UDC 539.172

TESTING NEUTRON CROSS-SECTION FILES FROM THE BROND-2 AND ENDF/B-6 LIBRARIES IN BENCHMARK EXPERIMENTS ON NEUTRON TRANSMISSION THROUGH SPHERICAL LAYERS

A.A. Androsenko, P.A. Androsenko, A.I. Blokhin, N.T. Kulagin, V.G. Pronyaev and S.P. Simakov

Institute of Physics and Power Engineering, Obninsk

ABSTRACT

The effect of angular anisotropy in inelastic secondary neutron scattering on neutron leakage spectra from the surface of spherical specimens is investigated. It is shown how inadequate representation of the cross-section structure in the neutron energy resonance region can affect the neutron leakage spectrum.

The international thermonuclear experimental reactor project ITER is entering a new phase - the engineering design phase. An evaluated nuclear data library FENDL [1] is being set up to facilitate the supplying by the international scientific community of the necessary constants for the nuclear physics part of the engineering calculations, this being co-ordinated by the IAEA. The library comprises files of evaluated neutron cross-sections from the national libraries ENDF/B-VI (USA), JENDL-3 (Japan), EFF-2 (Western Europe) and BROND-2 (CIS).

The requirements for nuclear data and also their contemporary status are discussed in the survey in Ref. [2]. The reports in Ref. [3], presented at the IAEA Advisory Group Meeting on FENDL-2 and Associated Benchmark Calculations, show that benchmark experiments for complex multi-component or extended systems are often reproduced unsatisfactorily in calculations. As a rule, this is explained by gross errors in the macroscopic group cross-sections, whose cause is to be found either in the methods of presenting the original files of evaluated microscopic nuclear cross-sections or in the procedure for preparing the group cross-sections from these files.

At the same time another possible cause of the notable discrepancies may be the generally unsatisfactory quality of the microscopic data. A clear answer to the question of the quality of the microscopic evaluated data for different materials can be given only by analysing benchmark experiments carried out in simple geometry for single component materials. Such experiments include measurements of the partial or total leakage of neutrons and their energy spectra from a 14 MeV neutron source located at the centre of a spherical shell made of the material under investigation. A large number of benchmark experiments and calculations of this kind have served to improve the representation of secondary neutron emission spectra in the hard region and to provide indications as to the quality of description of the (n,2n) cross-sections in the evaluated data files.

The purpose of this work is to try and answer two questions concerning the representation of nuclear data in evaluated cross-section files and the calculation of neutron transport in systems with spectra characteristic of thermonuclear devices:

1. Does allowance for anisotropy in the shape of the angular distributions for the continuous part of the secondary neutron spectrum have a great effect on the neutron leakage spectra?

2. Is the fact that the experimental data considerably exceed the calculated values for the leakage spectra of secondary neutrons with energies 1-5 MeV from thick spherical shells (more than three free path lengths for 14 MeV neutrons) not due to inadequate representation of the cross-section structure in the evaluated neutron cross-section files?

Effect of allowance for anisotropy in the form of the angular distributions of the continuous part of the secondary spectrum on neutron leakage

From experimental [5] and theoretical [6] investigations of secondary neutron spectra in reactions induced by 14 MeV neutrons it is well known that the angular distributions in the hard part of emission spectra possess appreciable anisotropy with predominant leakage of neutrons at forward angles. It is evident that this circumstance may affect calculations of neutron transport in systems with geometry close to that of a thermonuclear reactor by increasing the penetration or leakage of neutrons with energies greater than 2 MeV. This also determines the higher requirements for accuracy of double differential neutron emission cross-sections (error not more than 10%) in the world list of nuclear data requirements - WRENDA [2].

