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L26P3S34 - A 26-Group Library for the Computation of Neutron Transfer in Shielding Media

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A B S T R A C T

A 26-group 34-material library prepared by a modified version of SUPERTOG from the ENDL-2 evaluated data file is presented. A brief description of the algorithm of Legendre's polynomial expansion is given. This algorithm constitutes the basis of converting the tabulated anisotropy data of ENDL-2 into a form suitable for SUPERTOG processing. The performance of the algorithm is discussed and the library format is outlined. Additional data, facilitating the use of the library, are assembled in 3 tables.

The L26P3S34 library (ENDL 26-group up-to-P3 library prepared by SUPERTOG for 34 materials) is produced from the Evaluated Nuclear Data File ENDL-2 by means of a modified version /1/ of the SUPERTOG-3 code /2/.

SUPERTOG computes the average scattering cross sections for given energy groups as well as the P_n-matrices of elastic, inelastic and (n,2n) scattering.

The use of SUPERTOG for converting the evaluated data of ENDL into multigroup constants displays at least two peculiarities:

(a) The cross-section smooth and resonance parts are combined in ENDL-2 /3/; therefore, the SUPERTOG routines for resonance processing are skipped;

(b) The elastic-scattering anisotropy data in ENDL-2 have the form of tabulated values of the probability-density function which depends on the scattering angle and on the incident energy. The standard version of SUPERTOG-3, however, is able to compute the P_n-matrices of elastic scattering if and only if this function is represented by its expansion coefficients in a Legendre polynomial series. In our modified version of the same program /1/ these coefficients are computed from the tabulated values in a preparatory routine within a single SUPERTOG run, before the P_n elastic-scattering matrices are calculated.

The present report contains a brief description of the algorithm of Legendre's polynomial expansion, some observations on the performance of this algorithm, and the format specifications of the L26P3S34 library.

1. Calculation of the expansion coefficients

To compute the P_n elastic-scattering matrices SUPERTOG needs (a) the average values of cross sections over energy groups involved, and (b) scattering anisotropy data in the centre-of-mass system. The latter are represented in the evaluated nuclear data files of the ENDF/B format as:

either (i) tabulated values of $p(\mu, E)$, the probability-density function for scattering a neutron with incident energy E at angle $\cos^{-1}\mu$. In this case the LTT flag of ENDF/B equals 2;

or (ii) coefficients $f_\ell(E)$ of the function $p(\mu, E)$ in the form of truncated series over Legendre's polynomials

$$p(\mu, E) = \sum_{\ell=0}^{N} \frac{2\ell+1}{2} f_\ell(E) L_\ell(\mu), \qquad (1)$$

where N is the optimum order of truncation. Here LTT=1.

The anisotropy data in ENDL-2 correspond to LTT=2, while the standard version of SUPERTOG-3 requires data with LTT=1. Hence, the necessity arises of modifying SUPERTOG in a way that input data with LTT=2 be also accepted. By means of the LTTAS1 package the modified version of SUPERTOG /1/ solves the following problem.

At given sets

$$\{\mu_i\};\ \{p(\mu_i, E)\}_{i=1,2,\ldots,m},$$

corresponding to a fixed energy E, find the optimum order N ($N \leq 30$, $N \leq m-1$) and the set of coefficients

$$\{f_\ell(E)\}_{\ell=0,1,\ldots,N}$$

which, when substituted in (1), restore the tabulated values of $p(\mu, E)$ with an accuracy no worse than that of the input data.

The use of a special-class polynomials /4,5,6/ is an essential feature of the computation of $\{f_\ell(E)\}$.

We start with the generation of a polynomial family $\{P_\ell(\mu)\}_{\ell=0,1,\ldots,J}$, $J \leq 30$, $J \leq m-1$, orthonormal over the ordered point set $\{\mu_i\}$ $i = 1, 2, \ldots, m$ with positive weights $\{\omega_i\}$ defined as follows:

$$\omega_1 = c\,(\mu_2 - \mu_1)$$
$$\omega_i = c\,(\mu_{i+1} - \mu_{i-1}) \qquad , \; i = 2,3,\ldots,m-1$$
$$\omega_m = c\,(\mu_m - \mu_{m-1}) \; ,$$

where c is a coefficient whose value is recovered from the unit probability of scattering at some angle between 0 and π

$$\int_{-1}^{1} p(\mu, E)\, d\mu = 1 \, .$$

This weight set takes into account both the grid $\{\mu_i\}$ non-uniformity and the linear interpolation model used in ENDL-2 to compute the values of $p(\mu, E)$ at inter-grid points.

