4. FILE 4, ANGULAR DISTRIBUTIONS OF SECONDARY PARTICLES

4.1. General Description

File 4 is used to describe the angular distribution of emitted particles. It is used for reactions with incident neutrons only, and should not be used for any other incident particle. Angular distributions of emitted neutrons should be given for elastically scattered neutrons, and for the neutrons resulting from discrete level excitation due to inelastic scattering. However, angular distributions must also be given for particles resulting from (n,n′ continuum), (n,2n), and other neutron emitting reactions. In these cases, the angular distributions will be integrated over all final energies. File 4 may also contain angular distributions of emitted charged particles for a reaction where only a single outgoing charged particle is possible (MT=600 through 849, see section 3.4.6). Emitted photon angular distributions are given in File 14 when the particle angular distributions are given in File 4.

The use of File 6 to describe all emitted particle angular distributions is preferred when charged particles are emitted, or when the emitted particle's energy and angular distributions are strongly correlated. In these cases, Files 4 and 14 should not be used.

In some cases, it may be possible to compute the angular distributions in the resolved range from resonance parameters (see section 2.4.22 for further discussion). In such cases, the computed distributions may be preferable to the distributions from File 4 for deep penetration calculations. However, for many practical applications, the smoothed distributions in File 4 will be adequate.

Angular distributions for a specific reaction type (MT number) are given for a series of incident energies, in order of increasing energy. The energy range covered should be the same as that for the same reaction type in File 3. Angular distributions for several different reaction types (MT's) may be given in File 4 for each material, in ascending order of MT number.

The angular distributions are expressed as normalized probability distributions, *i.e.*,

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

where $f(\mu,E)d\mu$ is the probability that a particle of incident energy E will be scattered into the interval $d\mu$ about an angle whose cosine is μ. The units of $f(\mu,E)$ are (unit cosine)$^{-1}$. Since the angular distribution of scattered neutrons is generally assumed to have azimuthal symmetry, the distribution may be represented as a Legendre polynomial series,

$$f(\mu,E) = \frac{2\pi}{\sigma_s(E)}\sigma(\mu,E) = \sum_{l=0}^{NL}\frac{2l+1}{2}a_l(E)P_l(\mu)$$

where

μ	=	cosine of the scattered angle in either the laboratory or the center-of-mass system
E	=	energy of the incident particle in the laboratory system
$\sigma_s(E)$	=	the scattering cross section, *e.g.*, elastic scattering at energy E as given in File 3 for the particular reaction type (MT)
l	=	order of the Legendre polynomial
$\sigma(\mu,E)$	=	differential scattering cross section in units of barns per steradian
a_l	=	the l^{th} Legendre polynomial coefficient and it is understood that a_0 = 1.0.

The angular distributions may be given by one of two methods, and in either the center-of-mass (CM) or laboratory (LAB) systems. Using the first method, the distributions are given by tabulating the normalized probability distribution, $f(\mu,E)$, as a function of incident energy. Using the second method, the Legendre polynomial expansion coefficients, $a_l(E)$, are tabulated as a function of incident neutron energy.

Absolute differential cross sections are obtained by combining data from Files 3 and 4. If tabulated distributions are given, the absolute differential cross section (in barns per steradian) is obtained by

$$\sigma(\mu,E) = \frac{\sigma_s(E)}{2\pi} f(\mu,E)$$

where $\sigma_s(E)$ is given in File 3 (for the same MT number) and $f(\mu,E)$ is given in File 4. If the angular distributions are represented as Legendre polynomial coefficients, the absolute differential cross sections are obtained by

$$\sigma(\mu,E) = \frac{\sigma_s(E)}{2\pi} \sum_{l=0}^{NL} \frac{2l+1}{2} a_l(E) P_l(\mu)$$

where $\sigma_s(E)$ is given in File 3 (for the same MT number) and the coefficients $a_l(E)$ are given in File 4.