However, only after switching to the evaluated neutron cross-section format in ENDF/B-6 [7] was it possible to represent the double differential cross-sections in files for the continuous spectrum region. The files of evaluated neutron cross-sections included in the FENDL library contain such data. Existing systems of programs for processing files into constants for calculating neutron transport are not sufficiently well adapted at present for operating with the ENDF/B-6 format. Therefore the question as to how much allowance for angular anisotropy in the secondary neutron emission spectra affects the description of neutron passage through media has remained open until recently. An oblique answer to this question was obtained by the authors of Ref. [8] in calculations by the discrete ordinates method of neutron leakage spectra for Be and Fe spheres with a 14 MeV source at the centre and with allowance for angular anisotropy of double differential cross-sections. The results of calculations by the Monte Carlo method in the approximation of angular isotropy of double differential cross-sections are presented in these works. As calculations have shown, allowance for angular anisotropy has practically no effect on the magnitude of the total leakage but can appreciably affect the leakage spectrum in the neutron energy region above 2 MeV. Thus, in the case of an iron sphere 30.45 cm thick, the leakage spectrum for neutrons with energy from 2 to 12 MeV is ~ 50% higher in calculations based on files containing anisotropy in the form of angular distributions for the continuous spectrum region.

To obtain a straight answer to this question, we performed calculations of the total leakage of neutrons and their energy spectra for spherical layers of beryllium and iron for neutrons from a 14 MeV source by the Monte Carlo and discrete ordinates methods. The calculations were based on files of evaluated neutron cross-sections from the ENDF/B-6 and BROND-2 libraries containing energy-angle distributions for secondary neutrons in the continuous spectrum region in tabular form or in the form of Kalbach parametrization [12]. In the calculations account was taken of the real geometry of the sphere and the ion guide channel, the geometry of the target, absorption of neutrons by the target holder, and the energy-angle distribution of source neutrons. All the information necessary for the calculations apart from the design of the target holder is supplied in Tables 1 and 2. The effect of the target holder design on neutron yield is discussed in Ref. [9]. In comparing the experimentally-observed partial leakage spectra with the theoretical ones, the latter were not averaged over the energy with the spectrometer resolution function determined experimentally.

The results of calculations of the 4π neutron leakage spectra in comparison with experimental data are shown in Figs 1 and 2. The calculations were performed both by the Monte Carlo method with and without allowance for angular anisotropy in the continuous part of the secondary neutron spectra and by the discrete ordinates method with group description of the cross-sections and the transfer matrices. For greater clarity, Fig. 3 shows the ratio of calculations allowing for angular anisotropy in the secondary neutron spectra to calculations in the isotropic approximation. For performing calculations by the Monte Carlo method, the BRAND [10] program was adapted so that the files of evaluated cross-sections in ENDF/B-6 format could be used directly. The calculations were performed for neutron *energies above 0.2 MeV for beryllium and 1.0 MeV for iron. For calculations by the* discrete ordinates method we used the ANISN program [11], the group constants for which were prepared with the aid of the NJOY-87 program. The S16P11 approximation was performed in calculations of neutron transport with allowance for angular anisotropy for all processes in the 100 group representation (GAM grouping).

The results of calculations of partial leakage with very arbitrary energy grouping of source neutrons (10-20 MeV), scattered neutrons (5-10 MeV), (n,2n) reaction neutrons (1-5 MeV) and slow neutrons (below 1 MeV) are presented in Tables 3-5 in comparison with experimental data.

After analysing these data, we come to the conclusion that allowance for angular anisotropy for the continuous part of the neutron emission spectrum:

(a) has practically no effect on the magnitude of the integral neutron leakage for spheres with a thickness several times the free path length;

(b) leads to an increase by several tens of per cent in the leakage in the "scattered" neutron group when there is a low absolute contribution by this group to the total leakage.

In view of this, the accuracy requirement for presentation of double differential cross-sections (above 10%) in the WRENDA list for thermonuclear applications is evidently exaggerated. It is possible that such a requirement needs to be maintained for the representation of energy spectra but the accuracy requirement for the representation of angular distributions for the continuous part of the spectrum appears unjustified, and in any case it is already achieved with Kalbach and Mann's parametrization [12].

Representation of the cross-section energy structure in evaluated data files when performing benchmark calculations

The fraction of the neutron leakage spectrum with energy below a few MeV for large thicknesses of the spherical layers becomes predominant for a 14 MeV neutron source. Comparison of measurements and calculations of leakage spectra for iron spheres with a thickness of around 7 free path lengths (Δd = 30.45 cm) shows experimental values considerably - up to several times - in excess of theory [13] for the leakage spectrum in the region $1 < E_n < 5$ MeV. Such a trend was also observed for large-diameter lead spheres [14]. Attempts to attribute these discrepancies to deficiencies in the experimental data are unsatisfactory in our opinion.

