Neutron heating of metastables with NJOY

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Abstract

- Metastable nuclides with complete secondary distributions are increasingly more available in major evaluations, allowing for the calculation of their KERMA values. When processing these metastable nuclides using NJOY's `heatr` module, negative total energy release values are being calculated for certain nuclides.
- On investigation, the method by which NJOY calculates the heating for inelastic reactions is incorrectly handling the Q-values for metastable materials, resulting in significant negative values equivalent to the metastable energy level, which may be greater than the contribution from all other reactions. The cause for these values have been identified and further questions have been raised for the processing of metastable nuclides.

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Introduction

- Nuclear data evaluations are including increasing numbers of metastable nuclides
  - TENDL includes all nuclides with half life > 1s (hundreds of metastables)
  - ENDF/B-VIII includes all nuclides with half life > 1 year (21 metastables)
- Metastables are provided with secondary distributions allowing the calculation of neutron induced energy release (KERMA)
- After processing ENDF/B-VIII.0 with NJOY2016* into multigroup data, certain metastables were found to have a negative total KERMA in some energy groups – this flagged various errors in post-processing codes.
- An investigation was performed to find the cause of these negative values

* NJOY2016.62 - Los Alamos National Laboratory

NJOY - `heatr`

- `heatr` is used for the calculation of neutron induced energy release by NJOY
- Processing method:
  - `reconr` – resonance reconstruction
  - `broadr` – Doppler broadening
  - `heatr` – neutron induced heating
- Possible to then process into pointwise, groupwise….

```
moder
21 -22
reconr
-22 -23
'001-H-001'/
125 1 0 /
0.001 0.0 0.001 1.0e-12/
'reconr input 0.001 0.0 0.001 default'/
0/
broadr
-22 -23 -24
125 1 0 1 0.0
0.001 1.e6 0.001 1.0e-12/
290.11/
0/
heatr
-22 -24 -25 /
125 0 0 0 1 1/
stop
```

Options for partial kermas, user q values, multi temps, gammas transported/deposited, print level

heatr – Overview

- heatr calculates neutron heating through 'direct' method:

$$k(E) = \sum_i \bar{E}_i(E)\,\sigma(E)$$

where *i* is the *i*th species of secondary charged particle including nucleus

- Or the 'energy balance' method in absence of data for all species of particle:

$$k(E) = (E_n + Q_{MD} - \overline{E_n}' - \overline{E_\gamma}')\sigma(E)$$

Gamma energy may be transported or deposited – user's choice

- For an elastic reaction $k(E) = E_n - \overline{E_n}' = E_{recoil}$

Need $\overline{E_n}'$ to be calculated

`heatr` – elastic, inelastic reaction (MT 2, 51-90)

- `heatr` calculates average outgoing neutron energy $\overline{E_n{}'}$ and subtracts this from the incoming neutron energy E_n to calculate recoil energy $\overline{E_R}$.
- Elastic reactions to calculate $\overline{E_n{}'}$:

$$\overline{E_n{}'} = \frac{E_n}{(A+1)^2}(R^2 + 2R\bar{\mu} + 1)$$

μ - scattering cosine read from ENDF file MF4

- For elastic reactions $R = A$.
- For inelastic reactions R is dependent on the energy threshold:

$$R = A\sqrt{1 - \frac{(A+1)S}{AE_n}} \qquad \text{where } S = -Q$$

- R ranges between A(0) and A(1) from the threshold

`heatr` - inelastic

- Inelastic reactions may de-excite through gamma emission or charged particle production. ENDF-6 uses Latent Reaction (LR) flag to indicate this.
- Two Q-values are provided:
  - QM: Mass-difference Q $(m_a + m_A) - (m_b + m_c + \cdots + m_B)$
  - QI: Reaction Q including energy state E_x $(m_a + m_A + E_x) - (m_b + m_c + \cdots + m_B + E_y)$
- The calculated KERMA for partial inelastic reactions is dependent on the LR flag.
- For decays through gamma emission:

$$k(E) = \left(E_n - \overline{E_n{}'} - \overline{E_\gamma{}'}\right)\sigma(E)$$

