# 6 HEATR

The HEATR module generates pointwise heat production cross sections and radiation damage energy production for specified reactions and adds them to an existing PENDF file. The heating and damage numbers can then be easily group averaged, plotted, or reformatted for other purposes. An option of use to evaluators checks ENDF/B files for neutron/photon energy-balance consistency. The advantages of HEATR include

- Heating and damage are computed in a consistent way.
- All ENDF/B neutron and photon data are used.
- ENDF/B-6 charged-particle distributions are used when available.
- Kinematic checks are available to improve future evaluations.
- Both energy-balance and kinematic KERMA factors can be produced.

This chapter describes the HEATR module in NJOY2016.0.

## 6.1 Theory of Nuclear Heating

Heating is an important parameter of any nuclear system. It may represent the product being sold – as in a power reactor – or it may affect the design of peripheral systems such as shields and structural components.

Nuclear heating can be conveniently divided into neutron heating and photon heating (see Fig. 8). Neutron heating at a given location is proportional to the local neutron flux and arises from the kinetic energy of the charged products of a neutron induced reaction (including both charged secondary particles and the recoil nucleus itself). Similarly, photon heating is proportional to the flux of secondary photons transported from the site of previous neutron reactions. It is also traceable to the kinetic energy of charged particles (for example, electron-positron pairs and recoil induced by photoelectric capture).

Heating, therefore, is often described by KERMA[30] (Kinetic Energy Release in Materials) coefficients $k_{ij}(E)$ defined such that the heating rate in a mixture is given by

$$H(E) = \sum_i \sum_j \rho_i k_{ij}(E)\phi(E) \ , \tag{160}$$

where $\rho_i$ is the number density of material $i$, $k_{ij}(E)$ is the KERMA coefficient for material $i$ and reaction $j$ at incident energy $E$, and $\phi(E)$ is the neutron or

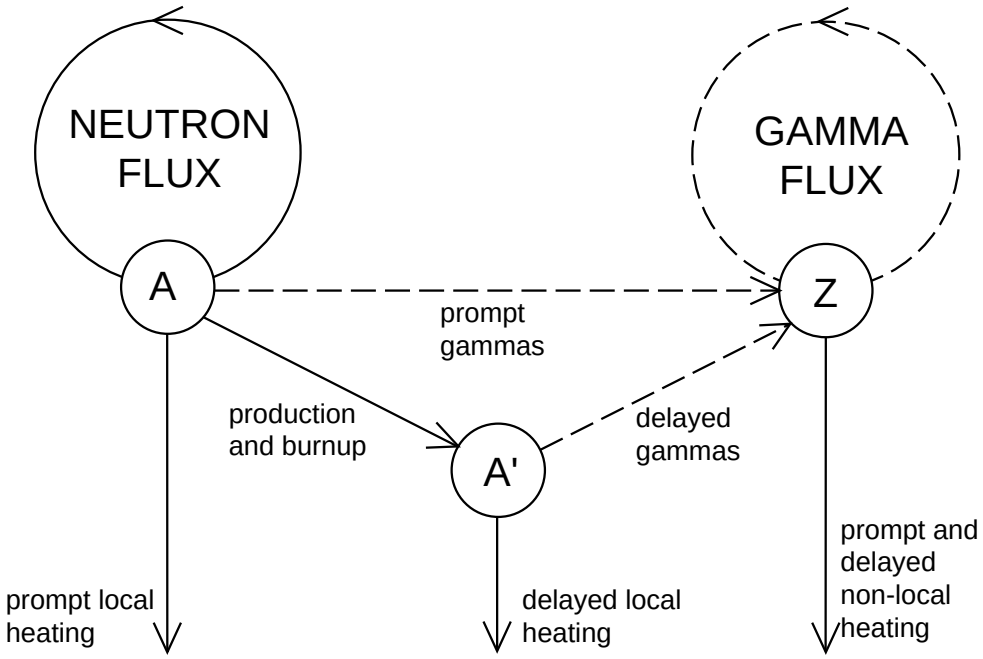


Figure 8: Components of nuclear heating. HEATR treats the prompt local neutron heating only. Gamma heating is computed in GAMINR. Delayed local heating and photon production are not treated by NJOY, and they must be added at a later stage.

photon scalar flux at $E$. KERMA is used just like a microscopic reaction cross section except that its units are energy $\times$ cross section (eV-barns for HEATR). When multiplied by a flux and number density, the result would give heating in eV/s.

The "direct method" for computing the KERMA coefficient is

$$k_{ij}(E) = \sum_{\ell} \overline{E}_{ij\ell}(E)\sigma_{ij}(E) \ , \tag{161}$$

where the sum is carried out over all charged products of the reaction including the recoil nucleus, and $\overline{E}_{ij\ell}$ is the total kinetic energy carried away by the $\ell^{th}$ species of secondary particle. These kinds of data are now becoming available for some materials with the advent of ENDF/B-VI and later, but earlier ENDF/B versions did not include the detailed spectral information needed to evaluate Eq. 161.

For this reason, NJOY computes KERMA factors for many materials by the "energy-balance method"[42]. The energy allocated to neutrons and photons is simply subtracted from the available energy to obtain the energy carried away by charged particles:

$$k_{ij}(E) = \left(E + Q_{ij} - \overline{E}_{ijn} - \overline{E}_{ij\gamma}\right) \sigma_{ij}(E) \ , \tag{162}$$

where $Q_{ij}$ is the mass-difference $Q$-value for material $i$ and reaction $j$, $\overline{E}_n$ is the total energy of secondary neutrons including multiplicity, and $\overline{E}_\gamma$ is the energy of secondary photons including photon yields.

This method was well suited for use with ENDF/B-V, or any other evaluation containing neutron and photon spectral data, but not the particle spectra required by the direct method. The disadvantage of this method is that the KERMA factor sometimes depends on a difference between large numbers. In order to obtain accurate results, care must be taken by the evaluator to ensure that photon and neutron yields and average energies are consistent. In fact, the lack of consistency in ENDF/B-V often revealed itself as negative KERMA coefficients[43].

However, a negative KERMA coefficient is not always the defect it seems to be. It must be remembered that heating has both neutron and photon components. A negative KERMA might indicate that too much energy has been included with the photon production in the evaluation. This will result in excessive photon heating if most of the photons stay in the system. However, the negative KERMA will have just the right magnitude to cancel this excess heating. The energy-balance method guarantees conservation of total energy in large homogeneous systems.

In this context, large and homogeneous means that most neutrons and photons stay in their source regions. It is clear that energy-balance errors in the evaluation affect the spatial distribution of heat and not the total system heating when the energy-balance method is employed.

A final problem with the energy-balance method occurs for the elemental evaluations common in earlier versions of ENDF/B. Isotopic $Q$-values and cross sections are not available in the files. It will usually be possible to define adequate cross sections, yields, and spectra for the element. However, it is clear that the available energy should be computed with an effective Q given by

$$\overline{Q} = \frac{\sum_i \rho_i \sigma_i Q_i}{\sum_i \rho_i \sigma_i} \ , \tag{163}$$

where $\rho_i$ is the atomic fraction of isotope $i$ in the element. This number is energy

dependent and can be represented only approximately by the single constant Q allowed in ENDF/B. HEATR allows the user to input an auxiliary energy-dependent Q for elements.

For elastic and discrete-level inelastic scattering, the neutron KERMA coefficient can be evaluated directly without reference to photon data. For other reactions, conservation of momentum and energy can be used to estimate the KERMA or to compute minimum and maximum limits for the heating. HEATR includes an option that tests the energy-balance KERMA factors against these kinematic limits, thereby providing a valuable test of the neutron-photon consistency of the evaluation. If the energy-balance heating numbers for a particular isotope should fail these tests, and if the isotope is important for a "small" system, an improved evaluation is probably required. The alternative of making *ad hoc* fixes to improve the local heat production is dangerous because the faults in the neutron and/or photon data revealed by the tests may lead to significant errors in neutron transport and/or photon dose and nonlocal energy deposition.

In practice, an exception to this conclusion must be made for the radiative capture reaction (n,$\gamma$). The difference between the available energy $E$+$Q$ and the total energy of the emitted photons is such a small fraction of $E$+$Q$ that it is difficult to hold enough precision to get reasonable recoil energies. Moreover, the emitted photons cause a component of recoil whose effect is not normally included in evaluated capture spectra. Finally, the "element problem" cited above is especially troublesome for capture because the available energy may change by several MeV between energies dominated by resonances in different isotopes of the element, giving rise to many negative or absurdly large heating numbers. These problems are more important for damage calculations (see below) where the entire effect comes from recoil and the compensation provided by later deposition of the photon energy is absent.

For these reasons, HEATR estimates the recoil due to radiative capture using conservation of momentum. The recoil is the vector sum of the "kick" caused by the incident neutron and the kicks due to the emission of all subsequent photons. Assuming that all photon emission is isotropic and that the directions of photon emission are uncorrelated, the photon component of recoil depends on the average of $E_\gamma^2$ over the entire photon spectrum

$$E_R = \frac{E}{A+1} + \frac{\overline{E_\gamma^2}}{2(A+1)mc^2} \ , \tag{164}$$

where $mc^2$ is the neutron mass energy. The second term is important below 25 – 100 keV. This formula gives an estimate that works for both isotopes and elements and has no precision problems. However, it does not explicitly conserve energy, and isotopes with bad capture photon data can still cause problems.

## 6.2 Theory of Damage Energy

Damage to materials caused by neutron irradiation is an important design consideration in fission reactors and is expected to be an even more important problem in fusion power systems. There are many radiation effects that may cause damage, for example, direct heating, gas production (*e.g.*, helium embrittlement), and the production of lattice defects.

A large cluster of lattice defects can be produced by the primary recoil nucleus of a nuclear reaction as it slows down in a lattice. It has been shown that there is an empirical correlation between the number of displaced atoms (DPA, displacements per atom) and various properties of metals, such as elasticity. The number of displaced atoms depends on the total available energy $E_a$ and the energy required to displace an atom from its lattice position $E_d$. Since the available energy is used up by producing pairs,

$$\text{DPA} = \frac{E_a}{2E_d} \ . \tag{165}$$

The values of $E_d$ used in practice are chosen to represent the empirical correlations, and a wide range of values is found in the literature[44, 45, 46]. Table 2 gives the default values used in NJOY2016. The energy available to cause displacements is what HEATR calculates. It depends on the recoil spectrum and the partition of recoil energy between electronic excitations and atomic motion. The partition function used is given by Robinson[47] based on the electronic screening theory of Lindhard[48] (see Fig. 9).

The damage output from HEATR is the damage energy production cross section (eV-barns). As in Eq. 160, multiplying by the density and flux gives eV/s. Dividing by $2E_d$ gives displacements/s. This result is often reduced by an efficiency factor (say 80%) to improve the fit to the empirical correlations.

Table 2: Typical Values for the Atomic Displacement Energy Needed to Compute DPA[46].

| Element | $E_d$, eV | Element | $E_d$, eV |
|---|---|---|---|
| Be | 31 | Co | 40 |
| C | 31 | Ni | 40 |
| Mg | 25 | Cu | 40 |
| Al | 27 | Zr | 40 |
| Si | 25 | Nb | 40 |
| Ca | 40 | Mo | 60 |
| Ti | 40 | Ag | 60 |
| V | 40 | Ta | 90 |
| Cr | 40 | W | 90 |
| Mn | 40 | Au | 30 |
| Fe | 40 | Pb | 25 |

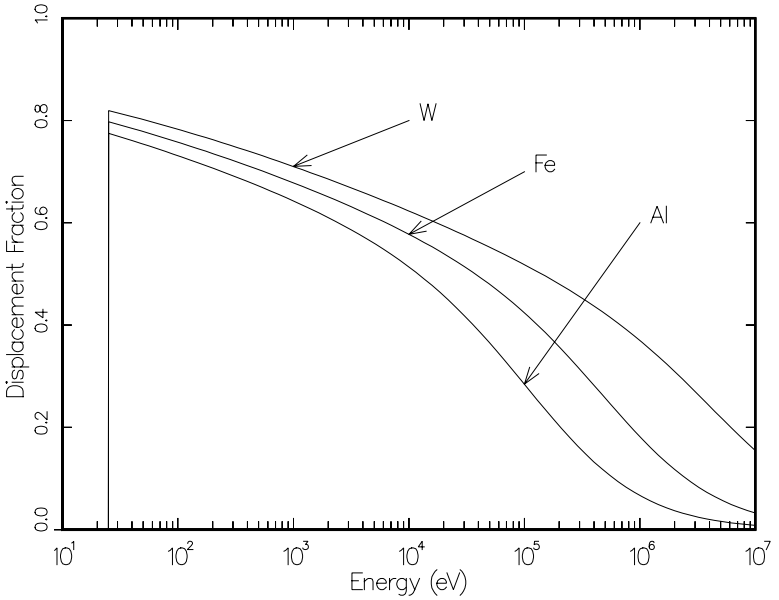


Figure 9: Examples of the portion of the primary recoil energy that is available to cause lattice displacements in metallic lattices. The remaining energy leads to electronic excitation. The quantity plotted is $P(E)$ from Eq. 200 divided by $E$. The 25 eV cutoff is also discussed in connection with Eq. 200.

## 6.3 Computation of KERMA Factors By Energy Balance

### 6.3.1 The general case

The older ENDF/B files do not usually give photon production data for all partial reactions. Summation reactions such as nonelastic (MT=3) and inelastic

(MT=4) are often used. It is still possible to compute partial KERMA factors for those summation reactions by reordering Eq. 162 as follows:

$$k_{ij} = \sum_{j \in J} k_{ij}^{n}(E) - \sum_{\ell \in J} \overline{E}_{i\ell\gamma}\sigma_{i\ell}(E) \ , \tag{166}$$

where $j$ runs over all neutron partials contained in $J$, and $\ell$ runs over all photon partials in $J$. The total KERMA is well defined, but partial KERMAS should be used only with caution.