Now the probability-density function is expressed as

$$p(\mu, E) = \sum_{j=0}^{N} a_j(E)\, P_j(\mu_i) \, ,$$

where the $a_j(E)$ coefficients are calculated as scalar products

$$a_j(E) = \sum_{i=1}^{m} p(\mu_i, E)\, \omega_i\, P_j(\mu_i) \qquad (2)$$

and $N \leq 30$, $N \leq m-1$; the optimum value of N is the one that minimizes the product of

- the value of χ^2 per one degree of freedom;
- the maximum relative deviation of fit from tabulated values of $p(\mu, E)$ at grid points;
- the maximum absolute deviation of fit from tabulated values of $p(\mu, E)$ over the same points.

Numerical experiments convinced us that such a combined criterion performs better than any of its individual components.

Once N and $\{a_j(E)\}$ have been determined, the latter should be transformed into $\{f_\ell(E)\}$ from eq. (1). This transformation proves most precise and numerically stable when carried out in the orthonormal basis $\{P_\ell(\mu)\}$. To this end we decompose each Legendre's polynomial in the new basis

$$L_\ell(\mu) = \sum_{j=0}^{\ell} c_j^{(\ell)} P_j(\mu) , \tag{3}$$

where, in analogy with (2),

$$c_j^{(\ell)} = \sum_{i=1}^{m} L_\ell(\mu_i)\,\omega_i\, P_j(\mu_i) . \tag{4}$$

Substituting (3) and (4) in (1) we obtain

$$\sum_{j=0}^{N} a_j(E) P_j(\mu) = \sum_{j=0}^{N} \frac{2j+1}{2} f_j(E) \sum_{K=0}^{j} c_K^{(j)} P_K(\mu)$$

which is easily reduced to a triangular linear algebraic system with respect to the unknown coefficients

$$f_N(E) = \frac{2}{2N+1} \frac{a_N}{c_N^{(N)}}$$

$$f_i(E) = \frac{2}{2i+1} \frac{1}{c_i^{(i)}} \left[a_i(E) - \sum_{j=i+1}^{N} \frac{2j+1}{2} c_i^{(j)} f_j(E) \right] , \quad i = N-1, \ldots, 1, 0.$$

This formula corresponds to eq. (9) in ref. /1/ where, due to a technical mistake, $a_i^{(j)}$ took the place of the correct $\frac{2j+1}{2} \cdot c_i^{(j)}$.

2. Discussion

It should be borne in mind that the L26P3S34 library was compiled by means of SUPERTOG from a micro cross-section library where the data on anisotropy of elastic scattering are given in the form of tabulated function $p(\mu, E)$. No essential changes were introduced in the methods programmed in the standard SUPERTOG version. Therefore, the credibility and reliability of data in L26P3S34 rest both with the quality of information in the files of evaluated micro cross-sections and with the accuracy of expressing the anisotropy in terms of spherical harmonics.

Our experience in using the modified version of SUPERTOG-3 generally confirms the assessment already reported in /1/. Most often and for the majority of materials processed the relative error of fit at the grid points $\{\mu_i\}$ is negligible (less than 1% in many cases). Concurrently, the truncation parameter N in our fits is higher than the respective value in the ENDF/B-4 library, i.e. for identical energies and materials we find a smooth approximation which suits better the local variations of the density function $p(\mu, E)$.

Previous conclusions about the causes of unsatisfactory numerical fits of $p(\mu, E)$ for isolated energies and/or materials were also confirmed. Unsatisfactory fits are obtained either when the grid is sparse or if the density function variations at a fixed energy exceed 4-5 decimal orders of magnitude. In the former case more detailed measurements of the anisotropy might be expected to be a good remedy, while the latter reveals a much deeper fault of numerical polynomial fits of any kind and, therefore, non-polynomial fits should be considered. This raises a whole set of new problems which are outside the scope of the present paper.

In addition, we observed that unsatisfactory polynomial fits are to a certain extent clustered around some materials. Such a clustering might be interpreted as due to insufficiently accurate data preparation within the limits of the linear interpolation model for these materials in ENDL-2.

The library package L26P3S34 is accompanied by two examples: the SUPERTOG printouts for Cu-nat and ^{181}Ta nuclides with tables of the fitting accuracy. These examples are typical for successful (Cu-nat) and not-always-acceptable (^{181}Ta) numerical fits of $p(\mu, E)$ at various values of the energy E.