Possible causes of such discrepancies may be: inadequate representation of neutron cross-section structure in evaluated nuclear data files for neutrons with energy above the resonance region, too low a value of the (n,2n) reaction cross-section and too hard a form of the secondary particle emission spectrum. For iron the upper limit of the resonance region in contemporary files is 850 keV. The cross-sections were given above in the pointwise representation with structures taken from experimental data possessing the best energy resolution. As a rule these are measurements performed on the ORELA accelerator at Oak Ridge. However as shown in Ref. [15], even data from experiments with high resolution do not enable one to describe the "observed" self-shielding factors of the total cross-section in experiments with poor resolution. The reason for this is that, even in experiments with the highest resolution for energies above the resonance region, the true structure of the cross-sections in not fully resolved. Figure 4 shows the self-shielding factors of the total cross-sections determined in experiments with poor resolution for transmission through thick specimens in comparison with data calculated from experimental data obtained with high resolution.

To demonstrate the effect of the cross-section structure on neutron leakage, we carried out calculations of leakage spectra for an iron sphere 30.45 cm thick with different groupings and a 14 MeV neutron source. In the calculations we used the ^{nat}Fe file from the BROND-2 library, where the total cross-sections for energy above 850 keV (up to 2.1 MeV) are the total cross-sections for natural iron, measured on ORELA, while below 850 keV they are represented as the resolved resonance region. With the aid of the NJOY-87 programme, the systems of group constants were prepared in which the 19-group constant system having group boundaries above 100 keV as in the BNAB system was used as the base. It may be assumed that in the pointwise representation of the cross-sections reconstructed from the resonance parameters their structure for energies below 850 keV is on average correctly reproduced. Calculations of the total and partial neutron leakage for the energy interval 400-800 keV were performed with the aid of the ANISN programmes in the S16P3 approximation. The calculations were performed for a one-group cross-section representation in this interval for a seven-group division (GAM grouping, average group width 60 keV), for a 20-group division (20 keV) and for an 80-group division (5 keV). The group boundaries outside this energy interval were unchanged.

The results of calculations of partial neutron leakage in the energy interval 400-800 keV, based on different groupings, are shown in Table 6. The leakage spectra for 20-group and 80-group divisions are shown in Fig. 5. It should be noted that grouping with a group width less than 5 keV makes it possible to reproduce details of the cross-section structure conditioned by the contribution of the s-wave and, in particular, large dips in cross-sections occurring with interference of resonance and potential scattering. It can be seen from the Table that partial leakage in the 400-800 keV energy interval increases by 40% with a more detailed representation of cross-sections. The total leakage in this case increases by only 1.5%, since a certain amount of compensation arises owing to its reduction in the lower groups. Evidently, in order to allow for the structure of cross-sections conditioned by the contributions of higher waves (from resonances of small width), it is necessary to have either a finer grouping or to make correct allowance in the transport calculations for self-shielding of the cross-sections.

The conclusions obtained for the 400-800 keV neutron energy interval can also be applied to higher energies (for iron and other constructional materials up to energy 3-4 MeV). This is because even with the detailed pattern of the cross-sections given in the files it is not possible to obtain the correct value of the total cross-section self-shielding coefficient (Fig. 4).

Ref. [16] presents a simple formula for improving the description of total cross-section self-shielding for the neutron energy region above resonance. This involves artificially increasing the cross-sections at the maxima and reducing them at the minima whilst maintaining the energy-averaged cross-sections. It is possible that multigroup calculations (with number of groups ~ 1000 for E_n = 1-5 MeV) in the discrete ordinates method, using nuclear data files corrected by this method, will enable better agreement to be obtained with experimental results for neutron leakage spectra from thick spherical layers.

