An explanation of the ENDEP code

G. W. Hedstrom

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1   Overview of `endep`

This note gives a description of the operation of the `endep` code, and it is an updated version of Chapter III of the Omega manual [3]. The purpose of `endep` is to determine the average energies of secondary particles, residual nuclei, and gammas, when the given data includes angular distributions or energy distributions of secondary particles. One difference between the current `endep` and that discussed in Chapter III of [3] is that the treatment of reactions induced by incident gammas is no longer done by `endep` but is done separately as described by the note [2]. I also wish to point out that much of the theory presented here is also given in Perkins's PD-note [5]. I have made some repetition here for the sake of completeness.

   At the end of this section I explain the usage of the `endep_diff` code, to compare two sets of energy-deposition files for a target.

   The reader should also be aware of the related code `nxgam`, which has the purpose of modelling gamma energy spectra when only average gamma energies are available. The theoretical basis for `nxgam` is given in [4], and the instructions for use of that code are contained in the note [6].

   The `endep` code handles the following basic reactions:

1. The modelling of discrete two-body reactions is discussed in Section 2. For these reactions the user must supply a file in `ENDL` format of angular distributions for the secondary particle (`I_number` = 1 data).

2. Section 3 discusses the treatment of continuum two-body reactions. For these reactions the user must supply a file in `ENDL` format of energy distributions for the secondary particle (`I_number` = 4 data).

3. Either of the above types of reactions may produce an unstable residual nucleus. The continuum decay of such a nucleus is described in Section 4. For each particle emitted the user must supply a file in `ENDL` format of energy distributions (`I_number` = 4 data).

   In addition, as explained in Section 5, `endep` has special coding for the treatment of gamma production, fission, and the breakup of deuterium, carbon, and beryllium.

1.1   Usage of `endep`

The best way to run `endep` is via the script

$$/\text{nds}/\text{bin}/\text{endep.script}$$

and the usage is

$$\text{endep.script } [\texttt{directory\_name}]$$

The command-line parameter is the name of the directory of files on which you want to run `endep`. If no directory name is given on the command line, the script asks the user to

supply one. Note that it is assumed that the data in this directory are for a single target only. In fact, the `endep` code will stop if it sees data from two different targets.

It is assumed that the files in this directory are in the `ENDL` format. Before running `endep`, the script runs `endlret` in order to concatenate the data into the order required by `endep`. This requires that your directory contain a `.index` file listing the names of the data files that you want to be processed by `endep`. If the script finds no `.index` file, it makes one, based on the assumption that you have used the usual `ENDL` file naming convention, namely, that data file names start out `yo...`. Hence, if you have named your data files `roulade` and `skinka`, then you have to provide a `.index` file consisting of these two file names on separate lines.

The script is set up so that the output from `endlret` is a file called `endl.asc`. The next step in `endep.script` is to use the Perl script `zacis.pl` to parse the `endl.asc` file and to write the structure to a file `endep.zacis`, which is used as input to `endep`.

Note that `endep.script` gets the `bdfls` file as an input to `endep`. The reason for this is that `endep` uses `bdfls` for its list of atomic masses, and these are used in the calculation of the mass-difference component of the energy of each reaction.

The user has the option of supplying an `endep.input` file, which has the following purpose. For discrete 2-body reactions the input data for `endep` consists of angular distributions of secondary particles in terms of center-of-mass coordinates, and it is assumed that this data may be interpolated linearly. But linear interpolation in the center-of-mass system transforms into parabolas in the laboratory frame. Because we also want to be able to do linear interpolation of the output from `endep`, the code inserts points on these parabolas to guarantee an interpolation accuracy given by the parameter `endep_tol`. The default value of `endep_tol` is 0.01, giving at least a 1% accuracy on the linear interpolation of the parabolas. If the user wants to have, say, 1/2% accuracy on the linear interpolation, he should supply an `endep.input` file in Fortran 90 namelist form,

```
&endep_opt
endep_tol = 0.005/
```

1.2 The output from `endep`

The script `endep.script` makes sure that where you are running the code there exists a subdirectory `data.new`. The output of `endep` is a collection of files `yo??c??i010s???` and `yo??c??i011s???` in the `data.new` directory. The file naming convention is as usual in `ENDL`. That is, `yo` identifies the emitted particle, `c` specifies the type of the reaction, the `i` number is 10 for average energy to secondary particles and 11 for average energy to the residual nucleus, and `s` indicates the identity of some of the numbers in the file header. The script makes a `.index` file for the `data.new` directory and then runs `endlret` to concatenate them into a `lib.new` file.