Also, a transformation matrix may be given in File 4 that can be used to transform a set of Legendre expansion coefficients, which are given to describe elastic scattering angular distributions, from one frame of reference to the other. The Legendre expansion coefficients $a_l(E)$ in the two systems are related through an energy-independent transformation matrix, U_{lm}, and its inverse, U^{-1}_{lm}:

$$a_l^{LAB}(E) = \sum_{m=0}^{NM} U_{lm} a_m^{CM}(E)$$

and

$$a_l^{CM} = \sum_{m=0}^{NM} U_{lm}^{-1} a_m^{LAB}(E)$$

Expressions for the matrix elements of U and U^{-1} may be found in papers by Zweifel and Hurwitz[1] and Amster.[2] Transformation matrices for nonelastic reactions are not incident energy independent and are not given in File 4.

The transformation matrix, if included, should be square, with the number of rows equal to NM + 1, where NM is the maximum order of the Legendre polynomial series used to describe any elastic angular distribution in this file. The transformation matrix is given as an array of numbers, V_K, where K = 1,....NK, and NK = (NM + 1)2, and where K = 1 + l + m (NM + 1). The value of K indicates how the $(l,m)^{th}$ element of the matrix may be found in array V_K. This means that the elements of the matrix $U_{l,m}$, or $U^{-1}{}_{l,m}$ are given column-wise in the array V_K:

$U_{0,0}$, $U_{0,1}$, ...$U_{0,NM}$
$U_{1,0}$, $U_{1,1}$, ...$U_{1,NM}$
. ...
. ...
$U_{NM,0}$, $U_{NM,1}$, ...$U_{NM,NM}$

[1] P.F. Zweifel and H. Hurwitz, Jr., J.Appl.Phys. 25, 1241 (1954).

[2] H. Amster, J.Appl.Phys. 29, 623 (1958).

4.2. Formats

File 4 is divided into sections, each containing data for a particular reaction type (MT number) and ordered by increasing MT number. Each section always starts with a HEAD record and ends with a SEND record. If the section contains a description of the angular distributions for elastic scattering, the transformation matrix is given first (if present) and this is followed by the representation of the angular distributions.

The following quantities are defined.

LTT Flag to specify the representation used and it may have the following values:
LTT=0, all angular distributions are isotropic
LTT=l, the data are given as Legendre expansion coefficients, $a_l(E)$
LTT=2, the data are given as normalized probability distributions, $f(\mu,E)$
LTT=3, low energy region is represented by as Legendre coefficients; higher region is represented by tabulated data.

LI Flag to specify whether all the angular distributions are isotropic
LI=0, not all isotropic
LI=1, all isotropic

LCT Flag to specify the frame of reference used
LCT=l, the data are given in the LAB system
LCT=2, the data are given in the CM system

LVT Flag to specify whether a transformation matrix is given for elastic scattering
LVT=0, a transformation matrix is not given (always use this value for all non-elastic scattering reactions)
LVT=l, a transformation matrix is given

NE Number of incident energy points at which angular distributions are given (NE≤1200)

NL Highest order Legendre polynomial that is given at each energy (NL≤64)

NK Number of elements in the transformation matrix (NK≤4225)
$NK = (NM + 1)^2$

NM Maximum order Legendre polynomial that will be required (NM≤64) to describe the angular distributions of elastic scattering in either the center-of-mass or the laboratory system. NM should be an even number.

V_K Matrix elements of the transformation matrices
$V_K=U^{-1}_{l,m}$, if LCT=1 (data given in LAB system)
$V_K=U_{l,m}$, if LCT=2 (data are given in CM system)

NP Number of angular points (cosines) used to give the tabulated probability distributions for each energy (NP≤l0l)

Other commonly used variables are given in the Glossary (Appendix A).