Conclusions

Consideration of the results of benchmark experiments on iron enables the following conclusions to be drawn and recommendations made for improving the file of evaluated neutron cross-sections for iron in the BROND-2 library:

1. Partial leakage in the source neutron group ($E_n > 10$ MeV) is appreciably too high, indicating too high an elastic scattering cross-section (by about 10%) at energies above 10 MeV;
2. Partial leakage in the scattered neutron group is also too high which is caused by a too hard inelastically scattered neutron spectrum with excitation of discrete low-lying levels (contribution of direct processes too high);
3. Since the total cross-section for iron given in the BROND-2 library file is known with high accuracy, while the elastic cross-section is too high, the total cross-section for inelastic processes (mainly inelastic scattering and (n,2n) reaction cross-sections), which lead to substantial softening of the leakage spectra is too low, as can be seen from the figures and tables presented here;
4. For calculating the leakage spectra in the neutron energy region below 4 MeV and up to the upper limit of the resolved resonance region, it is necessary to have detailed knowledge of the cross-section structure and to perform calculations pointwise with respect to energy or by the multigroup approach. An alternative to this could be to use small-group approaches with successive allowance for self-shielding of cross-sections.

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TABLE 1. CHARACTERISTICS OF SPHERES USED IN THE CALCULATIONS

Material, reference	Density with respect to the basic material	Radius of sphere, cm		Radius of channel, cm	Allowance for impurities
		Internal	External		
Beryllium [17]		6.0	11.0	2.5	No
Iron [9]		4.5	12.0	3.1	No
Iron [19]	7.87	7.65	38.1		No

TABLE 2. ANGLE-ENERGY DISTRIBUTIONS AND SOURCE NEUTRON YIELDS PRESENTED IN THE FORM OF A HISTOGRAM

Interval of angles in the scale, cos (θ)	Source neutron energy interval, MeV	Neutron yield, I/d (cos(θ))
-1.0 - -0.8	13.358 - 13.504	0.09516
-0.8 - -0.6	13.504 - 13.651	0.09626
-0.6 - -0.4	13.651 - 13.800	0.09726
-0.4 - -0.2	13.800 - 13.951	0.09840
-0.2 - 0.0	13.951 - 14.103	0.09942
0.0 - 0.2	14.103 - 14.257	0.10050
0.2 - 0.4	14.257 - 14.413	0.10160
0.4 - 0.6	14.413 - 14.571	0.10270
0.6 - 0.8	14.571 - 14.730	0.10381
0.8 - 1.0	14.730 - 14.891	0.10496

TABLE 3. PARTIAL NEUTRON LEAKAGES FROM A BERYLLIUM SPHERE, $\Delta d = 5$ cm

Neutron energy, MeV	Experiment, [17]	Calculation using BRAND (^{56}Fe, ENDF/B-6)	
		With allowance for anisotropy in the "continuum"	Without allowance for anisotropy in the "continuum"
0.4 - 1.0	0.12	0.094	0.095
1.0 - 3.0	0.157	0.137	0.131
3.0 - 10.0	0.178	0.161	0.148
10.0 - 15.0	0.690	0.730	0.716

TABLE 4. PARTIAL NEUTRON LEAKAGES FROM AN IRON SPHERE, Δd = 7.5 cm

Neutron energy, MeV	FEhI experiment [9]	IAEh experiment [20]	Calculation	
			BRAND (ENDF/B-6)	ANISN (S16P11) (BROND)
1.0 - 5.0	0.295	0.362	0.244	0.272
5.0 - 10.0	0.0492	0.05	0.029	0.0396
10.0 - 15.0	0.511	0.427	0.364	0.448
1.0 - 15.0	0.8552	0.839	0.637	0.7596

FEhI = Institute of Physics and Power Engineering, Obninsk
IAEh = I.V. Kurchatov Institute of Atomic Energy

TABLE 5. PARTIAL NEUTRON LEAKAGES FROM AN IRON SPHERE, Δd = 30.45 cm

Neutron energy, MeV	Experiment [19]	Calculation ANISN (S16P11) (BROND)
1.0 - 2.2	0.19 ± 0.01	0.0657
2.2 - 5.0	0.023 ± 0.001	0.0184
5.0 - 10.0	$(5.3 \pm 2.2) \cdot 10^{3}$	$7.4 \cdot 10^{-3}$
10.0 - 15.0	0.02 ± 0.001	0.0396
2.2 - 15.0	0.0483	0.065

Note: Partial neutron leakages are the number of neutrons per source neutron in the given energy interval.

