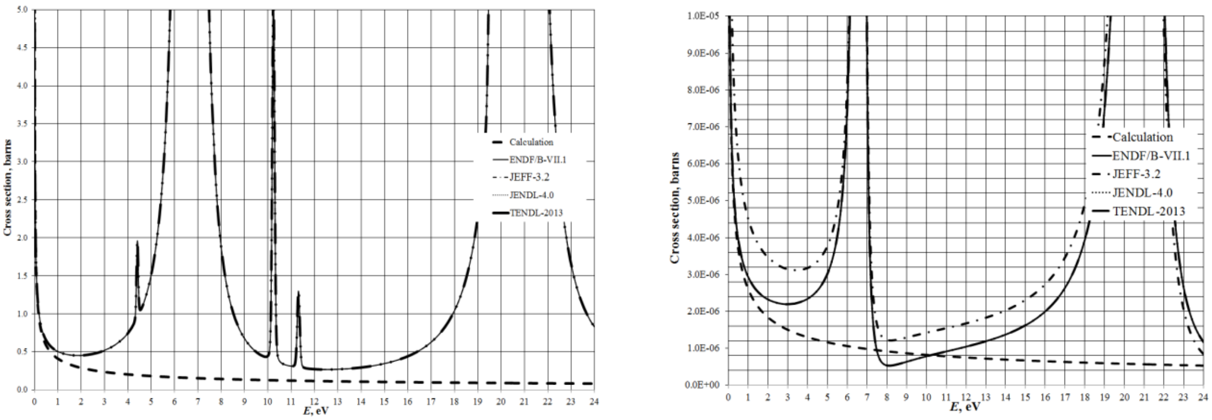
Taking into account relation (1) and the wavenumbers k_1 and k_2 found in solving the Schrödinger equation, the cross sections for ^{238}U and ^{232}Th were estimated in the energy range from 10^{-3} to 24 eV.

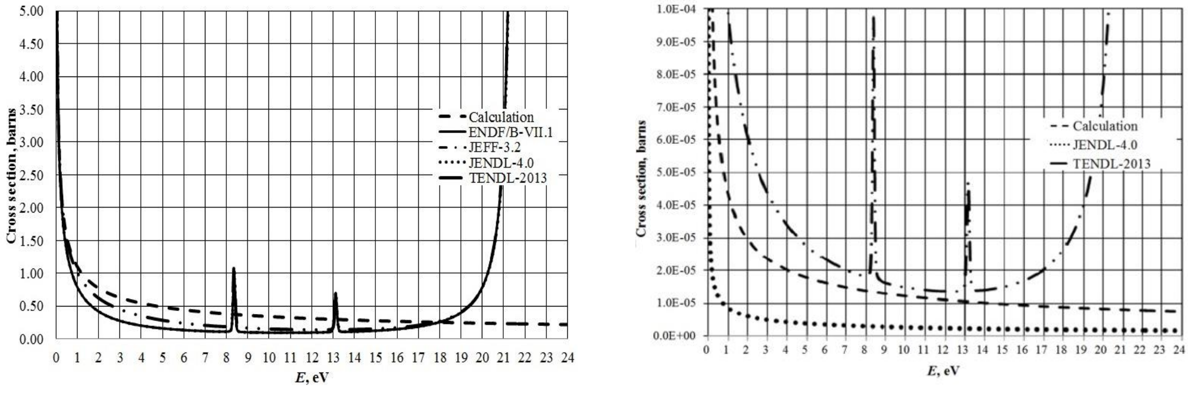
The found cross sections were compared with the data given in the ENDF/B-VII, JENDL-4.0, JEFF-3.1, and TENDL-2013 libraries. The results of comparisons are shown in Fig. 1 and 2.

The uncertainty in fission (σ_f) and radiative capture (σ_γ) cross sections for ^{238}U in the energy regions to 2.9 eV and 1.75 eV, respectively, does not exceed 30% (see Fig. 1). For ^{232}Th, the cross sections $\sigma\gamma$ with an accuracy of 30% can be found in the energy range from 10^{-3} to 0.8 eV (see Fig. 2).