The structure of a section depends on the values of LTT (representation used, $a_l(E)$ or $f(\mu,E)$),and LVT (transformation matrix given/not given), but it always starts with a HEAD record of the form

```
[MAT, 4, MT/ ZA, AWR, LVT, LTT,  0,  0]HEAD
```

4.2.l. Legendre Polynomial Coefficients and Transformation Matrix Given: LTT=1, LVT=1,and LI=0

When LTT=1 (angular distributions given in terms of Legendre polynomial coefficients) and LVT=1, the structure of the section is

```
[MAT, 4, MT/  ZA, AWR, LVT, LTT,  0,  0]HEAD        (LVT=1, LTT=1)
[MAT, 4, MT/ 0.0, AWR,  LI, LCT, NK, NM/ VK]LIST    (LI=0)
[MAT, 4, MT/ 0.0, 0.0,   0,   0, NR, NE/ Eint] TAB2
[MAT, 4, MT/   T,  E1,  LT,   0, NL,  0/al(E1)]LIST
[MAT, 4, MT/   T,  E2,  LT,   0, NL,  0/al(E2)]LIST
-------------------------------------------------
-------------------------------------------------
[MAT, 4, MT/   T,  ENE,  LT,   0, NL,  0/al(ENE)]LIST
[MAT, 4,  0/ 0.0, 0.0,   0,   0,  0,  0]SEND
```

Note that T and LT refer to temperature (in K) and a test for temperature dependence, respectively. These values are normally zero, however.

4.2.2. Legendre Polynomial Coefficients Given and the Transformation Matrix Not Given: LTT=1, LVT=0, and LI=0

If LTT=1 and LVT=0, the structure of a section is the same as above, except that the second record (a LIST record) is replaced by

```
[MAT, 4, MT/ 0.0, AWR,  LI, LCT,  0,  0] CONT  (LI=0)
```

This form is always used for angular distributions of nonelastically scattered particles when Legendre polynomial expansion coefficients are used.

4.2.3. Tabulated Probability Distributions and Transformation Matrix Given: LTT=2, LVT=1, and LI=0

If the angular distributions are given as tabulated probability distributions, LTT=2, and a transformation matrix is given for elastic scattering, the structure of a section is

```
[MAT, 4, MT/  ZA, AWR, LVT, LTT,  0,  0]HEAD        (LVT=1, LTT=2)
[MAT, 4, MT/ 0.0, AWR,  LI, LCT, NK, NM/VK] LIST    (LI=0)
[MAT, 4, MT/ 0.0, 0.0,   0,   0, NR, NE/Eint] TAB2
[MAT, 4, MT/   T,  E1 ,  LT,   0, NR, NP/μint /f(μ,E1)]TAB1
[MAT, 4, MT/   T,  E2 ,  LT,   0, NR, NP/μint /f(μ,E2)]TAB1
--------------------------------------
--------------------------------------
[MAT, 4, MT/   T,  ENE , LT,   0, NR, NP/μint /f(μ,ENE)]TAB1
[MAT, 4,  0/ 0.0, 0.0,   0,   0,  0,  0]SEND
```

T and LT are normally zero.

4.2.4.Tabulated Probability Distributions Given and Transformation Matrix Not Given: LTT=2, LVT=0, and LI=0

The structure of a section is the same as above, except that the second record (a LIST record) is replaced by

```
[MAT, 4, MT/ 0.0, AWR,  LI, LCT,  0,  0]CONT        (LI=0)
```

This form is always used for angular distributions of nonelastically scattered neutrons when tabulated angular distributions are given.

4.2.5. All angular Distributions are Isotropic: LTT=0, LVT=0, LI=1

When *all* angular distributions for a given MT are assumed to be isotropic then the section structure is:

```
[MAT, 4, MT/  ZA, AWR, LVT, LTT,  0,  0]HEAD        (LVT=0, LTT=0)
[MAT, 4, MT/ 0.0, AWR,  LI, LCT,  0,  0]CONT        (LI=1)
[MAT, 4,  0/ 0.0, 0.0,   0,   0,  0,  0]SEND
```