3. <u>Format and parameters of L26P3S34</u>

L26P3S34 is a 26-group library containing the group-to-group transition matrices up to and including the P_3-order. The ^{1}H data are obtained following the general method and taking into account the elastic-scattering anisotropy.

The ANISN-format with BCD fixed-field form is used. Each P-part for every nuclide covered is preceded by a card-image in the format

(1X, 2I6, I4, I6, 12A4)

which contains

NGPS, IHM, NF, ID, (TITLE(I), I=1,12),

where NGPS is the number of groups;

IHM is the table length;

NF is zero;

ID is the P-part index;

TITLE(I) is an alphanumerical string.

4. Appendix

Three tables are given below to facilitate the use of L26P3S34. Table 1 presents the 26-group structure of the library Table 2 contains the list of nuclides covered; each nuclide is accompanied by the appropriate ID-identifier and by the ENDL-2 number of the respective material. In Table 3 all the materials are collected for which at the energies reported certain fit values of $p(\mu, E)$ are negative at some grid point. Naturally, the interpretation of results calculated for these materials and energies should be paid special attention.

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Table 1

26-group structure of the L26P3S34 library

Group	Energy range (eV)	
1	1.492 + 7*	- 1.220 + 7
2	1.220 + 7	- 1.000 + 7
3	1.000 + 7	- 8.180 + 6
4	8.180 + 6	- 6.360 + 6
5	6.360 + 6	- 4.960 + 6
6	4.960 + 6	- 4.060 + 6
7	4.060 + 6	- 3.010 + 6
8	3.010 + 6	- 2.460 + 6
9	2.460 + 6	- 2.350 + 6
10	2.350 + 6	- 1.830 + 6
11	1.830 + 6	- 1.110 + 6
12	1.110 + 6	- 5.500 + 5
13	5.500 + 5	- 1.110 + 5
14	1.110 + 5	- 3.350 + 3
15	3.350 + 3	- 5.330 + 2
16	5.330 + 2	- 1.010 + 2
17	1.010 + 2	- 2.000 + 1
18	2.000 + 1	- 1.010 + 1
19	1.010 + 1	- 3.060
20	3.060	- 1.120
21	1.120	- 4.140 - 1
22	4.140 - 1	- 2.000 - 1
23	2.000 - 1	- 1.000 - 1
24	1.000 - 1	- 5.000 - 2
25	5.000 - 2	- 1.000 - 4
26	1.000 - 4	-

* 1.492 + 7 means 1.492×10^7

L26P3S34 - list of materials

Material	ID identifier of the P_o-part	ENDL-2 material No.	Material	ID identifier of the P_o-part	ENDL-2 material number
Ti	2	7128	Co^{59}	70	7135
Fe	6	7132	Ni	74	7136
Cu	10	7138	Mo	78	7144
H^1	14	7101	Nb^{93}	82	7143
C^{12}	18	7112	Sn	86	7150
N^{14}	22	7113	Li^6	90	7106
O^{16}	26	7114	Li^7	94	7107
F^{19}	30	7115	B^{10}	98	7110
Mg	34	7117	B^{11}	102	7111
Al^{27}	38	7119	He^4	106	7105
Si	42	7120	Zr	110	7141
Ar	46	7124	Ba^{138}	114	7151
Pb	50	7162	Cl	118	7123
P^{31}	54	7121	Ta^{181}	122	7155
S^{32}	58	7122	Pu^{239}	126	7176
Cr	62	7130	Pu^{240}	130	7177
Mn^{55}	66	7131	U^{235}	134	7168

Materials for which at the energies reported certain fit values of $\rho(\mu, E)$ are negative at some grid points

no	Material	Energy (MeV)
1	Fe	7.0, 14.6
2	Pb	3.3, 14.6, 16.0
3	P^{31}	4.8, 10.0, 12.0, 14.6
4	Mn^{55}	7.0, 11.0
5	Mo	3.5, 14.6
6	B^{10}	14.6, 20.0
7	B^{11}	14.6, 20.0
8	Zr	4.1, 7.0
9	Ta^{181}	12.0, 14.0, 15.0
10	Pu^{239}	10.0, 11.0, 16.0
11	Pu^{240}	10.0, 11.0, 16.0
12	U^{235}	10.0, 11.0, 16.0