HEATR loops through all the neutron reactions on the ENDF/B tape. If energy balance is to be used, it computes the neutron contributions needed for the first term. These are

$$k_{ij}^{n}(E) = \Big[E + Q_{ij} - \overline{E}_{ijn}(E)\Big]\sigma_{ij}(E) \ . \tag{167}$$

The $Q$-value is zero for elastic and inelastic scattering. For (n,n′) particle reactions represented by scattering with an LR flag set, Q is the ENDF "C1" field from MF=3. For most other reactions, Q is the "C2" field from MF=3. HEATR allows users to override any $Q$-value with their own numbers.

The $\overline{E}_n$ value as used in Eq. 167 is defined to include multiplicity. The multiplicity is either implicit — for example, 2 for (n,2n) — or is retrieved from the ENDF/B file (e.g. for the mt5 reaction). The average energy per neutron is computed differently for discrete two-body reactions and continuum reactions.

For elastic and discrete inelastic scattering (MT=2, 51-90),

$$\overline{E}_n = \frac{E}{(A+1)^2}\Big(1 + 2Rf_1 + R^2\Big) \ , \tag{168}$$

where $f_1$ is the center-of-mass (CM) average scattering cosine from MF=4 and $R$ is the effective mass ratio. For elastic scattering, $R$=$A$, but for threshold scattering,

$$R = A\sqrt{1 - \frac{(A+1)S}{AE}} \ , \tag{169}$$

where $S$ is the negative of the C2 field from MF=3.

For continuum scattering, the average energy per neutron is computed from the secondary neutron spectrum, $g$, in MF=5 using

$$\overline{E}_n(E) = \int_0^U E' g(E, E')\, dE' \ , \tag{170}$$

where $U$ is defined in MF=5. If $g$ is tabulated (LAW=1 or LAW=5), the integral is carried out analytically for each panel by making use of the ENDF/B interpolation laws. For the simple analytic representations (LAW=7, 9, or 11), the average energies are known[9].

The neutron cross sections required by Eq. 167 are obtained from an existing PENDF file (see RECONR, and BROADR).

When the neutron sum in Eq. 166 is complete, the code processes the photon production files. If the evaluation does not include photon data, HEATR returns only the first sum. This is equivalent to assuming that all photon energy is deposited locally, consistent with the fact that there will be no contribution to the photon transport source from this material. The same result can be forced by using the `local` parameter (see "User Input", Section 6.7, below).

Discrete photon yields and energies are obtained from MF=12 or 13. Continuum photon data are obtained from MF=15, and the average photon energy and $\overline{E_\gamma^2}$ are computed. For radiative capture, the photon term becomes

$$E_\gamma \sigma_\gamma = \left( E + Q - \frac{E}{A+1} + \frac{\overline{E_\gamma^2}}{2(A+1)mc^2} Y_\gamma \right) \sigma_\gamma \ , \tag{171}$$

[9] where $Y_\gamma$ is the capture photon yield from MF=12. This corrects the capture contribution from Eq. 167 by conservation of momentum. For other reactions, Eq. 167 is sufficient, and the product of $\overline{E}_\gamma$, $Y_\gamma$, and $\sigma_\gamma$ is subtracted from the neutron contribution.

### 6.3.2 The special case of fission

The partial KERMA for fission is a special case due to the particular problems with obtaining the $Q$-value for fission. First, the fission $Q$-value given in the C1 field of MF=3 includes delayed neutron and gamma contributions that we need to exclude, and second, the $Q$-value for fission is energy dependent.

As a result, the KERMA for fission will be calculated differently when compared to the other reactions which use Eq. 167 as is. Theoretically speaking, there is no difference with Eq. 167 as we will show here.

Energy dependent fission energy release and its components are given in the MT=458 section of MF=1 on the ENDF file. This section of the ENDF file defines the following components to the fission energy release:

- $Q_k$ : the kinetic energy of the fission fragments
- $Q_{n,p}$ and $Q_{n,d}$ : the kinetic energy of the prompt and delayed fission neutrons
- $Q_{\gamma,p}$ and $Q_{\gamma,d}$ : the energy of the prompt and delayed gamma rays
- $Q_\beta$ : the energy of the delayed beta radiation
- $Q_\nu$ : the energy carried away by the neutrinos

With these components, we can now define the total energy release from fission $Q_t$, the total energy release from fission excluding neutrinos $Q_r$ and the total prompt energy release from fission $Q_p$ as as follows:

$$Q_t(E) = Q_k(E) + Q_{n,p} + Q_{n,d} + Q_{\gamma,p} + Q_{\gamma,d} + Q_\beta + Q_\nu \ , \tag{172}$$

$$Q_r(E) = Q_t(E) - Q_\nu \ , \tag{173}$$

$$Q_p(E) = Q_r(E) - Q_{n,d} - Q_{\gamma,d} - Q_\beta = Q_k(E) + Q_{n,p} + Q_{\gamma,p} \ . \tag{174}$$

Using these fission energy release components, we can define the fission reaction $Q$-value (i.e. the energy released through the fission reaction) as the prompt fission energy release minus the incident neutron energy:

$$Q(E) = Q_p(E) - E = Q_k(E) + Q_{n,p} + Q_{\gamma,p} - E \ . \tag{175}$$

It should be noted that we have chosen to ignore the energy dependence of delayed beta and gamma emission because we don't yet treat it in subsequent codes. However, the impact of such an approximation is somewhat limited due to the amount of energy involved. For example, for U235 the value of $Q_k$ is roughly 169 MeV at 1e-5 eV while the sum of $Q_{n,d}$, $Q_{\gamma,d}$ and $Q_\beta$ is roughly 12 MeV at 1e-5 eV.

For the calculation of the fission KERMA factor, we also need to know the energy of the outgoing neutrons (i.e. $\overline{E}$ from Eq. 167). Because we are considering the prompt energy release only, this is simply equal to the prompt neutron energy release $Q_{n,p}$.

As a result, the partial fission KERMA factor $k_f^n$ will be given by:

$$k_f^n(E) = \Big[E + Q(E) - \overline{E}(E)\Big]\sigma_f(E) = \Big[Q_k(E) + Q_{\gamma,p}(E)\Big]\sigma_f(E) \ . \tag{176}$$

The fission KERMA is thus equal to the fission cross section times the sum of the kinetic energy of the fission products and the prompt gamma energy release.

This value will then be used in Eq. 166 to calculate the total KERMA.

In some cases it is possible that a fissile nuclide does not have an MT458 section. In this case, Eq. 167 will be used directly as follows:

$$k_f^n(E) = \Big[E + Q(E) - \overline{\nu}(E)\overline{E}(E)\Big]\sigma_f(E) \tag{177}$$

where the fission $Q$-value is approximated using the thermal point energy dependencies defined for MT458:

$$Q(E) = Q_{\text{ENDF}} - 8070000\,(\overline{\nu}(E) - \overline{\nu}(0)) + 0.307E \tag{178}$$

In this equation, $Q_{\text{ENDF}}$ is the reaction $Q$-value for fission as given in MF3.

## 6.4 Kinematic Limits

As an option provided mainly as an aid to evaluators, HEATR will compute the kinematic maximum and minimum KERMA coefficients and compare them with the energy-balance results. The formulas are as follows. For elastic scattering (MT=2), the expected recoil energy is

$$\overline{E}_R = \frac{2AE}{(A+1)^2}(1 - f_1)\ . \tag{179}$$

For discrete-inelastic scattering (MT=51-90), the photon momentum is neglected to obtain

$$\overline{E}_R = \frac{2AE}{(A+1)^2}\left[1 - f_1\sqrt{1 - \frac{(A+1)E_\gamma}{AE}}\ \right] - \frac{E_\gamma}{A+1}\ , \tag{180}$$

where $E_\gamma$=−C2 from MF=3. For continuum inelastic scattering (MT=91), secondary neutrons are assumed to be isotropic in the laboratory system (LAB) giving

$$\overline{E}_R = \frac{E - E_n}{A}\ , \tag{181}$$

and

$$\overline{E}_\gamma = \frac{(A-1)E - (A+1)\overline{E}_n}{A}\ , \tag{182}$$

where $\overline{E}_\gamma$ is the average photon energy expected for this representation. For radiative capture (MT=102),

$$\overline{E}_R = \frac{E}{A+1} + E_K \tag{183}$$

and

$$\overline{E}_\gamma = Q + \frac{AE}{A+1} - E_K \ , \tag{184}$$

where

$$E_K = \frac{1}{2M_R c^2}\left[\frac{AE}{A+1} + Q\right]^2 \left\{1 - \frac{1}{M_R c^2}\left[\frac{AE}{A+1} + Q\right]\right\} \ , \tag{185}$$

with

$$M_R c^2 = (939.565 \times 10^6)(A+1) - Q \tag{186}$$

being the mass energy in eV. The value of this constant is actually computed from fundamental constants in NJOY2016.

For two-body scattering followed by particle emission (MT=51-91, LR flag set), a minimum and maximum can be defined:

$$(E'_R + E_x)_{\min} = \overline{E}_R \ , \text{ and} \tag{187}$$

$$(E'_R + E_x)_{\max} = \overline{E}_R + Q + (E_\gamma)_{\max} \ , \tag{188}$$

where $\overline{E}_R$ is the value from Eq. 180 or (181), $Q$ is the C2 field from File 3, and $(E_\gamma)_{\max}$ is the negative of the C2 field from File 3. In these equations, $E'_R$ is the recoil energy and $E_x$ is the energy of the charged product. For absorption followed by particle emission (MT=103-120),

$$(E_R + E_x)_{\min} = \frac{E}{A+1-x} \ , \tag{189}$$

$$(E_\gamma)_{\max} = Q + \frac{A-x}{A+1-x}\,E \ , \text{ and} \tag{190}$$

$$(E_R + E_x)_{\max} = E + Q \ , \tag{191}$$

where $Q$ is the C2 field from MF=3 and $x$ is the particle mass ratio ($x$=1 gives a minimum for all reactions). For (n,2n) reactions,

$$(E_R)_{\min} = 0 \text{ , and} \tag{192}$$
$$(E_R)_{\max} = \frac{E+\overline{E}_n}{A-1} \text{ ,} \tag{193}$$

and for (n,3n) reactions,

$$(E_R)_{\min} = 0 \text{ , and} \tag{194}$$
$$(E_R)_{\max} = \frac{E+2\overline{E}_n}{A-2} \text{ .} \tag{195}$$

For both (n,2n) and (n,3n), if $(E_R)_{\max}$ is greater than $E_R$, it is set equal to $E_R$. In addition, these formulas are not used for $A<10$; $(E_R)_{\max}$ is set to $E_R$. For other neutron continuum scattering reactions (MT=22-45),

$$(E_R+E_x)_{\min} = 0 \text{ , and} \tag{196}$$
$$(E_R+E_x)_{\max} = E+Q-\overline{E}_n \text{ ,} \tag{197}$$

where $Q$ is the C2 field from File 3. Finally, for fission (MT=18-21, 38), the limits are

$$(E_R)_{\min} = E+Q-\frac{1}{2}\overline{E}_n - 15{\times}10^6 \text{ eV , and} \tag{198}$$
$$(E_R)_{\max} = E+Q-\overline{E}_n \text{ ,} \tag{199}$$

where $Q$ is the prompt fission Q-value less neutrinos. It is determined by taking the total (less neutrinos) value from File 3 and subtracting the delayed energy obtained from MF=1/MT=458.

These values are intended to be very conservative. Note that $E_K$ is only significant at very low neutron energy. In order to reduce unimportant error messages, a tolerance band is applied to the above limits. If all checks are satisfied, the resulting KERMA coefficients should give good local heating results even when 99.8% of the photons escape the local region. More information on using the kinematic checks to diagnose energy-balance problems in evaluations will be found in "Diagnosing Energy-Balance Problems", Section 6.9.

The upper kinematic limit can also be written out to the output tape as

MT=443 if desired. It is similar to the KERMA factors generated by the MACK code[30], and it is sometimes preferable to the energy-balance KERMA for calculating local heating for evaluations with severe energy-balance problems. The kinematic value in MT=443 is useful for plots (see the examples in this report).

### 6.5 Computation of Damage Energy

The formulas used for calculating damage energy are derived from the same sources as the heating formulas given above, except in this case, the effects of scattering angle do not result in simple factors like $f_1$ because the Robinson partition function is not linear. Instead, it is calculated as follows:

$$P(E) = \frac{E_R}{1 + F_L(3.4008\epsilon^{1/6} + 0.40244\epsilon^{3/4} + \epsilon)} \ , \tag{200}$$

if $E_R \geq 25.0$ eV, and zero otherwise. In Eq. 200, $E_R$ is the primary recoil energy,

$$\epsilon = \frac{E_R}{E_L} \ , \tag{201}$$

$$E_L = 30.724 Z_R Z_L \left(Z_R^{2/3} + Z_L^{2/3}\right)^{1/2} (A_R + A_L)/A_L \ , \text{ and} \tag{202}$$

$$F_L = \frac{0.0793 Z_R^{2/3} Z_L^{1/2} (A_R + A_L)^{3/2}}{\left(Z_R^{2/3} + Z_L^{2/3}\right)^{3/4} A_R^{3/2} A_L^{1/2}} \ , \tag{203}$$

and $Z_i$ and $A_i$ refer to the charge and atomic number of the lattice nuclei (L) and the recoil nuclei (R). The function behaves like $E_R$ at low recoil energies and then levels out at higher energies. Therefore, the damage-energy production cross section is always less than the heat production cross section. See Fig. 9 for examples.

For elastic and two-body discrete-level inelastic scattering,

$$E_R(E, \mu) = \frac{AE}{(A+1)^2}\left(1 - 2R\mu + R^2\right) \ , \tag{204}$$

where the "effective mass" is given by

$$R = \sqrt{1 - \frac{(A+1)(-Q)}{AE}} \ , \tag{205}$$

and $\mu$ is the CM scattering cosine. The damage energy production cross section

is then obtained from

$$D(E) = \sigma(E) \int_{-1}^{1} f(E,\mu)\, P(E_R[E,\mu])\, d\mu \ , \tag{206}$$

where $f$ is the angular distribution from the ENDF/B File 4. This integration is performed with a 20-point Gauss-Legendre quadrature. Discrete-level reactions with LR flags to indicate, for example, (n,n′)$\alpha$ reactions, are treated in the same way at present. The additional emitted particles are ignored.