4.2.6. Angular Distribution over Two Energy Ranges: LTT=3, LVT=0, LI=0

If LTT=3, angular distributions are given as Legendre coefficients over the lower energy range and as Probability Distributions over the higher energy range. The structure of a subsection is

```
[MAT, 4, MT/  ZA, AWR,  LVT,  LTT,  0,  0]HEAD      (LVT=0, LTT=3)
[MAT, 4, MT/ 0.0, AWR,   LI,  LCT,  0, NM]CONT      (LI=0)
              (Legendre coefficients)
[MAT, 4, MT/ 0.0, 0.0,    0,   0,  NR, NE1/Eint]TAB2
[MAT, 4, MT/   T,  E1,   LT,    0,  NL,  0/al(E1)]LIST
     -----------------------------
     -----------------------------
[MAT, 4, MT/   T,  ENE,  LT,   0,   NL,  0/al(ENE1)]LIST
              (Tabulated data)
[MAT, 4, MT/ 0.0, 0.0,   0,   0,   NR, NE2/Eint]TAB2
[MAT, 4, MT/   T,   E1,  LT,   0,  NR,  NP/μint /f(μ,ENE1)]TAB1
    ------------------------------
    ------------------------------
[MAT, 4, MT/   T,  ENE,  LT,   0,   NR, NP/μint /f(μ,ENET)]TAB1
           (NET = NE1+NE2-1)
[MAT, 4,  0/ 0.0, 0.0,   0,   0,    0,   0]SEND
```

Note that there is a double energy point at the boundary.

4.3. Procedures

The angular distributions for two-body reactions should be given in the CM system (LCT=2). It is recommended that other reactions (such as continuum inelastic, fission, *etc*.) should be given in *LAB system*. All angular distribution data should be given at the minimum number of incident energy points that will accurately describe the energy variation of the distributions. Legendre coefficients are preferred unless they cannot give an adequate representation of the data.

When the data are represented as *Legendre polynomial coefficients*, certain procedures should be followed. Enough Legendre coefficients should be used to accurately represent the recommended angular distribution at a particular energy point, and to ensure that the interpolated distribution is everywhere positive. The number of coefficients (NL) may vary from energy point to energy point; in general, NL will increase with increasing incident energy. A linear-linear interpolation scheme (INT=2) must be used to obtain coefficients at intermediate energies. This is required to ensure that the interpolated distribution is positive over the cosine interval from −1.0 to +1.0; it is also required because some coefficients may be negative. In no case should NL exceed a value of 64. If more than 64 coefficients appear to be required to obtain a non-negative distribution, a constrained Legendre polynomial fit to the data should be given. NL=1 is allowed at low energies to specify an isotropic angular distribution.

When angular distributions are represented as tabular data, certain procedures should be followed. Sufficient angular points (cosine values) should be given to accurately represent the recommended distribution. The number of angular points may vary from distribution to distribution. The cosine interval must be from −1.0 to +1.0. The interpolation scheme for $f(\mu,E)$ vs. μ should be log-linear (INT=4), and that for $f(\mu,E)$ vs. E should be linear-linear (INT=2).

Accurate angular distributions for the thermal energy range can be obtained by using File 7 or a detailed free-gas calculation. File 4 contains distributions for stationary free targets only.

The formats given above do not allow an energy-dependent transformation matrix to be given, so transformation matrices may not be given for nonelastic scattering reaction types. When a processing code wishes to transfer inelastic level angular distributions expressed as Legendre polynomial coefficients from the LAB to the CM system, or CM to LAB system, a distribution should be generated and transformed point by point to the desired frame of reference. The point-wise angular distributions can then be converted to Legendre polynomial coefficients in the new frame of reference.

(paragraph deleted)

4.4. Procedures for Specific Reactions

4.4.l. Elastic Scattering (MT=2)

1. A transformation matrix may be given in File 4 for elastic scattering. In general, this matrix is no longer required in ENDF/B because it is no longer needed in data processing codes. If the angular distributions are given for the center-of-mass system, the matrix should be for CM to LAB conversion. The parameter NM should be even, and it must be equal to or grater than $l_{\max}$ used in any of the angular distributions (if Legendre coefficients are given). The parameter NK is equal to $(\mathrm{NM} + 1)^2$.