1.3 The `endep_diff` code to compare energy depositions

Because the user may want to monitor differences between energy-deposition files, I have written an `endep_diff` code to do that. This code is also for use on reactions for a one

target at a time, and the best way to run it is with the script

$$/\text{nds}/\text{bin}/\text{endep\_diff.script}$$

The usage of that script is

```
endep_diff.script [-Dir_1 dir_name_1] [-Dir_2 dir_name_2] \
  [-Lib_1 lib_name_1] [-Lib_2 lib_name_2]
```

The first set of data may either be in an ENDL-type directory such as `dir_name_1` or in the form of an `endl.asc` file, as given by `lib_name_1`, and analogously for the second data set.

For example, a common use of `endep_diff` would be to compare a new set of energy depositions with the corresponding current ENDL data. Because the output of `endep.script` includes a `lib.new` file in `endl.asc` format, a natural way to compare this with ENDL data, e.g., for lithium 6, is to run

```
endep_diff.script -Dir_1 /nds/data/endl/za003006 -Lib_2 lib.new
```

The default threshold for flagging differences in energy deposition is 1%, but the user may set a different threshold in an `endep.input` file. For example, if you want a 2% threshold, include the lines

```
&endep_diff_opt
diff_tol = 0.02/
```

in your `endep.input` file. Note that the same `endep.input` file may be used for both the `endep` and `endep_diff` codes, basically because the namelists have different identifiers.

The output of `endep_diff` is a file `endep_diff.log`, and the format of this file is as follows. The results are ordered by reaction (`c` identifier) and by secondary particle. If the energy depositions for a data set agree to within the prescribed tolerance, no further data is printed. Otherwise, the energies of the incident particle for both data sets are given, along with the energy depositions from the first library. When the relative difference exceeds the tolerance, the deposition from the second library is also given, as well as the relative difference.

2 Discrete two-body reactions

In this section we discuss the calculation of energy depositon to secondary particles for discrete two-body reactions. Suppose that particles 1 and 2 interact to form paricles x and y. Let m_j denote the mass of particle j for $j = 1$, 2, x, and y, and let v_j be its velocity in the laboratory frame. Then the kinetic of particle j in the laboratory frame is

$$E_j = \frac{1}{2} m_j v_j^2,$$

We let W_j^* denote the excitation level of the j-th particle, and Q_0 the contribution of the mass difference to the energy of the reaction,

$$Q_0 = (m_1 + m_2 - m_x - m_y)c^2. \tag{1}$$

If particle 2 is at rest in the laboratory frame, then conservation of energy implies that

$$E_1 + Q = E_x + E_y, \tag{2}$$

where

$$Q = Q_0 + (W_1^* + W_2^*) - (W_x^* + W_y^*).$$

The kinetic energies E_x and E_y of the particles x and y depend on the angles at which they are ejected. The `endep` code calculates the average values of E_x and E_y based on the probability-density data for the angles (`I_number = 1` data). Because this data is given in terms of the center-of-mass frame, we have to make a transformation to laboratory coordinates before we compute the average. The arguments given here are based on Newtonian mechanics, so it is assumed that we are dealing with particles that are not too energetic. We shall concentrate our attention on E_x since by a choice of the labels x and y, this represents the kinetic energy of either secondary particle.

The following derivation of a formula for E_x in terms of E_1 and Q is based on the reference [1, pp. 91–94]. The plan of attack is to transform to center-of-mass coordinates and work out the kinematics there, and then transform back to the laboratory frame. We use primes to denote quantities in center-of-mass coordinates. Thus, if V_0 denotes the velocity of the center of mass,

$$V_0 = \frac{m_1 v_1 + m_2 v_2}{m_1 + m_2}, \tag{3}$$

then $v_1' = v_1 - V_0$, etc. It follows from conservation of momentum that

$$m_1 v_1' = -m_2 v_2',$$

and from this we may derive the relations

$$v_1' = \frac{m_2}{m_1 + m_2}(v_1' - v_2') \quad \text{and} \quad v_2' = \frac{-m_1}{m_1 + m_2}(v_1' - v_2'). \tag{4}$$