Continuum reactions like (n,n′) give a recoil spectrum

$$E_R(E,E',\mu) = \frac{1}{A}\Big(E - 2\sqrt{EE'}\mu + E'\Big) \ , \tag{207}$$

where $E'$ is the secondary neutron energy, $\mu$ is the laboratory cosine, and the photon momentum has been neglected. The damage becomes

$$D(E) = \sigma(E) \int_0^\infty dE' \int_{-1}^{1} d\mu\, f(E,\mu)\, g(E,E')\, P(E_R[E,E',\mu]) \ , \tag{208}$$

where $g$ is the secondary energy distribution from File 5. In the code, the angular distribution is defaulted to isotropic, and a 4-point Gaussian quadrature is used for the angular integration. For analytic representations of $g$, an adaptive integration to 5% accuracy is used for $E'$; for tabulated File 5 data, a trapezoidal integration is performed using the energy grid of the file. The same procedure is used for (n,2n), (n,3n), etc., but it is not realistic for reactions like (n,n′p) or (n,n′$\alpha$). The neutron in these types of reactions can get out of the nucleus quite easily; thus, much of the energy available to secondary particles is typically carried away by the charged particles[49]. HEATR treats these reactions in the same way as (n,p) or (n,$\alpha$).

The recoil for radiative capture must include the momentum of the emitted photons below 25 – 100 keV giving

$$E_R = \frac{E}{A+1} - 2\sqrt{\frac{E}{A+1}}\sqrt{\frac{E_\gamma^2}{2(A+1)mc^2}}\cos\phi + \frac{\overline{E_\gamma^2}}{2(A+1)mc^2} \ , \tag{209}$$

where $\phi$ is the angle between the incident neutron direction and emitted photon direction. If subsequent photons are emitted in a cascade, each one will add an additional term of $\overline{E_\gamma^2}$ and an additional angle. A complete averaging of Eq. 209 with respect to $P(E_R)$ would be very difficult and would require angular

correlations not present in ENDF/B evaluations. However, damage calculations are still fairly crude, and an estimate for the damage obtained by treating the neutron "kick" and all the photon kicks independently should give a reasonable upper limit because

$$\int_{-1}^{1} D(E_R)\, d\cos\phi \le D\left(\frac{E}{A+1}\right) + \sum_{\gamma} D\left(\frac{\overline{E_\gamma^2}}{2M_R c^2}\right) \ . \tag{210}$$

The actual formula used in the code is

$$\begin{aligned} D(E) &= D\left(\frac{E}{A+1}\right) + D\left(\frac{1}{2M_R c^2}\left[\frac{AE}{A+1}+Q\right]^2\right) \\ &+ \sum_{\gamma} D\left(\frac{\overline{E_\gamma^2}}{2M_R c^2}\right) - D\left(\frac{1}{2M_R c^2}\left[\frac{AE}{A+1}+Q\right]^2\right) \ , \end{aligned} \tag{211}$$

where the first line is computed in the neutron section, and the second line is computed in the photon section. This form also provides a reasonable default when no photons are given.

Finally, for the (n,particle) reactions, the primary recoil is given by

$$E_R = \frac{1}{A+1}\left(E^* - 2\sqrt{aE^*E_a}\cos\phi + aE_a\right) \ , \tag{212}$$

where $a$ is the mass ratio of the emitted particle to the neutron, $E^*$ is given by

$$E^* = \frac{A+1-a}{A+1}\, E \ , \tag{213}$$

and the particle energy $E_a$ is approximated as being equal to the smaller of the available energy

$$Q + \frac{AE}{A+1} \ , \tag{214}$$

or the Coulomb barrier energy

$$\frac{1.029\times 10^6\, zZ}{a^{1/3}+A^{1/3}} \text{ in eV} \ , \tag{215}$$

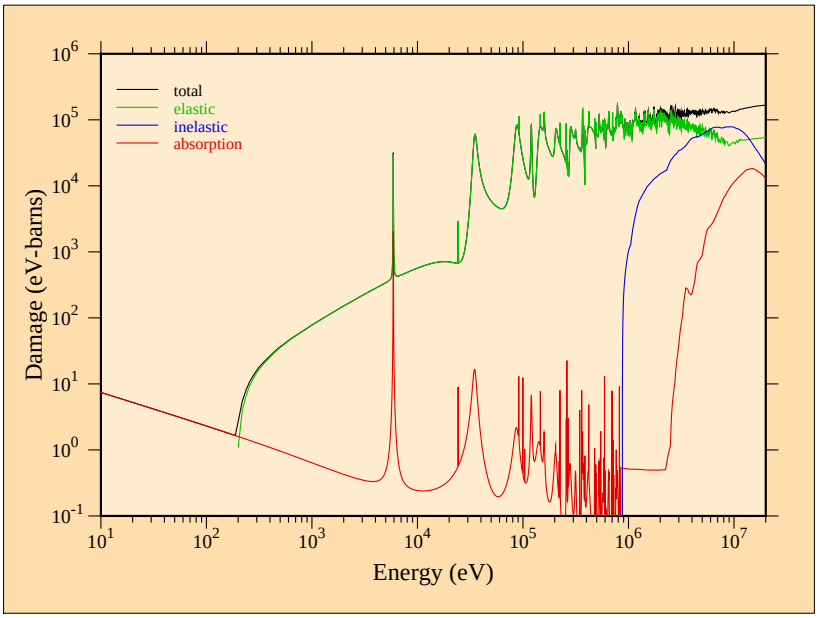


Figure 10: Components of radiation damage energy production for $^{27}$Al from ENDF/B-VII.0. Note that capture dominates at very low energies, then elastic dominates, and finally inelastic begins to contribute at very high energies.

where $z$ is the charge of the emitted particle and $Z$ is the charge of the target. A more reasonable distribution would be desirable[49], but this one has the advantage of eliminating an integration, and most results are dominated by the kick imparted by the incident neutron anyway. The angular distribution for the emitted particle is taken as isotropic in the lab. At high incident energies, direct interaction processes would be expected to give rise to a forward-peaked distribution, thereby reducing the damage. However, the importance of this effect is also reduced by the dominance of the neutron kick.

Fig. 10 gives a typical result for a damage energy production calculation, showing the separate contributions of elastic, inelastic, and absorption processes.

## 6.6 Heating and Damage from File 6

A number of the evaluations in ENDF/B-VI and later include complete energy-angle distributions for all of the particles produced by a reaction, including the residual nucleus. In these cases, HEATR can compute the contributions to KERMA by calculating the average energy in the spectrum of each outgoing charged particle or residual nucleus and using Eq. 161.

A fully-populated section of File 6 contains subsections for all of the particles

and photons produced by the reaction, including the recoil nucleus. There are a number of different schemes used to represent the energy-angle distributions for these outgoing particles. The most important ones for HEATR follow:

- *No distribution.* In this case, the subsection is inadequate for use in heating and damage calculations. A warning message is issued.
- *Two-body angular distribution.* These are basically the same as distributions in File 4.
- *Recoil distribution.* This particle is a recoil nucleus from a two-body reaction. Its angular distribution is assumed to be the complement of the angular distribution for the first subsection in this section.
- *CM Kalbach distribution.* This format is often used by LANL evaluations, and transformation to the laboratory frame is required. The looping order for the data is $E$, $E'$, $\mu$.
- *LAB Legendre distribution.* This format is used in most of the ORNL evaluations for ENDF/B-VI. It is already in the laboratory frame, and the angular information can be simply ignored.
- *LAB angle-energy distribution.* This format is used for the $^9$Be evaluation of ENDF/B-VI by LLNL. The looping order is $E$, $\mu$, $E'$.

The normal procedure is to loop through all of these subsections. The subsections producing neutrons are processed to be used in a total energy check, but they contribute nothing to the heating or to the damage. Subsections describing charged particles and residual nuclei are processed into heating and damage contributions. Finally, the photon subsection is processed for the photon energy check and the total energy check, even though it does not affect either heating or damage. Any remaining difference between the eV-barns available for the reaction and the eV-barns carried away by the neutrons, photons, particles, and recoil is added into the heating to help preserve the total energy deposition in the spirit of the energy-balance method.

For "two-body" sections, the emitted particle energy is given by

$$E' = \frac{A'E}{A+1}\Big(1 + 2R\mu + R^2\Big) \ , \tag{216}$$

where

$$R = \sqrt{\frac{A(A+1-A')}{A'}} \ , \tag{217}$$

and $A'$ is the ratio of the mass of the outgoing particle to that of the incident

particle. The heating is obtained by doing a simple integral over $\mu$, and the damage is computed using the integral over $\mu$ given in Eq. 206. In both cases, the integrals are performed using either a 20-point Gauss-Legendre quadrature (for Legendre representations) or a trapezoidal integration (for tabulated data).

For "recoil" sections, the code backs up to the particle distribution and calculates the recoil using the same method described above with the sign of $\mu$ changed.

For laboratory distributions that use the $E$, $E'$, $\mu$ ordering, the angular part can be ignored, and the heating and damage become

$$K(E) = \int g(E \to E') E' \, dE' \ , \tag{218}$$

and

$$D(E) = \int g(E \to E') P(E') \, dE' \ , \tag{219}$$

where $g(E \to E')$ is the angle-integrated energy distribution from File 6, and $P(E')$ is the damage partition function. Trapezoidal integration is used for the continuum, and the integrand is simply added into the sum for the delta functions (if any).

Heating for subsections that use the ordering $E$, $\mu$, $E'$ is computed using the formula

$$K(E) = \int \left\{ \int g(E \to E', \mu) E' \, dE' \right\} d\mu \ , \tag{220}$$

where an inner integral is performed using trapezoidal integration for each value in the $\mu$ grid. The results are then used in a second trapezoidal integration over $\mu$. The damage integral is performed at the same time in a parallel manner.

The problem is somewhat more difficult for subsections represented in the center-of-mass frame. The definitions for $K(E)$ and $D(E)$ are the same as those given above, except that the quantity $g(E \to E')$ has to be generated in the lab system. The methods used to do the transformation are basically the same in HEATR and GROUPR. The first step is to set up an adaptive integration over $E'$. The first value needed to prime the stack is obtained by calling `h6cm` with $E'$=0. It returns the corresponding value of $g$ in the lab system and a value for `epnext`. The second value for the stack is computed for $E$=`epnext`. The routine then subdivides this interval until 2% convergence is achieved, accumulating the contributions to the heating and damage integrals as it goes. It then moves up

to a new panel. This process continues until the entire range of $E'$ has been covered.

The key to this process is `h6cm`. As described in more detail in the GROUPR chapter of this manual, it performs integrals of the form

$$g_L(E \to E'_L) = \int_{\mu_{\min}}^{+1} g_C(E \to E'_C, \mu_C)\, J\, d\mu_L \ , \tag{221}$$

where $L$ and $C$ denote the laboratory and center-of-mass systems, respectively, and $J$ is the Jacobian for the transformation. The contours in the $E'_C$,$\mu_C$ frame that are used for these integrals have constant $E'_L$. The limiting cosine, $\mu_{\min}$, depends on kinematic factors and the maximum possible value for $E'_C$ in the File 6 tabulation.

The ENDF/B-VII library contains a few abbreviated versions of File 6 that contain an energy-angle distribution for neutron emission, but no recoil or photon data. In order to get semi-reasonable results for both heating and damage for such cases, HEATR applies a "one-particle recoil approximation," where the first particle emitted is assumed to induce all the recoil. There are also some cases where capture photons are described in MF=6/MT=102 with no corresponding recoil data. Here, the recoil can be added using the same logic described above for capture represented using File 15. The difference between the eV-barns available for the reaction and the energy accounted for by the emitted neutrons, photons, particles, and the approximated recoil is added into the heating in order to preserve the total heating in the spirit of the energy-balance method.

## 6.7 User Input

The input instructions that follow were reproduced from the comment cards in the current version of HEATR.

```
!---input specifications (free format)-----------------------
!
! card 1
!    nendf    unit for endf tape
!    nin      unit for input pendf tape
!    nout     unit for output pendf tape
!    nplot    unit for graphical check output
! card 2
!    matd     material to be processed
!    npk      number of partial kermas desired (default=0)
```

```
!    nqa      number of user q values (default=0)
!    ntemp    number of temperatures to process
!             (default=0, meaning all on pendf)
!    local    0/1=gamma rays transported/deposited locally
!             (default=0)
!    iprint   print (0 min, 1 max, 2 check) (default=0)
!    ed       displacement energy for damage
!             (default from built-in table)
! card 3      for npk gt 0 only
!    mtk      mt numbers for partial kermas desired
!             total (mt301) will be provided automatically.
!             partial kerma for reaction mt is mt+300
!             and may not be properly defined unless
!             a gamma file for mt is on endf tape.
!             special values allowed--
!               303   non-elastic (all but mt2)
!               304   inelastic (mt51 thru 91)
!               318   fission (mt18 or mt19, 20, 21, 38)
!               401   disappearance (mt102 thru 120)
!               442   total ev-barns
!               443   total kinematic kerma (high limit)
!             damage energy production values--
!               444   total
!               445   elastic (mt2)
!               446   inelastic (mt51 thru 91)
!               447   disappearance (mt102 thru 120)
!          cards 4 and 5 for nqa gt 0 only
! card 4
!    mta      mt numbers for users q values
! card 5
!    qa       user specified q values (ev)
!               (if qa.ge.99.e6, read in variable qbar
!                  for this reaction)
! card 5a     variable qbar (for reactions with qa flag only)
!    qbar      tab1 record giving qbar versus e (1000 words max)
!
!--------------------------------------------------------------
```

Card 1 specifies the input and output units for HEATR. They are all ENDF-type files. The input PENDF file has normally been through RECONR and BROADR, but it is possible to run HEATR directly on an ENDF file in order

to do kinematic checks. In this case, the results in the resonance range should be ignored. Defining `nplot` will produce a file of input for the VIEWR module containing detailed energy-balance test results. This option should only be used together with `iprint`=2.