2. Legendre polynomial representations should be used for the elastic scattering angular distributions and discrete channel scattering, and must be given in the CM system. When this representation is given, the maximum order of the polynomial for each incident energy should be even and $l_{\max}$ must be ≤ 64.

3. Care must be exercised in selecting an incident energy mesh for certain light-to-medium mass materials. Here it is important to relate any known structure in the elastic scattering cross section to the energy dependent variations in the angular distributions. These two features of the cross sections cannot be analyzed independent of one another. Remember, processing codes operate on MT=2 data are given in Files 3 and 4. (Structure of the total cross section is not considered when generating energy transfer arrays). It is better to maintain consistency in any structure effects between File 3 and File 4 data than to introduce structure in one File and ignore it in the other.

4. Consistency must be maintained between angular distribution data given for elastic and inelastic scattering. This applies not only to structural effects, but also to how the distributions were obtained.

Frequently, the evaluated elastic scattering angular distributions are based on experimental results that, at times, contain contributions from inelastic scattering to low-lying levels (which in turn may contain direct interaction effects). If inelastic contributions have been subtracted from the experimental angular distributions, this process must be done in a consistent manner. The same contributions must be subtracted from both the integrated elastic scattering and the angular distribution. Be sure that these contributions are included in the inelastic scattering cross section (both integrated data and angular distributions). This is particularly important when the inelastic contributions are due to direct interaction, since the angular distributions are not isotropic or symmetric about 90°, but they are generally forward peaked.

5. Do not use an excessive number of incident energy points for the angular distributions. The number used should be determined by the amount of variation in the angular distributions.

6. An incident energy point must be given at 10^{-5} eV. A point must be given at the highest energy point for which the angular distribution is isotropic. The highest incident energy must be the highest energy for which cross section data are given in File 3, at least 20 MeV.

7. In the case of neutrons, a relationship exists between the total cross section and the differential cross section at forward angles (Wick's limit or optical theorem).

$$\sigma(0°) \geq \sigma_W = \left(\frac{\sigma_T}{4\pi\lambda\!\!\!^{-}}\right)^2$$

$$\sigma_W = X\,E_0 \frac{AWR^2}{(1+AWR)^2}\,\sigma_T^2 \qquad \frac{\text{barns}}{\text{steradian}}$$

where E_0 is in eV and σ_T in barns; see Appendix H for value of X.

Care should be taken to observe this inequality, especially at high energies.

4.4.2. Inelastic Scattering Cross Sections

1. Do not give angular distribution data for MT = 4.

2. Always give angular distribution data for any one of the following if they are given in File 3: MT = 51 through 91.

3. Discrete channel (two body) angular distributions (*e.g.*, MT = 2, 51 - 90, 701...) should be given as Legendre coefficients in the CM system.

4. The continuum reaction (MT = 91) should be given in the LAB system.

5. Isotropic angular distributions should be used unless the degree of the isotropy exceeds 5%. If any level excitation cross sections contain significant direct interaction contributions, angular distributions are very important.

6. Use the precautions outlined above when dealing with the level excitation cross sections that contain a large amount of structure.

7. Do not overcomplicate the data files. Restrict the number of distributions to the minimum required to accurately represent the data.

4.4.3. Other Neutron Producing Reactions

Neutron angular distribution data must be given for all other neutron producing reactions, such as fission, (n,n′α), or (n,2n) in File 4 or File 6. File 4 is only appropriate if the distributions are fairly isotropic without strong pre-equilibrium components. The LAB system should be used.

4.4.4. Charged-Particle Producing Reactions

Distributions for charged particles from two-body reactions in the 600 series can be given in File 4 using the CM system, if desired. (Continuum reactions where only one charged particle is possible (*e.g.*, 649, 699, *etc*.) can also be given in File 4 using the LAB system. If angular data is needed for more complex reactions, File 6 is more appropriate.)