These relations are useful because they represent v_1' and v_2' in terms of

$$v_1' - v_2' = v_1 - v_2 = v_1. \tag{5}$$

The same momentum conservation argument applied to the secondary particles shows that

$$v'_x = \frac{m_y}{m_x + m_y}(v'_x - v'_y) \quad \text{and} \quad v'_y = \frac{-m_x}{m_x + m_y}(v'_x - v'_y). \tag{6}$$

Let us now consider the consequences of energy conservation in the center-of-mass system. It follows from the definition (3) of V_0 that

$$m_1 v_1^2 + m_2 v_2^2 = (m_1 + m_2)V_0^2 + m_1 v_1'^2 + m_2 v_2'^2,$$

so that E_1 in the the energy equation (2) may be replaced by

$$E_1 = \frac{1}{2}(m_1 + m_2)V_0^2 + E'_1 + E'_2.$$

Likewise, under the assumption that $m_1 + m_2 \approx m_x + m_y$, we may write the right-hand side of (2) as

$$E_x + E_y = \frac{1}{2}(m_x + m_y)V_0^2 + E'_x + E'_y.$$

In writing this equation, we have neglected a term equal to

$$(m_x + m_y)\left(\frac{m_x v_x + m_y v_y}{m_x + m_y} - V_0\right)V_0,$$

and if this difference is not small relative to Q, we should not be using Newtonian mechanics. In this same vein, upon neglecting the difference

$$\frac{1}{2}(m_x + m_y - m_1 - m_2)V_0^2,$$

the energy equation in center-of-mass coordinates takes the form

$$E'_1 + E'_2 + Q = E'_x + E'_y. \tag{7}$$

We now perform some algebraic manipulations, using (4) and (6) to derive from (7) an equation for E'_x in terms of E_1. We begin by expressing all of the kinetic energies in terms of squares of velocity differences,

$$\frac{m_1}{2}\left(\frac{m_2}{m_1 + m_2}(v'_1 - v'_2)\right)^2 + \frac{m_2}{2}\left(\frac{m_1}{m_1 + m_2}(v'_1 - v'_2)\right)^2 + Q$$
$$= \frac{m_x}{2}\left(\frac{m_y}{m_x + m_y}(v'_x - v'_y)\right)^2 + \frac{m_y}{2}\left(\frac{m_x}{m_x + m_y}(v'_x - v'_y)\right)^2.$$

Upon combining terms and using the relation (5), we find that

$$\frac{m_2 E_1}{m_1 + m_2} + Q = \frac{m_x m_y}{2(m_x + m_y)}(v'_x - v'_y)^2.$$
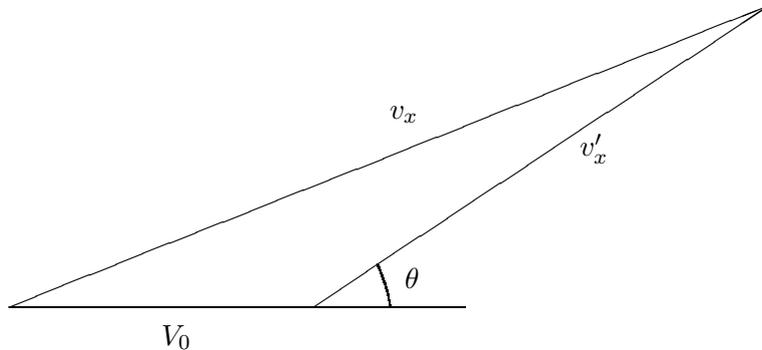
5

Figure 1: The relationship between velocities.

If we again use the first of equations (6), we obtain an expression for E'_x,

$$E'_x = \frac{m_x}{2} v'^2_x = \left(\frac{m_y}{m_x + m_y}\right)\left(\frac{m_2 E_1}{m_1 + m_2} + Q\right). \tag{8}$$