On Card 2, the default value for `npk` is zero, which instructs the code to process the energy-balance total KERMA (MT=301) only. Most often, the user will also want to include MT=443 and MT=444 (`npk`=2). The kinematic KERMA computed when MT=443 is requested is very useful for judging the energy-balance consistency of an evaluation (see the subsection on "Diagnosing Energy-Balance Problems", Section 6.9, below). It can also be used instead of the energy-balance value in MT=301 when local heating effects are important and the evaluation scores poorly in an energy-balance check. Damage energy production cross sections (MT=444) should be computed for important structural materials; this expensive calculation can be omitted for other materials.

When kinematic checks are desired, a number of additional `npk` values can be included. They can be determined by checking the evaluation to see what partial KERMA factors are well defined. For old-style evaluations that do not use File 6, look for the MT values used in Files 12 and 13. Many evaluations use only MT=3 and MT=102 (or 3, 18, and 102 for fissionable materials); in these cases, the only `mtk` values that make sense are 302, 303, and 402 (or 302, 303, 318, and 402 for fissionable materials). Caution: in many evaluations, MT=102 is used at low energies and taken to zero at some breakpoint. MT=3 is used at higher energies. In these evaluations, the partial KERMA MT=402 does not make sense above the breakpoint, and MT=3 does not make sense below it.

More complicated photon-production evaluations may include MT=4 and/or discrete-photon data in MT=51-90. In these cases, the user can request `mtk`=304. The same kind of energy-range restriction discussed for MT=102 can occur for the inelastic contributions. Other evaluations give additional partial reactions that can be used to check the photon production and energy-balance consistency of an evaluation in detail. HEATR can handle 6 additional reactions at a time. Multiple runs may be necessary in complex cases.

Note that several special `mtk` values are provided for the components of the damage-energy production cross section. They were used to prepare Fig. 10, and may be of interest to specialists, but they are not needed for most libraries.

In a few cases in the past, it has been necessary to change the $Q$-values that are normally retrieved from the ENDF tape. In addition, it is sometimes necessary to replace the single $Q$-value supplied in MF=3 with an energy-dependent

Q function for an element. One example of the former occurred for $^{16}$O for ENDF/B-V. The first inelastic level (MT=51) decays by pair production rather than the more normal mode of photon emission. In order to get the correct heating, it was necessary to change the $Q$-value by giving Card 4 and Card 5 as follows:

```
51
-5.0294e6
```

That is, the $Q$-value is increased by twice the electron energy of 0.511 MeV. Another example is the sequential (n,2n) reaction for $^{9}$Be in ENDF/B-V. It is necessary to include 4 changes to the $Q$-values:

```
46 47 48 49/
-1.6651e6 -1.6651e6 -1.6651e6 -1.6651e6/
```

The next example illustrates using energy-dependent $Q$-values for elemental titanium. Set `nqa` equal to 3 and give the following values on Cards 4, 5, and 5a:

```
16 103 107/
99e6 99e6 99e6/
0. 0. 0 0 1 8
8 2
8.0e6 -8.14e6 9.0e6 -8.14e6 1.1e7 -8.38e6
1.2e7 -8.74e6 1.3e7 -1.03e7 1.4e7 -1.091e7
1.5e7 -1.11e7 2.0e7 -1.125e7/
0. 0. 0 0 1 9
9 2
1.0e-5 1.82e5 4.0e6 1.82e5 5.0e6 -1.19e6
6.0e6 -2.01e6 7.0e6 -2.20e6 8.0e6 -2.27e6
1.4e7 -2.35e6 1.7e6 -2.43e6 2.0e7 -2.37e6/
0. 0. 0 0 1 9
9 2
1.0e-5 2.182e6 6.0e6 2.182e6 7.0e6 2.10e6
8.0e6 -3.11e5 9.0e6 -9.90e5 1.0e7 -1.20e6
```

```
 1.1e7 -1.27e6 1.4e6 -1.32e6 2.0e7 -1.48e6/
```

The next parameter on Card 2 is `ntemp`. For normal runs, use zero, and all the temperatures on the input PENDF tape will be processed. For kinematic check runs, use `ntemp`=1. The `local` parameter suppresses the processing of the photon-production files, if any. The photon energy appears in the KERMA factors as if the photons had very short range. A useful way to use the `iprint` parameter is to set it to zero for normal runs, which produce heating and damage values at all temperatures, and to use `iprint`=2 for the energy-balance check run, which is performed for the first temperature on `nin` only.

Card 3 gives the partial KERMA and damage selection MT numbers. Note that the user does not include MT=301 in this list. It is always inserted as the first value automatically. Giving MT=301 in this list will cause an informative message to be issued.

Cards 4, 5, and 5a give the user's changes to the ENDF Q values. The way in which to use these cards was described in connection with `nqa` on Card 2.

## 6.8 Reading HEATR Output

When full output and/or kinematic checks have been requested, HEATR loops through the reactions found in Files 3, 12, and 13. For each reaction, it prints out information about the energies, yields, cross sections, and contributions to heating. The energy grid used is a subset of the PENDF grid. At present, decade steps are used below 1 eV, factor-of-two steps are used from 1 eV to 100 keV, quarter-lethargy steps are used above 100 keV, and approximately 1 MeV steps are used above 2 MeV. An example of this printout for elastic scattering in ENDF/B-VII.0 $^{27}$Al is shown below:

```
neutron heating for mt  2   q0 =  0.0000E+00     q =  0.0000E+00
           e          ebar   ...       xsec       heating        damage
  1.0000E-05    9.3052E-06   ... 1.5694E+01    1.0903E-05    0.0000E+00
  1.0000E-04    9.3052E-05   ... 5.1179E+00    3.5557E-05    0.0000E+00
  1.0000E-03    9.3052E-04   ... 2.0644E+00    1.4342E-04    0.0000E+00
  1.0000E-02    9.3052E-03   ... 1.4925E+00    1.0369E-03    0.0000E+00
  1.0000E-01    9.3052E-02   ... 1.4318E+00    9.9474E-03    0.0000E+00
    ...
  1.0000E+03    9.3052E+02   ... 1.3662E+00    9.4914E+01    7.7171E+01
  2.0000E+03    1.8610E+03   ... 1.3196E+00    1.8337E+02    1.5115E+02
```

```
  5.0000E+03    4.6526E+03   ... 1.2130E+00    4.2136E+02    3.3998E+02
  1.0000E+04    9.3052E+03   ... 1.0367E+00    7.2028E+02    5.6725E+02
  2.0000E+04    1.8610E+04   ... 6.6204E-01    9.1991E+02    7.0347E+02
  5.0000E+04    4.6526E+04   ... 2.3220E+00    8.0660E+03    5.8732E+03
  1.0000E+05    9.3052E+04   ... 5.2976E+00    3.6805E+04    2.5521E+04
    ...
  1.0000E+07    9.7233E+06   ... 7.4942E-01    2.0738E+05    4.5689E+04
  1.1000E+07    1.0699E+07   ... 7.4953E-01    2.2576E+05    4.7347E+04
  1.2000E+07    1.1682E+07   ... 7.6363E-01    2.4286E+05    4.9202E+04
  1.3000E+07    1.2673E+07   ... 7.6329E-01    2.4980E+05    4.9559E+04
  1.4000E+07    1.3670E+07   ... 7.7918E-01    2.5737E+05    5.0566E+04
  1.5000E+07    1.4671E+07   ... 7.9297E-01    2.6088E+05    5.1189E+04
  1.6000E+07    1.5676E+07   ... 8.1414E-01    2.6347E+05    5.1973E+04
  1.7000E+07    1.6681E+07   ... 8.3429E-01    2.6577E+05    5.2680E+04
  1.8000E+07    1.7689E+07   ... 8.4524E-01    2.6246E+05    5.2747E+04
  1.9000E+07    1.8695E+07   ... 8.7093E-01    2.6568E+05    5.3787E+04
  2.0000E+07    1.9703E+07   ... 8.9326E-01    2.6547E+05    5.4573E+04
    ...
  1.4000E+08    1.3985E+08   ... 2.9730E-01    4.3523E+04    1.4994E+04
  1.4600E+08    1.4585E+08   ... 2.7580E-01    4.1851E+04    1.3890E+04
  1.5000E+08    1.4984E+08   ... 2.6510E-01    4.1161E+04    1.3339E+04
```

Note the identification and Q information printed on the first line; `q` is the ENDF $Q$-value from File 3, and `q0` is the corresponding mass-difference $Q$-value needed for Eq. 162. The `ebar`, `yield` (which was replaced by "..." to make this listing fit better), and `xsec` columns contain $\overline{E}_n$, $Y$, and $\sigma$, respectively. The `heating` column is just $(E+Q-Y\overline{E}_n)\sigma$. The results are similar for discrete inelastic levels represented using File 4. The heating due to the associated photons will be subtracted later while MF=12 or MF=13 is being processed. However, if an LR flag is set, the residual nucleus from the (n,n′) reaction breaks up by emitting additional particles. This extra breakup energy changes the `q0` value. An example of such a section for $^{27}$Al(n,n$_{25}$)p from ENDF/B-V follows:

```
neutron heating for mt 75   q0 = -8.2710e+06     q = -1.0750e+07
             e          ebar         yield          xsec       heating
    1.2000e+07    7.8653e+05    1.0000e+00    8.2242e-02    2.4199e+05
    1.3000e+07    1.7116e+06    1.0000e+00    8.0121e-02    2.4176e+05
    1.4000e+07    2.6427e+06    1.0000e+00    5.9282e-02    1.8296e+05
    1.5000e+07    3.5864e+06    1.0000e+00    4.1834e-02    1.3147e+05
```

```
    1.6000e+07    4.5096e+06    1.0000e+00    2.8880e-02    9.2977e+04
    1.7000e+07    5.4335e+06    1.0000e+00    1.9867e-02    6.5472e+04
    1.8000e+07    6.3848e+06    1.0000e+00    1.3677e-02    4.5739e+04
    1.9000e+07    7.2944e+06    1.0000e+00    9.4771e-03    3.2550e+04
    2.0000e+07    8.2479e+06    1.0000e+00    6.6142e-03    2.3025e+04
```

Starting with ENDF/B-VI, discrete-inelastic sections may also be given in File 6. Such sections contain their own photon production data, and the `heating` column will represent the entire recoil energy as in Eq. 180. (See below for detailed discussion of ENDF/B-VI output.)

For continuum reactions that use MF=4 and MF=5, such as (n,n′) or (n,2n), the neutron part of the display looks like this:

```
neutron heating for mt 16   q0 = -1.3057e+07     q = -1.3057e+07
             e          ebar         yield          xsec       heating
    1.4000e+07    1.9960e+05    2.0000e+00    2.4000e-02    1.3051e+04
    1.5000e+07    6.6850e+05    2.0000e+00    1.2320e-01    7.4659e+04
    1.6000e+07    1.0855e+06    2.0000e+00    2.0710e-01    1.5987e+05
    1.7000e+07    1.4308e+06    2.0000e+00    2.6510e-01    2.8667e+05
    1.8000e+07    1.6379e+06    2.0000e+00    3.0300e-01    5.0518e+05
    1.9000e+07    1.7659e+06    2.0000e+00    3.3000e-01    7.9567e+05
    2.0000e+07    1.8755e+06    2.0000e+00    3.5000e-01    1.1172e+06
```

Once again, the photon effects will be subtracted later.

Absorption reactions such as (n,γ) or (n,p), lead to similar displays, but the particle `ebar` columns will always be set to zero (no emitted neutrons). An example follows:

```
neutron heating for mt103   q0 = -1.8278e+06     q = -1.8278e+06
             e          ebar         yield          xsec       heating
    2.5000E+06    0.0000E+00    1.0000E+00    3.2800E-05    2.2048E+01
    3.0000E+06    0.0000E+00    1.0000E+00    1.3300E-03    1.5590E+03
    3.5000E+06    0.0000E+00    1.0000E+00    1.0100E-02    1.6889E+04
    4.0000E+06    0.0000E+00    1.0000E+00    6.9667E-03    1.5133E+04
    4.5000E+06    0.0000E+00    1.0000E+00    1.7000E-02    4.5427E+04
    5.0000E+06    0.0000E+00    1.0000E+00    2.3300E-02    7.3912E+04
       ...
    1.7000E+07    0.0000E+00    1.0000E+00    5.5200E-02    8.3751E+05
```

```
    1.8000E+07    0.0000E+00    1.0000E+00    4.7800E-02    7.7303E+05
    1.9000E+07    0.0000E+00    1.0000E+00    4.0200E-02    6.9032E+05
    2.0000E+07    0.0000E+00    1.0000E+00    3.2200E-02    5.8514E+05
```