TABLE 6. PARTIAL NEUTRON LEAKAGES IN THE ENERGY INTERVAL 0.4-0.8 MeV FOR AN IRON SPHERE WITH Δd = 30.45 cm FOR DIFFERENT GROUPINGS WITHIN THIS INTERVAL

Number of groups	Width of group, keV	Calculation ANISN (S16P11) (BROND)
1	400	0.196
7	~60	0.224
20	20	0.255
80	5	0.271
1	400*	0.326

* With allowance for self-shielding.

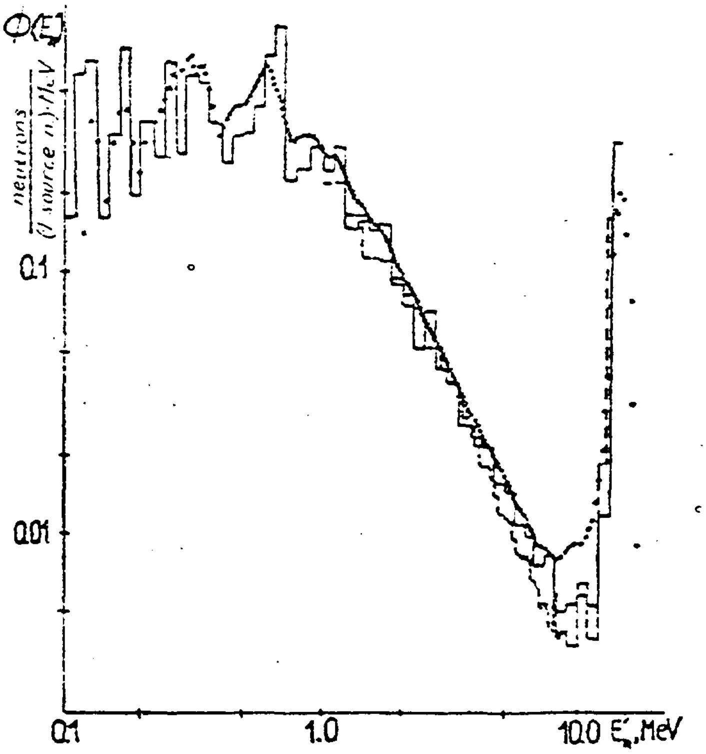

FIG. 1. Leakage neutron energy spectrum for an iron sphere with Δd = 7.5 cm. The points represent experimental data [9], the broken line the results of calculation by the Monte Carlo method with the BRAND program for ^{56}Fe from the ENDF/B-6 library, and the solid line the results of calculation by the discrete ordinates method with the ANISN program in the S16P11 approximation for ^{nat}Fe from the BROND library.

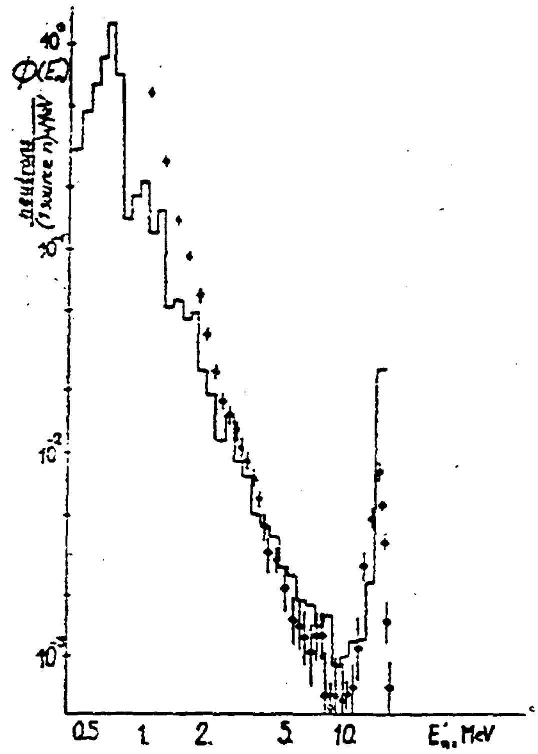

FIG. 2. Energy spectrum of leakage neutrons for an iron sphere with Δd = 30.45 cm. The points represent experimental data [19] and the solid line the results of calculation by the discrete ordinates method with the ANISN program in the S16P11 approximation for ^{nat}Fe from the BROND library.