(a) (b)

Figure 1. The results of calculated ^{238}U cross-sections are compared with evaluated nuclear data (ENDF/B, JEFF-3.2, JENDL-4.0, TENDL-2013) (a) Dependence of cross-section σ_γ of ^{238}U nucleus in the neutron energy range from 10^{-3} to 24 eV (b) Dependence of cross-section σ_f of ^{238}U nucleus in the neutron energy range from 10^{-3} to 24 eV.



(a) (b)

Figure 2. The results of calculated values of ^{232}Th cross-sections are compared with evaluated nuclear data (JENDL-4.0, TENDL-2013): (a) Dependence σ_γ of ^{232}Th nucleus in the neutron energy range form 10^{-3} to 24 eV (b) Dependence of ^{232}Th nucleus cross-section in the energy range from 10^{-3} to 24 eV.

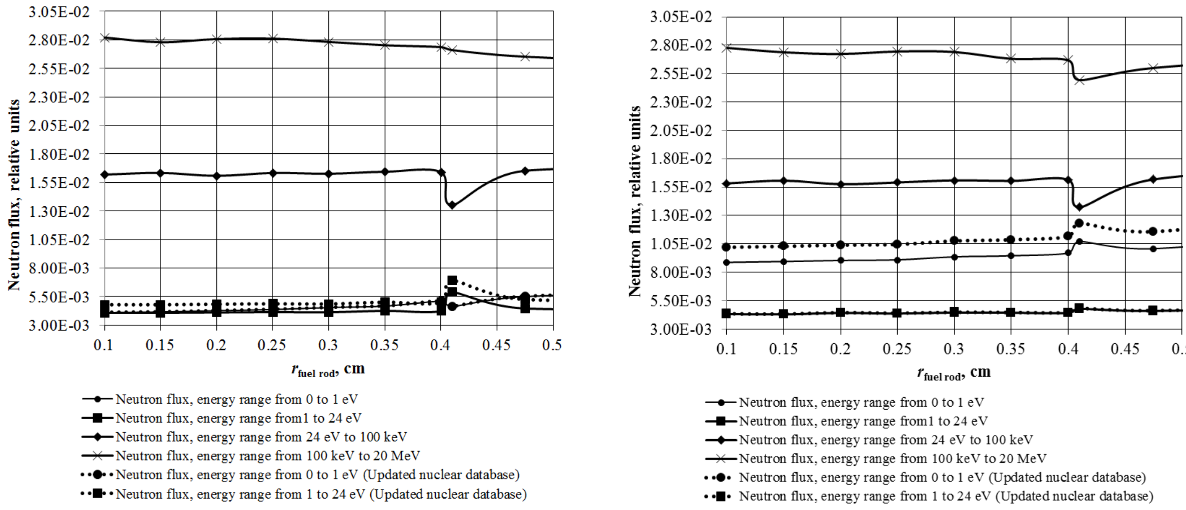
We note that the cross sections σf in the energy region to 4 eV, given in the TENDL for ^{232}Th differ significantly from those in the JENDL-4.0 (see Fig. 2), and the presence of the first two allowed resonances in the energy range from 6 to 14 eV seems doubtful.

In general, the structure of nuclear ^{232}Th absorption resonant region is enough in detail explored in the works [1, 2, 7–11]. Table №1 shows nuclear ^{232}Th absorption resonant region parameters convolution results for nuclear ^{232}Th in the range from 4 eV to 2,15 keV [9].

Table 1. Characteristics of ^{232}Th resonances.

Number group	The boundaries of the energy interval, eV	Number of resonance	E_r(eV)	σ_r,(b)	0,5Γ (eV)	$\overline{\sigma_r}$ (b)	$\overline{E_r}$ (eV)	$\overline{\Gamma}$ (eV)
21	4.65…10	–	–	–	–	–	–	–
20	10...21.5	–	–	–	–	–	–	–
19	21.5…46.5	1	22.5	1000	2	1000	34	4
18	46.5…100	2	60	1000	1.25	1000	73.3	4.25
		3	68	1000	3			
17	100…2150	4	114	425	1	405	157.5	2.2
		5	121.5	600	1			
		6	129	200	0.5			
		7	171	600	1.5			
		8	193	330	1.25			
		9	199	275	1.35			

Further nuclear-physical researches were carried out considering analytically corrected nuclear data and MCU5 program code [12].