If File 6 is present (which happens for evaluations in ENDF-6 format only, such as the evaluations in ENDFB-VII), each reaction will be divided into subsections, one for each emitted particle. The neutron subsections are displayed as part of the energy-balance checks, but they do not contribute to KERMA or damage. The subsection for each charged particle or residual nucleus will give the incident energy, average energy for the emitted particle, cross section, heating contribution, and (optionally) damage contribution as follows:

```
file six heating for mt 28, particle =     1     q =  -8.2721E+06
             e          ebar         yield          xsec       heating
    9.0000E+06    1.2303E+05    1.0000E+00    1.0385E-03    0.0000E+00
    1.0000E+07    4.6746E+05    1.0000E+00    1.3526E-02    0.0000E+00
    ...
    1.8000E+07    3.1862E+06    1.0000E+00    3.7721E-01    0.0000E+00
    1.9000E+07    3.4535E+06    1.0000E+00    3.7577E-01    0.0000E+00
    2.0000E+07    3.7207E+06    1.0000E+00    3.7434E-01    0.0000E+00

file six heating for mt 28, particle =  1001     q =  -8.2721E+06
             e          ebar         yield          xsec       heating
    9.0000E+06    4.5909E+05    1.0000E+00    1.0385E-03    4.7677E+02
    1.0000E+07    8.9616E+05    1.0000E+00    1.3526E-02    1.2121E+04
    ...
    1.8000E+07    3.5193E+06    1.0000E+00    3.7721E-01    1.3275E+06
    1.9000E+07    3.8257E+06    1.0000E+00    3.7577E-01    1.4376E+06
    2.0000E+07    4.1321E+06    1.0000E+00    3.7434E-01    1.5468E+06

file six heating for mt 28, particle = 12026     q =  -8.2721E+06
             e          ebar         yield          xsec       heating
    9.0000E+06    3.2104E+05    1.0000E+00    1.0385E-03    3.3340E+02
    1.0000E+07    3.8540E+05    1.0000E+00    1.3526E-02    5.2128E+03
    ...
    1.8000E+07    8.0820E+05    1.0000E+00    3.7721E-01    3.0486E+05
    1.9000E+07    8.6147E+05    1.0000E+00    3.7577E-01    3.2372E+05
    2.0000E+07    9.1475E+05    1.0000E+00    3.7434E-01    3.4243E+05

file six heating for mt 28, particle =     0     q =  -8.2721E+06
```

```
          e          ebar         yield          xsec       heating
 9.0000E+06    1.8347E+05    2.8104E-06    1.0385E-03    0.0000E+00
                                                ebal    -1.8204E+02
 1.0000E+07    4.4913E+05    3.0441E-05    1.3526E-02    0.0000E+00
                                                ebal    -2.8626E+02
 ...
 1.8000E+07    1.8309E+06    1.2028E+00    3.7721E-01    0.0000E+00
                                                ebal     4.5397E+03
 1.9000E+07    1.8856E+06    1.3695E+00    3.7577E-01    0.0000E+00
                                                ebal     1.8336E+03
 2.0000E+07    1.9403E+06    1.5363E+00    3.7434E-01    0.0000E+00
                                                ebal    -7.6798E+03
```

Note that the last subsection in this example was for emitted photons. Photons do not contribute to the KERMA or damage, but this information is used to check the total energy conservation for this reaction. The `ebal` lines show the difference between the available energy and the sum over all the outgoing particles. The values should be a small percentage of the total heating. If the `ebal` values are too large, there may be an error in the evaluation, or it may be necessary to refine the energy grids in the distributions. In addition, this photon production information is needed later for the photon energy check.

After all the sections corresponding to MT numbers in File 3 have been processed (using the File 4, File 4/5, or File 6 method as appropriate), the photon production sections in Files 12 and 13 are processed, if present. File 12 data are usually present for radiative capture (MT=102), at least at low energies. Simple files normally give a tabulated photon spectrum. The display gives the average energy for this spectrum in the `ebar` column and the negative contribution to the heating computed with Eq. 171 in the `heating` column. The `edam` column contains the $\overline{E_\gamma^2}$ term needed to compute the photon contribution to the damage, which is given in the `damage` column. See Eq. 211. The display also has an extra line for each incident energy containing the percent error "`-- pc`" between the total photon energy as computed from File 12 and the value $E{+}Q{-}E/(A{+}1)$ computed from File 3. As discussed above, HEATR does not guarantee energy balance in large systems if this error occurs. The following example shows some large errors due to mistakes in the ENDF/B-V evaluation for $^{55}$Mn. Two columns labeled `edam` and `xsec` have been removed to show the `heating` and `damage` columns. The text has also been shifted to the left of its normal position to fit better on the printed page.

```
photon energy (from yields) mf12, mt102
         e    ebar/err        egam ...      yield     heating      damage
1  continuum gammas
1.0000e-05  4.5088e+06  2.4237e+02 ... 2.4791e+00 -4.8477e+09  5.4975e+04
1.0000e-05    53.7 pc
1.0703e-04  4.5088e+06  2.4237e+02 ... 2.4791e+00 -1.4819e+09  1.6806e+04
1.0703e-04    53.7 pc
1.2520e-03  4.5088e+06  2.4237e+02 ... 2.4791e+00 -4.3347e+08  4.9159e+03
1.2520e-03    53.7 pc
  ...
1.3571e+04  4.4522e+06  2.3887e+02 ... 2.4836e+00 -7.3869e+03 -1.2406e-01
1.3571e+04    51.8 pc
2.7142e+04  4.3957e+06  2.3536e+02 ... 2.4881e+00 -3.7037e+05 -1.6487e+01
2.7142e+04    49.9 pc
5.4287e+04  4.2826e+06  2.2834e+02 ... 2.4972e+00 -2.5604e+04 -2.5340e+00
5.4287e+04    46.0 pc
1.0858e+05  4.0563e+06  2.1430e+02 ... 2.5154e+00 -1.3327e+04 -2.7289e+00
1.0858e+05    38.3 pc
```

Many MF=12, MT=102 sections give multiplicities for the production of discrete photons. In these cases, HEATR prints out data for all of the parts, and it provides a sum at the end. The balance error is printed with the sum. The following example shows a case with discrete photons. The last two columns have been removed (`heating`, `damage`), and the text has been compacted and shifted to the left to fit on the printed page.

```
photon energy (from yields) mf12, mt102
         e    ebar/err        egam        edam        xsec       yield
1   7.7260E+06 ev gamma
1.0000e-05  7.7260e+06  1.1448e+03  8.9780e+02  1.1677e+01  3.0000e-01
1.1406e-04  7.7260e+06  1.1448e+03  8.9780e+02  3.4574e+00  3.0000e-01
1.1406e-03  7.7260e+06  1.1448e+03  8.9780e+02  1.0934e+00  3.0000e-01
  ...
2.0000e+07  2.7005e+07  1.1448e+03  8.9780e+02  1.0000e-03  3.0000e-01
2   7.6950e+06 ev gamma
1.0000e-05  7.6950e+06  1.1356e+03  8.9091e+02  1.1677e+01  5.0000e-02
1.1406e-04  7.6950e+06  1.1356e+03  8.9091e+02  3.4574e+00  5.0000e-02
  ...
```

```
 2.0000e+07  2.6974e+07  1.1356e+03  8.9091e+02  1.0000e-03  5.0000e-02
 3   6.8630e+06 ev gamma
 1.0000e-05  6.8630e+06  9.0330e+02  7.1515e+02  1.1677e+01  1.2000e-03
 1.1406e-04  6.8630e+06  9.0330e+02  7.1515e+02  3.4574e+00  1.2000e-03
 1.1406e-03  6.8630e+06  9.0330e+02  7.1515e+02  1.0934e+00  1.2000e-03
   ...
89   3.1000e+04 eV gamma
 1.0000e-05  3.1000e+04  1.8430e-02  0.0000e+00  1.1677e+01  2.8884e-01
 1.0000e-05     0.0 pc
 1.1406e-04  3.1000e+04  1.8430e-02  0.0000e+00  3.4574e+00  2.8884e-01
 1.1406e-04     0.0 pc
 1.1406e-03  3.1000e+04  1.8430e-02  0.0000e+00  1.0934e+00  2.8884e-01
 1.1406e-03     0.0 pc
 1.1912e-02  3.1000e+04  1.8430e-02  0.0000e+00  3.3832e-01  2.8884e-01
 1.1912e-02     0.0 pc
   ...
 2.0000e+07  3.1000e+04  1.8430e-02  0.0000e+00  1.0000e-03  2.8884e-01
 2.0000e+07     0.0 pc
```

In this case ($^{27}$Al), the capture energy production checks out perfectly for the sum of all 89 discrete photons.

Other sections using either File 12 or File 13 generate displays similar to the following:

```
photon energy (from xsecs) mf13, mt  3
             e           ebar           xsec        energy       heating
    1  continuum gammas
    2.0000e+05    3.6753e+06    4.2076e-03    1.5464e+04   -1.5464e+04
    4.0500e+05    3.3863e+06    5.2873e-03    1.7904e+04   -1.7904e+04
    6.0031e+05    3.1097e+06    6.4478e-03    2.0051e+04   -2.0051e+04
    8.0182e+05    2.0089e+06    9.3236e-02    1.8730e+05   -1.8730e+05
    1.0000e+06    9.2622e+05    1.7859e-01    1.6541e+05   -1.6541e+05
    1.2000e+06    9.6151e+05    2.8329e-01    2.7239e+05   -2.7239e+05
  ...
```

Note that the photon $\overline{E}\sigma$ is simply subtracted from the `heating` column for each incident energy.

If the partial KERMA `mtk`=443 was requested in the user's input, HEATR will print out a special section that tests the total photon energy production

against the kinematic limits (see Section 6.4 above for the formulas used). An example follows:

```
photon energy production check
             e      ev-barns           min           max
    1.0000e-05    9.0215e+07    9.0187e+07    9.0200e+07
    1.1406e-04    2.6712e+07    2.6704e+07    2.6708e+07
    1.1406e-03    8.4479e+06    8.4453e+06    8.4466e+06
    1.1912e-02    2.6138e+06    2.6130e+06    2.6134e+06
    1.2812e-01    7.9895e+05    7.9871e+05    7.9883e+05
    1.2812e+00    2.5211e+05    2.5203e+05    2.5207e+05
    2.6875e+00    1.7420e+05    1.7415e+05    1.7417e+05
    5.5000e+00    1.2186e+05    1.2182e+05    1.2184e+05
    1.1406e+01    8.4662e+04    8.4636e+04    8.4648e+04
    2.4062e+01    5.8231e+04    5.8213e+04    5.8222e+04
    4.9375e+01    4.0614e+04    4.0601e+04    4.0607e+04
    1.0000e+02    2.8522e+04    2.8514e+04    2.8518e+04
  ...
    8.0000e+06    3.8972e+06    3.7964e+06    4.4880e+06
    9.0000e+06    4.4782e+06    4.4401e+06    5.4986e+06
    1.0000e+07    4.9645e+06    5.2078e+06    6.6176e+06
    1.1000e+07    5.3712e+06    6.1302e+06    7.8374e+06   ----
    1.2000e+07    5.3212e+06    5.8699e+06    8.0618e+06
    1.3000e+07    5.0984e+06    5.9333e+06    8.5312e+06   ----
    1.4000e+07    4.7415e+06    5.7172e+06    8.6605e+06   ----
    1.5000e+07    4.0795e+06    4.7419e+06    8.0409e+06   ----
    1.6000e+07    3.2521e+06    3.6806e+06    7.2734e+06   ----
    1.7000e+07    2.8079e+06    2.8418e+06    6.6927e+06
    1.8000e+07    2.7492e+06    2.2915e+06    6.2850e+06
    1.9000e+07    2.9626e+06    1.9674e+06    6.2330e+06
    2.0000e+07    3.4419e+06    1.7938e+06    6.1994e+06
```

The low and high kinematic limits will be the same at low energies where only kinematics affect the calculations. They may be the same for all energies for ENDF/B-VII evaluations that provide complete distributions for all outgoing charged particles and recoil nuclei. Normally, the limits diverge above the threshold for continuum reactions. Note that HEATR marks lines where the computed value goes more than a little way outside the limits with the symbols `++++` or `----`. It is often convenient to extract these numbers from the output listing and

plot them (see Fig. 11). Although the energy grid is a little coarse, such plots can often be useful (see below).

The last part of a full HEATR output listing is a tabulation of the computed KERMA and damage coefficients on the normal coarse energy grid. Columns are provided for the total KERMA and for each of the partial KERMA results requested with `mtk` values in the user's input. If kinematic checks were requested, the check values are written just above and below the corresponding partial KERMA values. In addition, `low` and `high` messages are written just above or just below the kinematic limits in every column where a significant violation of the limits occurs. Caution: if summation reactions (MT=3, MT=4) were used to define the photon production over some parts of the energy range, the partial KERMA results may not make sense at some energies. For example, consider the common pattern in ENDF/B-V where MT=102 is used for capture at low energies, but at higher energies, it is set to zero, and the capture contribution is included in MT=3 (nonelastic). Clearly, the partial KERMA MT=402 doesn't make sense above this breakpoint. The following example shows part of the final KERMA listing for ENDF/B-V.1 $^{55}$Mn. The damage column was removed and the columns compressed to fit on the printed page.