In order to transform (8) into the laboratory frame, we need a relation between the velocities v_x and v'_x depending on the collision angle θ in center-of-mass coordinates. In order to do this, we use the fact that v_x is the vector sum of v'_x and the velocity V_0 of the center of mass. See Fig. 1. With the notation that $|V_0|$ is the length of V_0, we find that

$$v^2_x = v'^2_x + V^2_0 + 2\,|v'_x|\,|V_0|\cos\theta.$$

In (8) we make the approximation that $m_x + m_y \approx m_1 + m_2$. Then, with the notation

$$\alpha = \frac{m_2 m_y}{(m_1 + m_2)^2}, \qquad \beta = \frac{m_y}{m_1 + m_2}, \qquad \gamma = \frac{m_1 m_x}{(m_1 + m_2)^2}, \tag{9}$$

it follows from (3) that we have

$$E_x = (\alpha + \gamma)E_1 + \beta Q + 2\left\{(\alpha E_1 + \beta Q)\gamma E_1\right\}^{1/2}\cos\theta. \tag{10}$$

The library data for the angular distribution (I_number $= 1$ data) is given as the probability density $p(E_1, \eta)$ with respect to the center-of-mass collision cosine

$$\eta = \cos\theta.$$

Consequently, in order to calculate the average secondary energy

$$\langle E_x \rangle = \int_{-1}^{1} E_x p(E_1, \eta)\, d\eta,$$

we multiply (10) by p and integrate with respect to η,

$$\langle E_x \rangle = (\alpha + \gamma)E_1 + \beta Q + 2\left\{(\alpha E_1 + \beta Q)\gamma E_1\right\}^{1/2}\int_{-1}^{1} p(E_1, \eta)\eta\, d\eta. \tag{11}$$

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2.1 The treatment of endothermic reactions near the threshold

At low incident energies the angular distribution of secondary particles is isotropic (with $p(E_1, \eta) = 1/2$), so that the integral in (11) vanishes, and we have

$$\langle E_x \rangle = (\alpha + \gamma)E_1 + \beta Q. \tag{12}$$

For endothermic reactions ($Q < 0$) and for E_1 near the threshold, the arithmetic on the right-hand side of this equation may lead to the subtraction of nearly equal numbers. In this circumstance we therefore modify the calculation of $\langle E_x \rangle$ as follows.

We begin by computing the threshold, which occurs when the secondary particles have zero energy in the center-of-mass system. Thus, we set $E'_x = 0$ and $E'_y = 0$ in (7) to get that the threshold is when

$$E'_1 + E'_2 = -Q.$$

In terms of laboratory coordinates with a stationary target ($v_2 = 0$), this equation takes the form

$$E_1 - \frac{1}{2}(m_1 + m_2)V_0^2 = -Q.$$

We may now use (3) to write the velocity V_0 of the center of mass in terms of v_1 to get that the threshold occurs when the incident energy E_1 is equal to $E_{\text{threshold}}$ with $E_{\text{threshold}}$ given by

$$E_{\text{threshold}} = -\left(\frac{m_1 + m_2}{m_2}\right)Q. \tag{13}$$

In laboratory coordinates at threshold the secondary particles are both moving at the velocity of the center of mass. The energy E_x is therefore equal to

$$E_x = \frac{1}{2}m_x V_0^2.$$

By (3) this is equal to

$$E_x = \frac{m_1 m_x}{(m_1 + m_2)^2}E_1,$$

and at the threshold $E_1 = E_{\text{threshold}}$ we find from (13) that

$$E_x = -\frac{m_1 m_x}{m_2(m_1 + m_2)}Q. \tag{14}$$

On the basis of these ideas, for an endothernmic reaction when the incident particle is near threshold and the angular distribution is isotropic, we calculate $\langle E_x \rangle$ by using the formula

$$\langle E_x \rangle = (\alpha + \gamma)(E_1 - E_{\text{threshold}}) - \frac{m_1 m_x}{m_2(m_1 + m_2)}Q. \tag{15}$$

It is easy to show that the two equations, (15) and (12), are mathematically equivalent. From the point of view of computer arithmetic, however, (15) is much more reliable.

3 Continuum two-body reactions

In the rest of this note, for reasons of clarity we shall use the notation that m_{targ} denotes the mass of the target and that W_{targ} is its excitation level. Similarly, we say that m_{yi} and E_{yi} are the mass and energy of the incident particle and m_{yo} and E_{yo} the mass and energy of the secondary particle. Furthermore, m_{res}, E_{res}, and W_{res} denote, respectively, the mass, kinetic energy, and excitation level of the residual.