(a) (b)

Figure 3. Space-energy distribution of neutron flux density in fuel element semi-array in IGR (a) Neutron flux distribution in fuel-rod arrays with thorium (5%Pu, 95%,Th)O_2; (b) Neutron flux distribution in fuel-rod arrays with thorium– (5%U, 95%Th)O_2.

Using the calculation code of MCU5 and evaluated data library files (ENDF/B and JENDL-4.0) and analytically calculated cross-sections values the nuclear constants used for determination of k_{eff} and evaluation of necessary functionals ($\sigma_i(E_i,r_i,\Omega)$ и $\varphi(\Delta E_i,r_i)$) were found. During preparation of the nuclear constants the technology developed in Nuclear Safety Institute, Russian Academy of Sciences

[13] was used. It is worth noting that macro constants for the spectrum part from 18 eV to 100 keV were determined using the MCU5 program code without correction of the nuclear data.

Such kind of approach allows not only to conduct correction of nuclear constants but to take into account fine structure of neutron absorption by nuclear ^{232}Th resonant region.

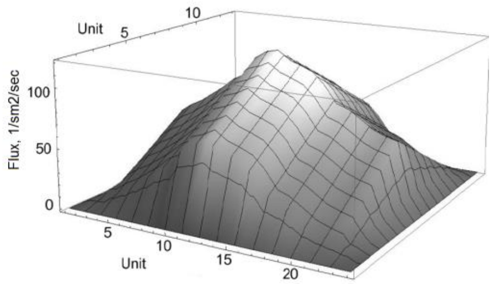
So we used the maximum opportunities theoretical analysis and nuclear data, which have long been received, evaluated and do not cause doubts. The results of calculations for multiplying systems with thorium are presented graphically in figure 3.

Neutron-physical researches of storage systems containing thorium were also carried out by the authors considering analytically corrected nuclear data. The calculation of k_{eff} and $\varphi(\Delta E_i,r_i)$ was made in the multigroup approximation using subgroup parameters during calculation of group coefficients in the decomposed Boltzmann equation (Scale 4.4) with the used of calculation methods [13, 14].

Figure 4 shows one of the DSSNF loading layouts allowing a decrease in the neutron radiation level at critical storage points to maximum allowable values (NRB-99/2009) [6]. The effective multiplication factor of the simulated system is $k_{eff} = 0.2148 \pm 0.0003$.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
11	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5
10	39	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	5
9	40	1	1	1	1	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	5
8	41	1	1	1	2	2	2	3	3	3	3	3	3	3	3	2	2	2	1	1	1	5
7	42	1	1	1	2	2	3	3	3	3	3	3	3	3	3	3	2	2	1	1	1	5
6	43	1	1	1	2	3	3	3	3	3	3	3	3	3	3	3	3	2	1	1	1	5
5	44	1	1	1	2	2	3	3	3	3	3	3	3	3	3	3	2	2	1	1	1	5
4	45	1	1	1	2	2	2	3	3	3	3	3	3	3	3	2	2	2	1	1	1	5
3	46	1	1	1	1	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	5
2	47	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	5
1	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69

(a)



(b)

Figure 4. Results of calculations of k_{eff} and $\varphi(\Delta E_i,r_i)$ of DSSNF systems with modified UGR fuel: (a) array 22×11 in size. Units 1, 2, 3 are seats with canisters, burnup fractions are 20, 25, 30 GW·day/tHM, respectively; Units 5, 39-69 are empty seats; (b) fast neutron flux as a function of unit layout in the array; INF storage is 10 years.

3. Conclusion

The work shows necessity of nuclear constants corrections which are used in the calculations of grids and thorium storage systems. The results of numerical experiments lattices and storage systems with thorium.

The performed theoretical studies and numerical experiments will make it possible to increase ecological, nuclear, and radiation safety of dry storage and transport systems for ceramic irradiated nuclear fuel of next generation reactor facilities.

Furthermore, the performed studies will allow the development of technical and regulating solutions for handling of promising irradiated nuclear fuel.

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