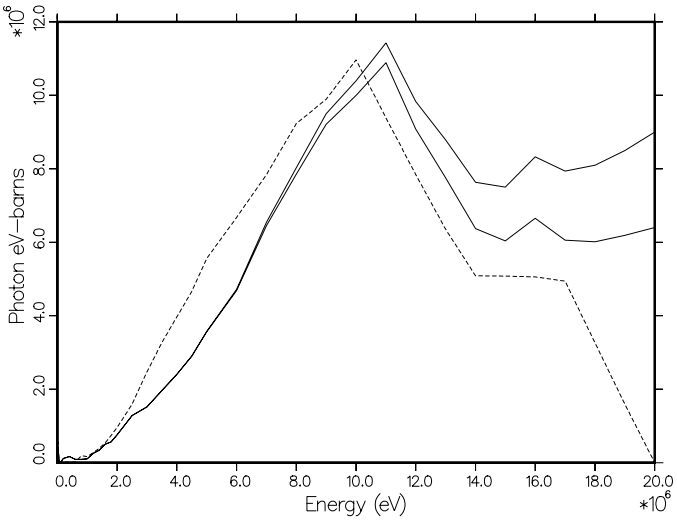


Figure 11: Example of a plot comparing the total photon energy production for $^{55}$Mn from ENDF/B-V.1 (dashed) with the kinematic limits (solid).

```
final kerma factors
          e           301           302           303           402           443

       min   1.2400e-04   3.7775e-06   1.2022e-04   1.2022e-04
 1.0000e-05   4.0068e+05   3.7775e-06   4.0068e+05   4.0068e+05   4.0068e+05
       max   3.3820e+05   3.7775e-06   3.3820e+05   3.3820e+05
               high                       high         high

  ...

       min   3.2373e+04   2.3497e+04   8.8759e+03   4.1114e+01
 6.0031e+05   1.0017e+05   2.3497e+04   7.6673e+04   2.9899e+04   3.2375e+04
       max   3.2375e+04   2.3497e+04   8.8781e+03   4.3366e+01
               high                       high         high

                low                        low
       min   7.3041e+04   5.9403e+04   1.3638e+04   4.4748e+01
 8.0182e+05  -2.4355e+04   5.9403e+04  -8.3758e+04   2.4987e+04   7.3043e+04
       max   7.3043e+04   5.9403e+04   1.3640e+04   4.6676e+01
                                                     high

               low                        low
       min   9.8973e+04   7.7075e+04   2.1898e+04   4.7777e+01
 1.0000e+06   3.7682e+04   7.7075e+04  -3.9393e+04   2.1917e+04   9.8974e+04
       max   9.8974e+04   7.7075e+04   2.1900e+04   4.9509e+01
                                                     high

               low                        low
       min   1.1397e+05   7.7800e+04   3.6168e+04   4.9760e+01
 1.2000e+06   9.5321e+04   7.7800e+04   1.7521e+04   1.9482e+04   1.1397e+05
       max   1.1397e+05   7.7800e+04   3.6169e+04   5.1335e+01
                                                     high

               low                        low
       min   1.4632e+05   1.0192e+05   4.4402e+04   5.3005e+01
 1.4000e+06   9.8251e+04   1.0192e+05  -3.6667e+03   1.8208e+04   1.4632e+05
       max   1.4632e+05   1.0192e+05   4.4403e+04   5.4511e+01
                                                     high

  ...
```

```
       min   2.3650e+05   1.6907e+05   6.7426e+04   1.7607e+02
1.9000e+07   7.1384e+06   1.6907e+05   6.9693e+06   1.3503e+04   2.5435e+06
       max   2.5435e+06   1.6907e+05   2.3744e+06   1.7939e+02
               high                       high         high

       min   2.4001e+05   1.8261e+05   5.7406e+04   1.4423e+02
2.0000e+07   9.2369e+06   1.8261e+05   9.0543e+06   1.0908e+04   2.8385e+06
       max   2.8385e+06   1.8261e+05   2.6559e+06   1.4701e+02
               high                       high         high
```

The following subsection discusses how to analyze the "check" output of HEATR in order to diagnose energy-balance errors in ENDF-format evaluations. The examples are drawn from ENDF/B-V testing[43]. In general, results like these are less likely to occur in modern evaluations.

## 6.9 Diagnosing Energy-Balance Problems

The analysis should start with MT=102, because if it is wrong, the guarantee of energy conservation for large systems breaks down. If the display for MF=12, MT=102 shows messages of the form "`-- pc`", there may be a problem. If these messages only show up at the higher energies, and if the size of the error increases with energy, it is probable that the evaluator has used a thermal spectrum over the entire energy range (this is very common). Of course, the total photon energy production from radiative capture should equal

$$\frac{A}{A+1}E + Q \ , \tag{222}$$

where the rest of the total energy $E$+$Q$ is carried away by recoil. If only a thermal spectrum is given, the $E$ term is being neglected, and errors will normally appear above about 1 MeV. The $E$ term can be included in evaluations that use tabulated data by giving $E$-dependent spectra in File 15; and it can be included for evaluations that use discrete photons by setting the "primary photon" flags in File 12 properly. In practice, the capture cross sections above 1 MeV are often comparatively small due to the $1/v$ tendency of capture, and the errors introduced by neglecting the $E$ term can be ignored.

If the MT=102 errors show up at low energies, there is probably an error in the average photon yield from File 12, in the average energy computed from File 15, or both. In the $^{55}$Mn case shown above, the yield had been incorrectly

entered. In addition, the spectrum didn't agree with the experimental data because the bin boundaries were shifted. Each case must be inspected in detail to find the problems.

The next common source of energy-balance errors in ENDF files arises from the representation used for inelastic scattering. Typically, the neutron scattering is described in detail using up to 40 levels for the (n,n′) reaction. However, the photon production is often described using MF=13/MT=3 or MF=13/MT=4 and rather coarse energy resolution. As a result, it is possible to find photons for $(n,n_1)$ being produced for incident neutron energies slightly below the MT=51 threshold! These photons would lead to a spike of negative KERMA factors. A more common effect of the coarse grid used for photon production is to lead to an underestimate or overestimate of the photon production by not following the detailed shape of the inelastic cross section. The HEATR "kinematic KERMA" is correct in this range since only two-body reactions are active. Therefore, a plot of MT=301 and MT=443 on the same frame normally shows these effects in detail. Fig. 12 is an example of such a plot.

Fig. 13 shows both the inelastic cross section from File 3 and the photon production cross section from File 13 to demonstrate the mismatch in the energy grids that contributes to the energy-balance errors. These kinds of errors are best removed by changing to a representation that uses File 12 to give photon

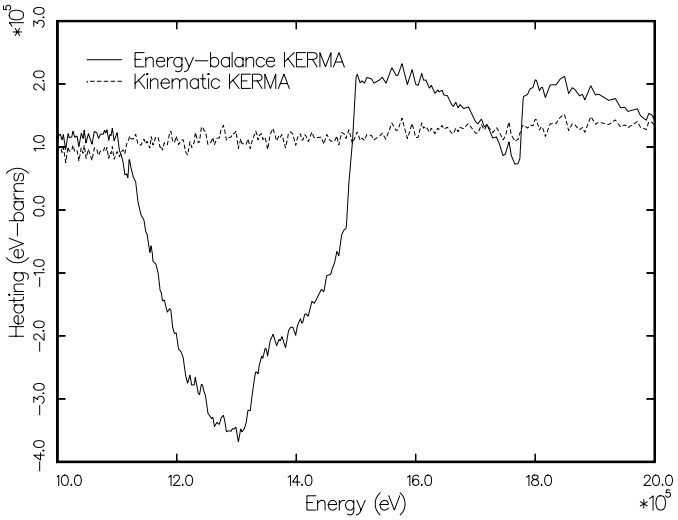


Figure 12: Comparison of MT=301 with MT=443 for the region of the discrete-inelastic thresholds for $^{59}$Co from ENDF/B-V.2. Note the large region of negative KERMA. The best way to remove this kind of problem is by using yields in File 12, MT=51, 52, 53, ... to represent the photon production.

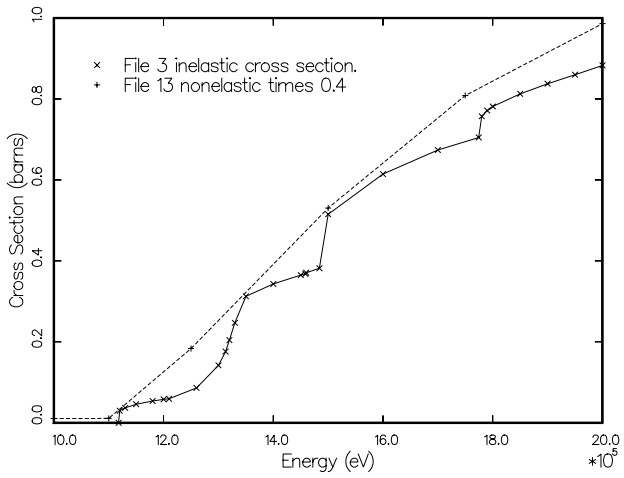


Figure 13: Plot showing the mismatch between the energy grids used for File 3 and File 13 in the region of the thresholds for discrete-inelastic scattering levels for the case shown in Fig. 12. The cross and ex symbols show the actual grid energies in the evaluation.

production yields for the separate reactions MT=51, MT=52, etc. This representation makes full use of the File 3 cross sections, and as long as each section of File 12 conserves energy, the total inelastic reaction is guaranteed to conserve energy, even at the finest energy resolution.

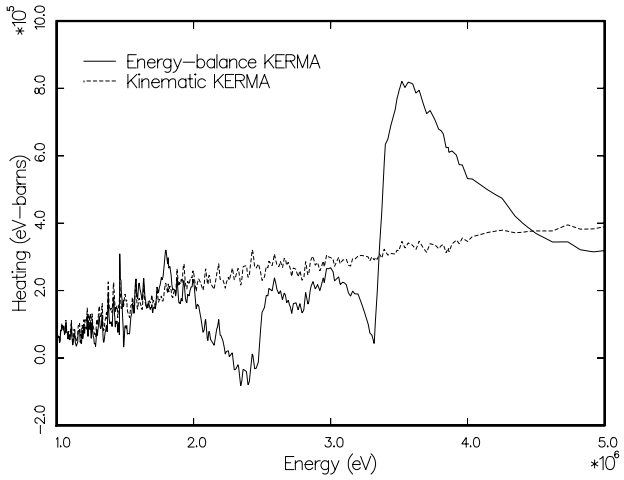


Figure 14: Typical energy-balance problems between points where balance is satisfied. Discrete photons were used below about 2 MeV, and energy balance is reasonably good there. The energy points in MF=13 for the continuum part are at 2, 3, and 5 MeV, and the balance is also good at those energies. Clearly, a grid in File 13 that used steps of about 0.25 MeV between 2 and 4 MeV would reduce the size of the deviations substantially and remove the negative KERMA factors.

A method that is frequently used by evaluators of photon production files is to select a number of nonelastic photon spectra on a fairly coarse incident-energy grid using theory or experiment, and then to readjust the photon yield on this energy grid so as to conserve energy at each grid point. However, the results do not, in general, conserve energy at intermediate points. If a very coarse energy grid is used for File 13, quite large deviations between MT=301 and MT=443 can result. Fig. 14 shows such a case. The solution to this kind of violation of energy balance is to add intermediate points in Files 13 and 15 until the magnitude of the deviations is small enough for practical calculations.

Especially large energy-balance errors of this type are caused by interpolating across the minimum formed by the decreasing capture heating and the increasing inelastic heating. Fig. 15 shows a dramatic example using a photon energy production comparison.

For energies above the threshold for continuum reactions like (n,n′) or (n,2n), it is difficult to use the results of the kinematic checks to fix evaluations. The representation of Eqs. 181 and 182 for continuum inelastic scattering is very rough. Comparison to other more accurate methods suggests that a CM formula

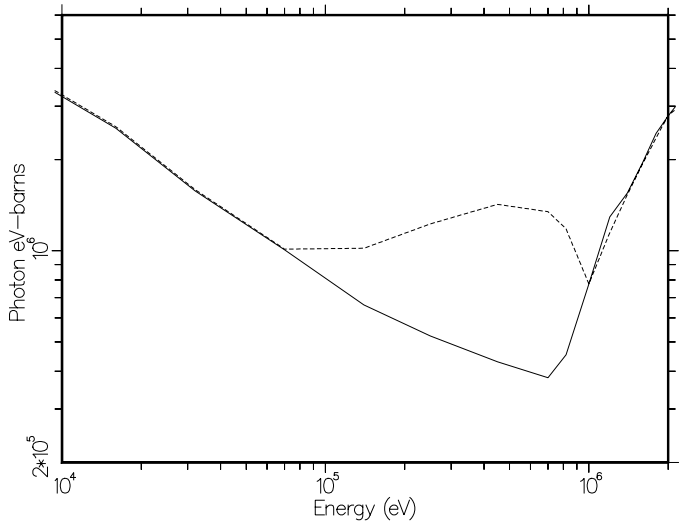


Figure 15: Computed photon energy production (dashed) compared with the kinematic value (solid) for $^{93}$Nb from ENDF/B-V. The original File 13 has grid points at 100 keV and 1 MeV. Interpolating across that wide bin gives a photon production rate that is much too large for energies in the vicinity of a few hundred keV. This will result in a large region of negative heating heating numbers. Since this is just the region of the peak flux in a fast reactor, niobium-clad regions could be cooled instead of heated!

would be better here[50], even though the ENDF file says "lab." Most other reactions give very wide low and high limits. Two exceptions are (n,2n) and (n,3n). If they dominate the cross section, the kinematic limits will be fairly close together. In the 14 MeV range, energy errors could be in the photon data, the neutron data, or both. The best way to eliminate balance errors is to construct a new evaluation based on up-to-date nuclear model codes.

## 6.10 Coding Details

The main subroutine is `heatr`, which is exported by module `heatm`. It starts by reading the user's input and locating the desired material on the PENDF file. The main loop is over temperature. For each temperature, a check is made to see if the user provided a value for the damage displacement energy. If not, a default value is provided. Next, `hinit` is called to examine the directory. Flags are set if MF=12 or 13 is present, if MT=18 or 19 is used, and if MT=458 is present (see `mgam`, `mt19`, and `mt458`). The flags `mt103`, `mt104`, `mt105`, `mt106` and `mt107` are set if the corresponding particle production levels are present. The MT numbers used for the levels depend on whether the input file used version 6 format or one of the earlier formats. For example, `mt103` is set if MT=600-649 is found for ENDF-6 data, or if MT=700-719 is found for earlier versions. The code also checks to see if the corresponding angular distribution data are present (see `nmiss4`). If any are not present, the code will assume they are isotropic. Note that `hinit` also collects a list of the File 6 MT numbers in `mt6(i6)`. For fissionable materials, the delayed fission energy values are retrieved from MF=1/MT=458, and the correction, `qdel`, is computed for later use when calculating the heating from prompt fission.

The next step in `hinit` is to make a copy of File 6 on a scratch file (if any sections of File 6 were found). While doing this, it searches through the subsections for each reaction accumulating the ZA residual remaining after each particle is given. If it comes to the photons (`zap`=0), which should be last, and there is still a ZA residual left, then it concludes that there is no subsection describing the residual. It loads a value into `mt6no(ii6)` that is the index to the subsection that the recoil should have followed had it been present. If it comes to the end of the subsection list without finding photons and still has a ZA residual, it sets `mt6no(ii6)` to `nk`; that is, the residual missing should follow the last subsection. In either case, the routine prints out messages about "photon recoil correction" or "one-particle recoil approximation."