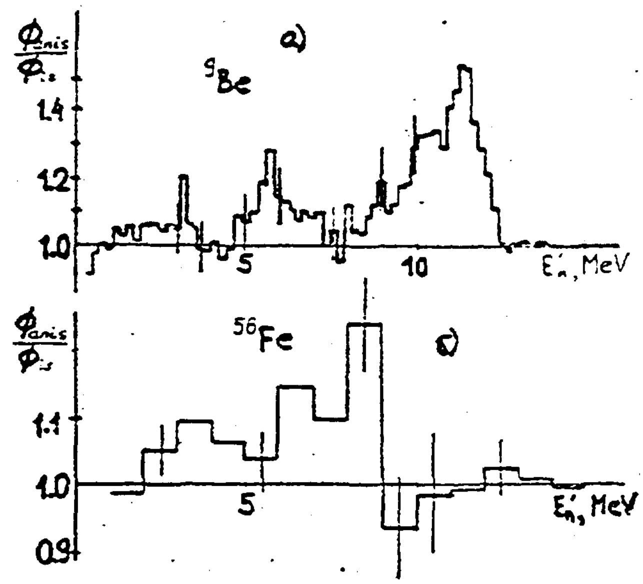

FIG. 3. Ratio of the leakage spectra calculated with allowance for anisotropy in the angular distributions of inelastic processes to the same spectra without such allowance (a) for a beryllium sphere with Δd = 5 cm and (b) for an iron sphere with Δd = 7.5 cm. In the calculations by the Monte Carlo method the ENDF/B-6 library files for ^{9}Be and ^{56}Fe were used. The statistical errors of the calculations are indicated.

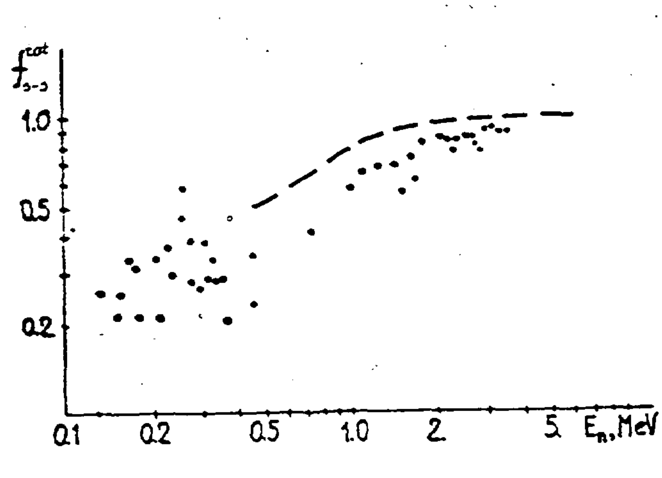

FIG. 4. Self-shielding factors of iron cross-sections from Ref. [15]. The points represent experimental data from measurements for transmission in thick specimens and the broken line the results of calculation from experimental data (point curves of cross-sections), measured with high resolution.

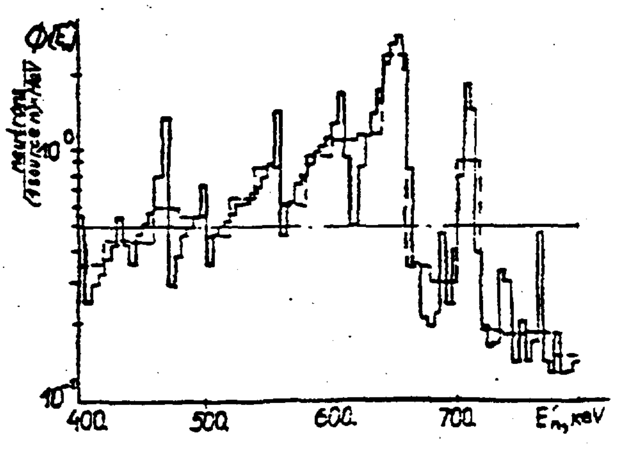

FIG. 5. Neutron leakage spectra from an iron sphere with Δd = 30.45 cm in calculations using the ANISN program with different groupings in the 400-800 keV energy interval. The solid line represents 80 groups and the broken line 20 groups.