For continuum two-body reactions the `endep` code works with energy-distribution data (`I_number` = 4) in the laboratory frame. That is, for a set of incident energies E_{yi}, we are given probability densities $P(E_{\text{yi}}, E_{\text{yo}})$ that the secondary particle has energy E_{yo}. The total average energy of the secondary particle corresponding to an incident particle at energy E_{yi} is therefore computed by evaluating the integral

$$\langle E_{\text{yo}} \rangle = \int E_{\text{yo}} P(E_{\text{yi}}, E_{\text{yo}}) \, dE_{\text{yo}}. \tag{16}$$

Here, the limits of integration are the minimum and maximum possible energies for the secondary particle.

If energy distributions are given for the gammas and if this residual decays only by gamma emission, then the average gamma energy $\langle E_{\gamma} \rangle$ is also calculated by using (16). In that case, the average energy of the residual $\langle E_{\text{res}} \rangle$ is obained from energy conservation (2),

$$\langle E_{\text{res}} \rangle = E_1 + Q - \langle E_{\text{yo}} \rangle - \langle E_{\gamma} \rangle. \tag{17}$$

Also, if the residual nucleus is an alpha or lighter, it is assumed that there is no gamma emission, and the average energy of the residual is taken to be

$$\langle E_{\text{res}} \rangle = E_1 + Q - \langle E_{\text{yo}} \rangle.$$

3.1 The average excitation energy

We devote the remainder of this section to explain how average gamma and residual energies are derived when no gamma energy distributions are given.

For continuum two-body reactions the kinematics is treated very much like that of discrete two-body reactions in the previous section. One difference is that the angular distribution is now assumed to be isotropic, so that (11) simplifies to (12). The other difference is that the energy of the reaction Q is an average value, dependent upon the average excitation energy of the residual nucleus, and both of these quantities are to be determined.

When the x-particle in (11) plays the rôle of the residual nucleus, then the mass ratios in (9) take the form

$$\alpha_{\text{res}} = \frac{m_{\text{targ}} m_{\text{yo}}}{(m_{\text{yi}} + m_{\text{targ}})^2}, \quad \beta_{\text{res}} = \frac{m_{\text{yo}}}{m_{\text{yi}} + m_{\text{targ}}}, \quad \gamma_{\text{res}} = \frac{m_{\text{yi}} m_{\text{res}}}{(m_{\text{yi}} + m_{\text{targ}})^2}. \tag{18}$$

Then, equation (12) provides us with a relation between the average kinetic energy to the residual $\langle E_{\text{res}} \rangle$ and the average energy of the reaction $\langle Q \rangle$,

$$\langle E_{\text{res}} \rangle = (\alpha_{\text{res}} + \gamma_{\text{res}}) E_{\text{yi}} + \beta_{\text{res}} \langle Q \rangle. \tag{19}$$

In terms of the energy Q_0 due to the mass difference (1) and the excitation levels W_{targ} and W_{res} of the target and residual, the average energy $\langle Q \rangle$ of the reaction is given by

$$\langle Q \rangle = Q_0 + W_{\text{targ}} - \langle W_{\text{res}} \rangle. \tag{20}$$

It therefore follows from energy conservation (2) that for a stationary target we have

$$E_{\text{yi}} + \langle Q \rangle = \langle E_{\text{yo}} \rangle + \langle E_{\text{res}} \rangle. \tag{21}$$

Upon solving equations (19) and (21) for the unknowns $\langle Q \rangle$ and $\langle E_{\text{res}} \rangle$, we find that

$$\langle Q \rangle = \frac{1}{1 - \beta_{\text{res}}} \{ E_{\text{yo}} + (\alpha_{\text{res}} + \gamma_{\text{res}} - 1) E_{\text{yi}} \}, \tag{22}$$

and

$$\langle E_{\text{res}} \rangle = \frac{1}{1 - \beta_{\text{res}}} \{ (\alpha_{\text{res}} + \gamma_{\text{res}} - \beta_{\text{res}}) E_{\text{yi}} + \beta_{\text{res}} \langle E_{\text{yo}} \rangle \}. \tag{23}$$

We conclude from (22) and (20) that the average excitation level W_{res} of the residual is given by

$$\langle W_{\text{res}} \rangle = Q_0 + W_{\text{targ}} - \frac{1}{1 - \beta_{\text{res}}} \{ \langle E_{\text{yo}} \rangle + (\alpha_{\text{res}} + \gamma_{\text{res}} - 1) E_{\text{yi}} \}. \tag{24}$$