Finally, `hinit` makes a standardized copy of the ENDF tape using `hconvr`,

and it also saves the grid of the total cross section (MT=1) on the `loada/finda` scratch file that will be used to accumulate the KERMA factors, damage, and kinematic checks (if requested). Note also `mt303`, which tells which of the requested edits is for nonelastic heating, MT=303. This is used later for writing out the photon energy production check.

Now `nheat` is called. Its basic function is to loop over the "nonredundant" reactions in File 3, and to accumulate the corresponding contributions to the partial heating and partial damage values into the appropriate elements of the `c` array on the `loada/finda` file. Redundant reactions are reactions that duplicate or include effects that can be obtained from another MT number. They are determined using a set of `if` statements just after the entry to the reaction loop at statement number 105. The structure of the `c` array depends on whether kinematic checks are being accumulated or not and whether photon production files are present. If neither occurs, the structure has `npk`+1 elements as follows:

| Element | Contents |
|---|---|
| `1` | energy |
| `2` | total heating |
| `3` | value for first partial |
| ... | |
| `npk`+1 | value for last partial |

where `npk` is the number of partial KERMA or damage values being accumulated, including the total. If checks are being accumulated, the `c` array has the following 3*`npk`+1 elements:

| Element | Contents |
|---|---|
| `1` | energy |
| `2` | total heating |
| `3` | value for first partial |
| ... | |
| 2+`npk` | lower kinematic limit for total |
| 3+`npk` | lower kinematic limit for first partial |
| ... | |
| 2+2*`npk` | upper kinematic limit for total |
| 3+2*`npk` | upper kinematic limit for first partial |
| ... | |
| 3*`npk`+1 | upper kinematic limit for last partial |

If photon production files are present in the evaluation, the total length of the

c array increases by the following three words (len is the old length from above plus three):

| Element | Contents |
|---|---|
| len-2 | photon capture correction |
| len-1 | total photon eV-barns |
| len | total energy yield for "subtot" |

Back inside the loop over nonredundant reactions, subroutine gety1 is initialized for this reaction. The code checks to see if this section uses File 6 for its distributions; if so, it arranges to make multiple passes through the reaction's energy grid, one pass for each subsection of the MF=6 section, and perhaps one additional pass to synthesize the missing recoil subsection. It is now possible to select the appropriate $Q$-value and particle yield, and to initialize the appropriate calculational routine. This routine will be sixbar for all reactions described in File 6, disbar for two-body reactions using File 4 (including charged-particle reactions in the 600 or 700 series of MT numbers), conbar for continuum reactions represented using File 5, and capdam for the neutron disappearance reactions (MT=102, 103, *etc.*) and the charged-particle continuum reactions from the 600 or 700 series of MT numbers. The last step before beginning the energy loop for this reaction is to call indx, which determines which element of the c array is to receive the heating or damage contribution from this reaction (see below).

The energy loop in nheat goes through statement number 190. For each energy, finda is called to retrieve the current values for the energy [see c(1)] and the partial heating and damage values as accumulated so far. On the first pass through the scratch file, the list of energies to be used for printing information on the listing is established in elist using a few if statements based on the range of the energy variable e. For each energy, the corresponding cross section is retrieved using gety1 and the appropriate $\overline{E}$ and damage numbers are computed by calling getsix, disbar, conbar, or capdam. The heating contribution is computed from the appropriate formula, and the heating and damage numbers are summed into the c array at location index. If requested, the kinematic limits on the heating are computed and summed into the c array at index+npk and index+2*npk. The completed results for this energy and reaction are written out onto the loada/finda scratch file, and the energy loop is continued.

When the energy loop is complete, the subroutine jumps to the next section (or subsection in the case of File 6) and repeats the entire energy loop for that reaction (or particle from File 6).

Subroutine `indx` is used to select what element of the `c` array is to receive the heating or damage contribution for a section with a particular MT number. The meaning of each element of the `c` array is obtained from the `mtp` array. Normally, a reaction MT contributes to the partial heating element with `mtp(i)`=MT+300. But it can also contribute to several other elements of `c`, such as nonelastic (MT=303), inelastic (MT=304), etc. Therefore, `indx` returns the count of reactions contributed to by `mt` in `nmt` and the indexes for the `c` array in `imt(nmt)`.

Subroutine `capdam` is used to compute the damage energy for neutron capture (or disappearance) reactions; that is, for MT=102, 103, etc. On the initialization entry (`ee`=0.0), the routine sets up various kinematics parameters, such as `zx` and `ax` to describe the outgoing particle, and initializes `df`. In order to save time, the routine only calculates the damage on a grid that increases by steps of 10%. Intermediate values are obtained by interpolation (see `el`, `daml`, `en`, and `damn`). The values at the grid points are computed using

$$D\left(\frac{E}{A+1}\right)+D\left(\frac{1}{2M_Rc^2}\left[\frac{AE}{A+1}+Q\right]^2\right) \tag{223}$$

for radiative capture (the corrections for multiple photon emission will be made later), or using Eq. 206 with $E_R$ from Eq. 212 and a 4-point Gauss-Legendre quadrature. The angular distribution for particle emission is taken to be isotropic.

Subroutine `disbar` is used by `nheat` to compute the average secondary energy and damage energy for elastic scattering (MT=2), discrete-inelastic scattering (MT=51-90), or discrete-level particle production (MT=600-648, 650-698, etc. for ENDF/B-VI or ENDF/B-VII, or MT=700-717, 720-737, etc. for earlier versions). It starts by initializing `hgtfle` (which is very similar to `getfle` in the GROUPR module), determining kinematic parameters like `awp` (the mass ratio to the neutron for the emitted particle), and initializing `df`. In order to save time, it only computes the heating and damage on a grid based on steps by a factor of 1.1 and the `enext` values from `hgtfle`. On a normal entry, it interpolates between these values (see `el`, `cl`, `daml`, `en`, `cn`, and `damn`). When the desired `ee` exceeds `en`, the old high values are moved down to the low positions, and new high values are calculated. The calculation of `cn` follows Eq. 168. The calculation of `damn` uses Eq. 206 with a 20-point Gauss-Legendre quadrature (see `nq`, `qp`, and `qw`).

Function `df` is used to compute the damage partition function given in Eq. 200. The constants that depend on the recoil atom or particle type and lattice type

(see zr, ar, zl, al) are computed in an initialization call with e=0.0. Thereafter, it can be called with any other value of e.

Similarly, conbar computes the average secondary energy and damage energy for continuous distributions described in File 5. Analytic representations use simple formulas coded into anabar or a combination of adaptive and Gaussian quadrature in anadam. Tabulated data are interpolated from the File 5 table using tabbar or integrated using trapezoidal and Gaussian quadratures in tabdam. As usual, the routine is initialized by calling it with e=0.0. The secondary-particle yield is either chosen from the MT number, or hgtyld is initialized. The desired section of File 5 is located on the input ENDF tape, and the kinematic constants are computed. The reactions with MT=22, 28, 32, 33, and 34 will be treated using the capdam method; if mtd has one of these values (see mtt), capdam is initialized. As is the case for getsed in the GROUPR module, this routine can handle some sections of File 5 that contain multiple subsections, but the analytic subsections must come first. As each analytic subsection is read, appropriate data are stored in in the external array c using pointers saved in the array loc. Only the first energy is read and stored for a tabulated subsection (lf=1). The idea is to have only two energy values in memory at a time in order to save storage; the second subsection will be read during the first normal entry to the subroutine. The final step in the initialization pass is to initialize df. For a normal entry into conbar, the energy-dependent fission yield is retrieved, if needed, and the loop over subsections is entered. Each subsection in File 5 starts with a fractional-probability record. The desired value for energy e is computed by interpolation using the standard NJOY utility routine terpa. For analytic subsections, the routine uses anabar to compute $\overline{E_n}$, and anadam or capdam to compute the damage energy. Note that in order to save time, anadam is only calculated on a fairly coarse grid based on steps by a factor of 1.5. The intermediate values are obtained by interpolation using terp1. For tabulated subsections, ebar and dame values are normally obtained by interpolation (see elo, flo, dlo, ehi, fhi, and dhi). However, for the first entry, or whenever e reaches ehi, the high data are moved into the low positions, new high data are read from the File 5 subsection, and the values for heating and damage are computed at ehi using tabbar and either tabdam or capdam.

Subroutine hgtyld is similar to getyld in the GROUPR module. It finds the required section on the ENDF tape and reads the entire LIST or TAB1 record into memory. On normal entries, it either computes the yield using the polynomial formula with constants from the LIST record, or it uses terpa to

interpolate for the yield in the TAB1 data.

Subroutine `anabar` is used to compute the average energy for a neutron described by an analytic subsection of File 5. The simple formulas used are tabulated in the ENDF format manual[9]. Similarly, `anadam` is used to compute the damage energy for an analytic subsection of File 5. Only LF=9 (the Simple Maxwellian Distribution) is supported; the routine returns zero for other laws. Note that a statement function is defined to compute the secondary energy distribution for this law (see `sed`). For each incident energy, the spectrum temperature `theta` is retrieved using `terpa`, and an adaptive integration stack is initialized with points at four secondary energies, namely, 1., .5($E-U$), $\theta$, and $E-U$, where $U$ is a parameter that sets the maximum possible value of $E'$. The adaptive procedure proceeds to solve Eq. 208 by subdividing this starting grid until trapezoidal integration can be used on each panel. The inner integral over emission cosine $\mu$ is performed using a 4-point Gauss-Legendre quadrature for each point on the adaptive grid. The function `sed` is used to compute $g(E')$, and `df` is used to compute the partition function.

Subroutine `tabbar` is used to compute the average energy of the emitted neutron for a tabulated subsection of File 5. It can also be used for a tabulated subsection of File 6. This option is flagged by `law` negative. The trick is to set the "stride" or "cycle" through the file to be larger than 2 (see `ncyc`). The angular part of the $g(E \rightarrow E')$ table is skipped, and only the $E'$ and $g$ values are retrieved. For File 5, this routine only works for laws 1 and 5; others cause a fatal error message to be issued. In both of these cases, the integral over $E'$ needed to compute the average energy is done analytically for each panel in the input data using a different formula for each interpolation scheme `int`.

Subroutine `tabdam` is used to compute the damage energy for a tabulated subsection of File 5. The integration that is needed is given in Eq. 208. The energy grid of the tabulation is assumed to be good enough to allow trapezoidal integration to be used for $E'$, and a 4-point Gauss-Legendre quadrature is used for $\mu$.

Subroutine `sixbar` is used to compute charged-particle average energy and damage energy represented by using a subsection of File 6. As is common with NJOY subroutines, `sixbar` is initialized by calling it with `e`=0.0. The initialization path is controlled by `j6`, which is the index to the current subsection in File 6; by `irec`, which is 1 when a recoil response is to be calculated, and by `jrec`, which tells the routine how to get back to the next subsection after a recoil calculation. If this is not a recoil subsection, the routine jumps to statement 110 and

starts reading in the data for the desired subsection. If it is flagged as a recoil (see `irec`), the routine backs up to the subsection describing the particle that induced the recoil and then continues by reading in the data for that particle.

The first step is to read in the TAB1 record that contains the particle yield, identity (`zap` and `awp`), and representation `law`. If this law describes a two-body recoil distribution, the routine sets `jrec` for a proper return, sets `irec` to back up to the corresponding direct emission subsection, and jumps back to the beginning of the routine to do the recoil calculation.

When the code finally arrives at statement number 210, it is ready to start processing the current subsection. It reads in the parameters for laws 3 and 6, or the TAB2 record and the data for the first energy point for the other laws. With the data in place, it computes the corresponding values for mean energy and damage energy using `getsix` or `tabsq6` and returns.

In the special case where the section contains only a single subsection that describes a neutron, the data stored in memory will be the data for that subsection, and the subroutine `tabbar` with a negative value for the law is used to produce the low values.

On a normal entry (`e`>0), `sixbar` checks to see whether `e` is in the current interpolation range. If it is, the code jumps to statement number 400. For the analytic laws (`law`=3 and `law`=6), it uses a direct call to `getsix` to compute the mean energy and damage energy. For the tabulated laws, it interpolates for the results using the low and high data (see `elo`, `flo`, `dlo`, `ehi`, `fhi`, and `dhi`). On the first entry, or whenever `e` increases to `ehi`, the code moves the high data to the low positions, and then it reads in the data for the next energy and computes a new set of high values for mean energy and damage using `getsix` or `tabsq6`.

Subroutine `getsix` is used to compute the mean energy and damage energy for one particular incident energy in a subsection of File 6. The method used depends on the value of `law` and the reference frame for the subsection. The first case in the coding is for `law`=1 with data in the CM system.

This case uses Eqs. 218 and 219 with an adaptive integration over $E'$. The integration stack is contained in the arrays `x` and `y`. It is primed with `x(2)`=0, and `h6cm` is called to compute `y(2)` and the next grid point `epnext`. The first panel is completed by calculating `y(1)` and `x(1)`=`epnext`. The panel is then divided in half, and the midpoint is tested to see if it is within `tol`=0.02 (*i.e.*, 2%) of the linearly interpolated value. If not, the midpoint is inserted in `x` and `y`, and the new top panel [that is `x(2)`−`x(3)`] is tested. This continues until convergence is achieved in the top panel. The contributions to the heating and

damage are added into the accumulating integrals at statement number 190, and `i` is decremented so that the process can be repeated for the next panel down. When `i` decreases to one, the current value of `epnext` is used to start the next higher $E'$ panel. This loop over panels continues until the entire $E'$ range has been integrated.