For continuum decay the order of operations in the `endep` code is as follows. We begin by calculating the average energy $\langle E_{\text{yo}} \rangle$ of the secondary particle by using the integral (16). We then use (24) to compute $\langle W_{\text{res}} \rangle$, the average excitation level of the residual. It sometimes happens that this calculation produces a negative result. If there is no further decay, we set $\langle W_{\text{res}} \rangle = 0$ and `endep` prints a warning. Otherwise, the `endep` code keeps the negative $\langle W_{\text{res}} \rangle$ and just prints a warning message. Finally, the average kinetic energy of the residual is obtained from energy conservation (20) and (21) as

$$\langle E_{\text{res}} \rangle = E_{\text{yi}} + Q_0 + W_{\text{targ}} - \langle W_{\text{res}} \rangle - \langle E_{\text{yo}} \rangle. \tag{25}$$

If there is no further particle emission, the average energy to the gammas, $\langle E_\gamma \rangle$, is taken to be $\langle E_\gamma \rangle = \langle W_{\text{res}} \rangle$. Otherwise, the average kinetic $\langle E_{\text{res}} \rangle$ and excitation $\langle W_{\text{res}} \rangle$ energies are used in the modelling of the continuum decay process, as described in the next section.

4 Continuum decay reactions

The kinematics of continuum decay reactions is derived from that for continuum two-body reactions. The difference is that the initial unstable nucleus plays the rôle of the incident particle, and the target is null. This unstable nucleus may now be in an excited state, either because the previous reaction was inelastic scattering to some excitation level or because we had a continuum reaction leading to an average excitation as given by (24). Note that the reactions discussed here include those like $(n, 2n\gamma)$, in which there is more than one secondary particle of the same kind. The special considerations required for such reactions are spelled out at the end of this section.

Let us introduce the notation that m_{prev} denotes the mass of the initial unstable nucleus and that E_{prev} and W_{prev} are, respectively, its kinetic energy and excitation level. We again use the integral (16) to calculate the average energy $\langle E_{\text{yo}} \rangle$ of the secondary particle emitted at this stage.

As with continuum 2-body reactions, the calculation of the average kinetic energy of the final residual depends on whether or not gamma energy distributions are given. If they are given, then the average gamma energy is obtained from the integral (16), and energy balance is used to determine the average energy of the stable residual nucleus. Likewise, if the residual is an alpha or lighter, we assume that there is no gamma emission, and the average kinetic energy of the residual is obained from energy balance.

If gamma energy distributions are not given and if the residual is heavier than an alpha, then as in Section 3.1 we use the reaction kinematics to determine the average kinetic energy and excitation level for the residual at each step of the decay process. Thus, for one decay step the mass ratios (18) take the form

$$\alpha_{\text{res}} = 0, \qquad \beta_{\text{res}} = \frac{m_{\text{yo}}}{m_{\text{prev}}}, \qquad \gamma_{\text{res}} = \frac{m_{\text{res}}}{m_{\text{prev}}}.$$

The equation for the average excitation level of the residual (24) simplifies to

$$\langle W_{\text{res}} \rangle = Q_0 + W_{\text{prev}} - \frac{1}{1 - \beta_{\text{res}}} \{ \langle E_{\text{yo}} \rangle + (\gamma_{\text{res}} - 1) \langle E_{\text{prev}} \rangle \},$$

where Q_0 is the result of the mass difference for this decay step,

$$Q_0 = (m_{\text{prev}} - m_{\text{yo}} - m_{\text{res}}) c^2.$$

What we do if the computed value of $\langle W_{\text{res}} \rangle$ comes out to be negative depends upon whether or not this is the final decay step. If this is the final decay process and the computed value of $\langle W_{\text{res}} \rangle$ is negative, we replace it by zero and print a warning message. For intermediate decay steps we keep the negative average excitation and print a warning to indicate that the model may be wrong and that the decay steps probably ought to be done in a different order.

The equation (25) for the average kinetic energy of the residual becomes

$$\langle E_{\text{res}} \rangle = \langle E_{\text{prev}} \rangle + \langle W_{\text{prev}} \rangle + Q_0 - \langle W_{\text{res}} \rangle - \langle E_{\text{yo}} \rangle.$$

If this is the final particle emission, the average gamma energy is taken to be $\langle E_\gamma \rangle = \langle W_{\text{res}} \rangle$.

4.1 Secondary particles with multiplicity greater than 1

The differences in the treatment of secondary particles with multiplicity exceeding 1, e.g., $(n, 2n\gamma)$ reactions, derive from the fact that the energy distribution data is the average for the two particles. Note also that the output of `endep` includes the particle multiplicity in the average energy deposition. That is, the output file contains pairs

$$(E_{\mathrm{yi}}, \mu\langle E_{\mathrm{yo}}\rangle)$$

where E_{yi} is the energy of the incident particle, $\langle E_{\mathrm{yo}}\rangle$ is the average energy of the secondary particle `yo` as computed from the integral (16), and μ is its multiplicity.

Another difference arises from the fact that some decision has to be made about how to apportion the energy between the multiple secondary particles. For the sake of clarity, I describe how `endep` handles $(n, 2n\gamma)$ reactions. This is treated as a 2-step reaction, with the first step being continuum inelastic scattering as described in Section 3. The second step is emission of the second neutron by continuum decay as discussed above. The important point to note is that the same average neutron energy, $\langle E_{\mathrm{yo}}\rangle$ from the integral (16), is used in both processes. If the model were changed, for example by apportioning more energy to the first neutron emitted than to the second, the average energies $\langle E_{\mathrm{res}}\rangle$ and $\langle E_{\gamma}\rangle$ would change, but the sum $\langle E_{\mathrm{res}}\rangle + \langle E_{\gamma}\rangle$ would stay constant.

5 Special reactions

Several reactions require special treatment in `endep`. These include fission, some gamma-production reactions, and the breakup of deuterium, carbon, and beryllium. Endothermic reactions on natural targets also require special handling. We discuss these cases here.

5.1 Gammas from neutron-capture reactions

For neutron-capture reations with no given gamma data, the `endep` code uses conservation of energy and momentum to determine the average kinetic and excitation energy of the residual nucleus. This average excitation energy is output as the average energy of the gammas. A subsequent application of the `nxgam` code may be used to model the gamma energy distribution. See the references [4] and [6].

5.2 Gammas from level excitation

For reactions such as inelastic scattering with the residual at a specific excitation level, this level is given in the header of the angular-distribution file for the scattered particle. In this case, one of the output files from `endep` simply contains pairs

$$(E_{\mathrm{yi}}, E_\gamma)$$

where E_{yi} is the energy of the incident particle, and E_γ is the excitation level of the residual nucleus.

5.3 Fission and reactions with multiple gammas

For fission reactions the multiplicity μ of the neutrons produced is given as a function of the energy E_{yi} of the incident neutron (`I_number = 7` data). The probability density $P(E_{\mathrm{yi}}, E_{\mathrm{yo}})$ that an incident neutron with energy E_{yi} will produce a fission neutron with energy E_{yo} is also given. In this case output file from `endep` for average fission neutron energy contains the pairs

$$(E_{\mathrm{yi}}, \mu(E_{\mathrm{yi}})\langle E_{\mathrm{yo}}\rangle), \tag{26}$$

where $\langle E_{\mathrm{yo}}\rangle$ is the average energy of a single fission neutron as calculated from the integral (16). Note that the energy of the delayed fission neutrons is not included.

For some reactions, e. g., fission, the energy distribution of the gammas is given, along with their multiplicity as a function of the energy of the incident particle (`I_number = 9` data). In these cases the output file from `endep` for average gamma energy includes the multiplicity as in (26).

5.4 Breakup of deuterium

The $^2\mathrm{H}\,(n, 2n)\,^1\mathrm{H}$ reaction is treated by `endep` as follows. First, the average energy of the secondary proton is computed from its energy distribution by evaluating the integral (16). Then the total average energy of the two neutrons is derived from energy balance.

5.5 Breakup of beryllium 7

For the $^7\mathrm{Be}\,(n,\alpha)\,^4\mathrm{He}$ reaction `endep` calculates the energy available, namely, the sum of the energy from the mass difference plus the energy of the incident neutron. It apportions this energy equally between the two alphas and writes two files, one for the alpha as secondary particle ($\mathtt{yo} = 6$) and one for the alpha as residual nucleus ($\mathtt{yo} = 16$).