The next special case is for tabulated distributions that use $E$, $E'$, $\mu$ ordering in the lab system. The angular part is ignored. A simple loop over the `NEP` points in $g(E \rightarrow E')$ is carried out. Trapezoidal integration is used for each panel for both heating and damage (`h` and `d`). If `nd`>0, the first `nd` entries are discrete energies, and the values of the integrand at those energies are added into `h` and `d`. Finally, `h` and `d` are copied into `ebar` and `dame`.

The block of coding starting at statement number 450 is used to compute particle mean energies for the emitted particles from two-body reactions, or to compute the mean recoil energy for a two-body reaction (see `irec`>0). The calculation follows Eq. 216. Note that the kinematic factors include `awp`, the mass ratio of the emitted particle to the incident particle. The parameter `beta` here is the same as $R$ in Eq. 217. If the angular distribution in File 6 is in Legendre form, the heating and damage integrals are performed using a 20-point Gauss-Legendre quadrature (see `nq`, `qp`, and `qw`). If the angular distribution is tabulated as $f(\mu)$ *versus* $\mu$, a trapezoidal integration is used for both heating and damage.

The final option in `getsix` is for lab distributions that use $E$, $\mu$, $E'$ ordering. See Eq. 220. The inner integrals are computed using trapezoidal integration. The outer integral over $\mu$ also uses trapezoidal integration on the results of the inner integrals for each $\mu$ grid point.

Note that `getsix` has an `irec` parameter in its calling list. When this parameter is greater than zero, the angular distribution is complemented and the charge and mass of the particle are modified to represent the recoil species. The value of `irec` is controlled by `sixbar`.

Subroutine `h6cm` is used by `getsix` to compute the lab distribution $g(E \rightarrow E'_L)$ of Eq. 221 using the CM data in File 6. This subroutine uses `h6dis`, `h6ddx` and `h6psp` to retrieve the CM discrete, tabulated or phase-space data from the file. These routines are basically the same as `f6cm`, `f6dis`, `f6ddx` and `f6psp`. See GROUPR for more details.

Subroutine `gheat` is used to correct the heating and damage values accumulated during the pass through the neutron sections. It loops through all of the reactions in File 12 and File 13 using two ENDF-type tapes. One is the input

PENDF tape, which is used to retrieve cross sections for use with the photon multiplicities in File 12. The other is a version of the input ENDF tape that has been passed through `hconvr` to put the photon data in a standard form (see Chapter 8 (GROUPR) of this manual for a more detailed discussion of `conver`). This scratch tape is used to retrieve the File 12 and File 13 data. It is very common to find reaction MT=3 (nonelastic) in File 12, but this reaction has been removed from the PENDF tape because it is redundant; that is, it is equal to MT1−MT2. Therefore, two passes are made through the File 12 data for MT=3, an addition pass with MT=1 from the PENDF tape, and a subtraction pass with MT=2 from the PENDF tape. Once the desired sections on the two tapes have been found, the subroutines `gambar`, `capdam`, and `disgam` are initialized.

The energy loop for `gheat` goes through statement number 190. For each energy, `finda` is used to retrieve the partial KERMA factors as computed from the pass through the neutron files. The yield or cross section is retrieved using `gety1` into the variable `y`. If necessary, the corresponding cross section `x` is retrieved using `gety2`. For cases where an energy-dependent Q is available, it is retrieved using `terp1` on the data stored at `lqx`. The next two lines correct the energy of "primary" photons (`lp`=2).

For radiative capture represented in File 12 (MT=102), `gambar`, `disgam`, and/or `capdam` are called to return $\overline{E}_\gamma$ and $\overline{E_\gamma^2}/(2m_Rc^2)$ for this photon spectrum or discrete photon and to correct the heating and values in the `c` array using Eq. 171 and the second line of Eq. 211. The capture contribution to the total photon eV-barns is added into `c(npkk-1)` and the photon energy yield is loaded into `c(npkk)` for each subsection. When the last subsection is reached, the capture energy check is made using this subtotal. Note that the capture error is loaded into `c(npkk-2)` for later use in calculating the kinematic limits for photon energy production.

For other photon-production reactions, the photon eV-barns contribution is subtracted from the energy-balance heating position, added into the total photon energy value in `c(npkk-1)`, and added into `c(npkk)` for the subtotal for a section with multiple subsections. After all the corrections have been completed for this energy, the revised values are written out using `loada`. The code then moves on to the next reaction and repeats the entire process.

When the reaction loop has been finished, `gheat` checks to see if it can print out a photon energy production check. It can do this if kinematic checks have been requested and if MT=303 was requested in the user's list of partial KERMA calculations. The code reads through the `loada/finda` file one more time. For

each energy in `elist`, it prints out the total photon eV-barns from `c(npkk-1)` and the kinematic limits `elo` and `ehi`. If the limits are violated by more than 10%, alarms consisting of the strings ++++ or `--` are printed after the eV-barns values.

Subroutine `gambar` is used to compute the mean energy for continuous photon spectra and the photon recoil correction for capture. When called with `e`=0.0, it locates the desired section of File 15 on the ENDF tape and reads in the first incident energy. On a normal entry, it checks to see if `e` is in the range of the data already computed (`elo`, `ehi`, etc.), and if so, it interpolates for the desired results. If not (or on the first real entry), it moves the high data down to the low positions, reads in the next energy from File 15, prepares new values at the new `ehi`, and checks the energy range again. The photon `ebar` is returned by `tabbar`, and the corrections to the heating value (`esqb`) and damage value (`esqd`) from photon production are generated using `tabsqr`.

Subroutine `tabsqr` is used to compute the average recoil energy

$$\frac{\overline{E_\gamma^2}}{2M_R c^2} \tag{224}$$

for radiative capture for a tabulated subsection of File 15. The corresponding damage energy is computed at the same time. The basic secondary-energy integral is over the panels defined by the grid points given in File 15. Inside each panel, the integral is computed using a 4-point Gauss-Legendre quadrature.

Subroutine `disgam` is used to compute the $\overline{E_\gamma^2}$ and corresponding damage energy for a discrete capture photon. The rest-mass constant is computed by calling `disgam` once with `e`=0.

Subroutine `hout` writes the new PENDF tape with the desired heating and damage MT numbers added. It also corrects the directory in MF=1/MT=451, and it prepares the output listing for printing. The first step is to loop through the partial KERMA factors requested and to write the data on the `loada/finda` file onto a scratch tape in ENDF File 3 format. While the first partial is being prepared, the code matches energies in `c(1)` against the energy list for printing in `elist`. When a match is found, the partial KERMA factors are checked against the kinematic limits, and the variables `klo` or `khi` are set if any of the comparisons are out of bounds. The KERMA factors, kinematic limits, and error flags are then printed on the output listing. When all of the new sections for File 3 have been prepared, the code updates the contents of the File 1 directory. It then loops through the rest of the input PENDF tapes copying sections to

the output and inserting the new sections in the appropriate places. When the new PENDF file has been completed, `hout` makes VIEWR input for a set of plots showing the total heating and the photon production compared to their kinematic limits in both lin-lin and log-log forms. The lin-lin plots show the high-energy range better, and the log-log plots expand the low-energy range.

### 6.11 Error Messages

`error in heatr***requested too many kerma mts`
: 6 values in addition to MT=301 are allowed with kinematic checks; otherwise, 25 can be requested. See `npkmax`=28. When checks are requested, the number of words needed is 3*`npk`+7; otherwise, `npk`+3 are needed.

`error in heatr***requested too many q values`
: Limited to 30 by the global parameter `nqamax`=30.

`error in heatr***too much energy-dependent q data`
: Limited to `maxqbar`=10000.

`error in heatr***mode conversion not allowed...`
: Both units must be BCD (positive) or blocked binary (negative).

`error in hinit***too many mf6 reactions`
: A maximum of 320 reactions are allowed. See the global parameter `maxmf6`=320.

`message from heatr--mt301 always calculated`
: MT=301 was given in the input list of partial KERMA factors. This is not necessary; it is always inserted automatically.

`message from hinit--mf4 and 6 missing, isotropy...`
: Cross sections were found for charged-particle levels in the 600 or 700 series of MT numbers, but no corresponding angular distributions were found. Isotropy is assumed to enable the calculation to proceed, but this evaluation should be upgraded to include the proper sections of File 4 or 6.

`message from hinit--mt18 is redundant...`
: If MT=19 is present, MT=18 will be ignored.

`message from hinit--mt19 has no spectrum...`
: In some evaluations, the partial fission reactions MT=19, 20, 21, and 38 are given in File 3, but no corresponding distributions are given. In these cases, it is assumed that MT=18 should be used for the fission neutron distributions.

`error in hinit***upper energy mismatch for ifc=... in mt=458`
: When using tabulated fission energy release components in mf1/mt458, NJOY detected different values for the upper energy limit of some of the components. This is an evaluation error.

`error in hinit***no tabulated fission q components found`
: mf1/mt458 contains no tabulated fission energy release components even thought the LFC value was set to 1. This is an evaluation error.

`error in hinit***bad LFC in mt=458`
: The LFC value in mf1/mt458 can only be equal to 0 or 1. This is an evaluation error.

`message from hinit--mt458 is missing for this mat`
: The fission $Q$-value cannot be adjusted for delayed effects.

`message from hinit--photon momentum recoil used`

`message from hinit--one-particle recoil approx. used`

`message from nheat--changed Q from -- to --`
: The fission $Q$-value is adjusted from the total (non-neutrino) value given in File 3 to a prompt value using the delayed neutron energy from MF=1/MT=458.

`error in nheat***binding energy for sequential n,2n needed`
: The user must enter special $Q$-values for the ENDF/B evaluation for $^{9}$Be. See the discussion in Section 6.7.

`error in nheat***storage exceeded`
: Insufficient storage for diagnostic energy grid. See the global parameter `ilmax`=100 at the start of the module.

`error in nheat***upper energy tabulated fission q components ...`
: The tabulated fission energy components are tabulated up to an upper energy value that is inconsistent with the upper energy value of the fission cross section. This is an evaluation error.

`error in conbar***nktot gt nkmax`
: More than 12 subsections found. See the parameter `nkmax`=12.

`error in conbar***insufficient storage for raw endf data`
: The allocatable array `a` in `nheat` is too small. Increase `na`=10000.

`error in hgtyld***illegal lnd, must be 6 or 8`
: The LND value in the ENDF file is not correct, only 6 or 8 are allowed.

`error in hgtyld***storage exceeded`
: Increase `nwmax` in `nheat`. Currently 7000.

`error in tabbar***coded for lf=1 and lf=5 only`
: Self-explanatory. Should not occur.

`message from sixbar--no distribution for mt -- ...`
: The ENDF-6 format allows the evaluator to describe a subsection of File 6 with "`law`=0"; that is, no distribution is given. Such sections are fine for giving particle yields for gas production and similar applications, but they are not adequate for computing heating and damage.

`error in h6ddx***too many legendre terms`
: See `nlmax`=65 in `h6ddx`.

`error in h6ddx***illegal lang`
: The allowed values for the angular law flag are 1, 2, and 11–15.

`error in h6dis***illegal lang`
: The allowed values for the angular law flag are 1, 2, and 11–15.

`error in bacha***dominant isotope not known for...`
: The Kalbach-systematics approach to computing angular distributions for particle emission requires the separation energy as computed by the liquid drop model. If the target for an evaluation is an element, it is necessary to choose a dominant isotope that adequately represents the effect for this element. Dominant isotopes for materials often evaluated as elements are given in `if` statements in this routine. If the desired value is missing, it must be added, and NJOY will have to be recompiled. See the corresponding routines in GROUPR and ACER as well.

`error in h6psp***3, 4, or 5 particles only`
: The phase-space law is defined for 3, 4, or 5 particles only.

`message from hgtfle--lab distribution changed to cm...`
: ENDF procedures require that two-body reactions be described in the CM system. Some earlier evaluations claim to be in the lab system. However, they are for relatively heavy targets, and changing to the CM frame will cause only a small change in the results.

`error in hgtfle***desired energy above highest energy...`
: Fault in the evaluation.

`error in getco***limited to 64 legendre coefficients`
: The upgraded ENDF limit.

`error in getco***lab to cm conversion not coded`
: Discrete scattering data should be in the CM system already.

`message from hconvr--mf3, mt... is missing`

`message from hconvr--mf12, mt... is missing`

`error in hconvr--missing mf3 mt's, probable endf error`
: All these messages indicate missing sections in either mf3 or mf6. This is an evaluation error.

`message from hconvr--gamma prod patch made for mt --`
: This reflects some problems in the old ENDF-III evaluations for Cl and K, which were also carried over to later ENDF versions.

`error in hconvr***too many lo=2 gammas`
: See `lmax`=500.

`error in hconvr***exceeded storage for nubar`
: See `nnu`=6000.

`error in gheat***lo=2 not coded`
: Will not occur since `lo`=2 data have been transformed to `lo`=1 format by `hconvr`.

`message from gheat--no file 12 for this material`

Information only.

`message from gheat--skipping mf.../mt... processed in mf6`

NJOY has found photon data for a given mt in both mf6 and mf12 - mf15. Only the mf6 data are used.

`error in gambar***storage exceeded in a`

Increase `nd`=10000 in `gheat`.

`error in gambar***requested energy gt highest given`

Probably reflects an error in the evaluation.

`error in hout***nin out of order. read mfh,mth = ...`

`error in hout***nscr out of order. read mfh,mth = ...`

These errors indicate that the various sections in the ENDF file are not sequentially ordered. Check the ENDF file and correct it if possible.

## 6.12 Storage Allocation

Allocatable arrays are used for most large data blocks. Storage requirements are dominated by the length of File 5 or File 15 for the evaluation. The `loada/finda` buffer size `nbuf` may be decreased or increased at will. The code is currently dimensioned as follows:

| | |
|---|---|
| 100 | coarse grid points |
| 30 | auxiliary $Q$-values |
| 25 | partial KERMAS (7 when kinematic limits are requested) |
| 10000 | words of energy-dependent Q data |
| 10000 | maximum for File 5 or 15 raw data |
| 7000 | maximum for fission yield data |
| 320 | File 6 reactions |