5.6 Breakup of beryllium 9

In `ENDL` the breakup of beryllium 9 is listed as an $(n,2n)$ reaction ($\mathtt{c\_ID} = 12$), giving $^9\mathrm{Be}\,(n,2n)\,^8\mathrm{Be}$, and `endep` produces two output files, one for the total average energy of the two neutrons ($\mathtt{yo} = 1$) and one for the total average energy of the two alphas as residual ($\mathtt{yo} = 16$). It might make more sense to list this reaction as $^9\mathrm{Be}\,(n,2n\alpha)\,^4\mathrm{He}$ with the identifier $\mathtt{c\_ID} = 33$.

This is the only `ENDL` reaction in which the data are joint energy-angle distributions. Specifically, for given energy of the incident neutron E_{yi} we have the probability distribution $p(E_{\mathrm{yi}}, \mu)$ of the direction cosine μ of the alphas, and for given E_{yi} and μ we have the probability distribution $P(E_{\mathrm{yi}}, \mu, E_{\mathrm{yo}})$ of the energy E_{yo} of the alphas. Therefore, the average alpha energy is obtained by calculating the double integral

$$\langle E_{\mathrm{yo}} \rangle = \int_{-1}^{1} \left(\int E_{\mathrm{yo}} P(E_{\mathrm{yi}}, \mu, E_{\mathrm{yo}}) \, dE_{\mathrm{yo}} \right) p(E_{\mathrm{yi}}, \mu) \, d\mu. \tag{27}$$

The ouput file of average alpha energies contains the pairs

$$(E_{\mathrm{yi}}, 2\langle E_{\mathrm{yo}} \rangle).$$

The average neutron energies are then obtained from energy balance. The `ENDL` library does contain joint energy-angle distributions for the secondary neutrons. Therefore, `endep` also calculates the double integrals (27) for this data and checks for consistency of the results.

5.7 Breakup of carbon 12

For the $^{12}\mathrm{C}\,(n,n'2\alpha)\,^4\mathrm{He}$ reaction the first step is inelastic scattering, with the residual either at a discrete excitation level or treated as an average of a continuum. In the case of discrete excitation we are given angular distributions and the excitation level, and we use (11) based on discrete two-body kinematics to calculate the average energy of the secondary neutron. For the continuum we are given energy distributions, and we use the integral (16) to calculate the average secondary neutron energy.

The remaining energy is split equally between the three alphas. The `endep` code writes a file of pairs

$$(E_{\mathrm{yi}}, 2\langle E_{\mathrm{yo}} \rangle)$$

for two of the alphas ($\mathtt{yo} = 6$), and it writes a file of pairs

$$(E_{\mathrm{yi}}, \langle E_{\mathrm{yo}} \rangle)$$

for the residual alpha ($\mathtt{yo} = 16$).

Note that $\mathtt{ENDL}$ also contains energy distributions for both types of alphas. The code therefore checks for consistency of the average energies.

5.8 Mass-difference energies for natural targets

For isotopic targets we may look up the masses of the particles in the $\mathtt{bdfls}$ mass tables and obtain the energy due to the mass difference by calculating the difference (1). For reactions on natural targets the $\mathtt{endep}$ code reads the mass-difference energy from the header of the $\mathtt{ENDL}$ data file. For scattering reactions this number is, of course, zero. But it means different things for exothermic and endothermic reactions.

For exothermic reactions on natural targets the mass-difference energy in the header of an $\mathtt{ENDL}$ data file is simply a weighted average, according to the natural isotopic abundances.

For endothermic reactions on a natural target there is no single number for the mass-difference energy, because different isotopes have different thresholds. Consequently, the weighting depends on which isotopes are above threshold, and strictly speaking, the mass-difference energy is a step function of the energy of the incident particle. Specifically, there is a jump discontinuity corresponding to the energy threshold for each isotope in the natural mixture. The way that these reactions are handled in $\mathtt{ENDL}$ is that the mass-difference energy value given in the file header corresponds to the lowest natural threshold. That is, it is the mass difference for the natural isotope which is the first to react, and the reason for this choice is that it puts the threshold at the proper energy. This has the consequence, however, that for incident particles at higher energies, the energies computed by $\mathtt{endep}$ for the gammas and the residual may well come out negative. The prime example of this difficulty in $\mathtt{ENDL}$ is natural zinc, and for some reactions the situation is so bad that the gamma and residual average-energy files are not included in the library.

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