`heatr` sets Q=0 and only reassigns if there is an LR flag (charged particle)

For decays through charged particle emission:

$$k(E) = \left(E_n + Q - \overline{E_n{}'} - \overline{E_\gamma{}'}\right)\sigma(E)$$

^{12}C - inelastic

- Example ^{12}C
  - MT51 results in gamma emission
  - MT52 results in 3α emission

```
<     ZA      ><    AWR    >           0           0           0           0 MATMF  MT
<     QM      ><    QI     >           0          LR          NR          NP

  6012.00000 11.8936500                0           0           0           0  625  3  51
        0.0 -4438900.00                0           0           1         585  625  3  51   Gamma emission

  6012.00000 11.8936500                0           0           0           0  625  3  52
-7275000.0 -7653000.00                 0          23           1          27  625  3  52   3α emission
```

This value included in KERMA calculation because of LR

^{12}C – inelastic MT 51

```
6012.00000 11.8936500          0          0          0          0 625 3 51
       0.0 -4438900.00         0          0          1        585 625 3 51
```

$$K = (E_n - \overline{E_n{}'})\,\sigma(E)$$

Gamma emission

E_n (eV)	$\overline{E_n{}'}$ (eV)	$\overline{E_R}$ (eV)	σ (b)	KERMA (eVb)
5.00E+6	2.10E+5	5.79E+5	4.55E-2	2.18E+5
6.00E+6	1.07E+6	4.93E+6	2.24E-1	1.11E+6
7.00E+6	1.90E+6	5.10E+6	1.70E-1	8.68E+5
8.00E+6	2.66E+6	5.34E+6	3.73E-1	1.99E+6
9.00E+6	3.61E+6	5.39E+6	2.98E-1	1.61E+6

Table 1: ^{12}C MT51 values of outgoing neutron and KERMA as calculated by heatr

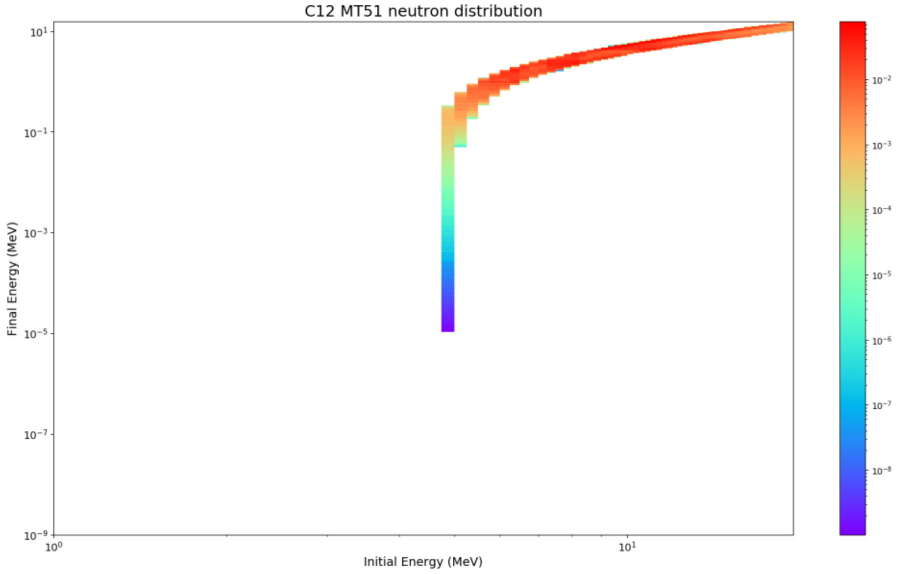

Figure 1: ^{12}C *(n,n')* ^{12}C values of outgoing neutron distribution (MT51)

^{12}C – inelastic MT 52

```
 6012.00000 11.8936500          0          0          0          0 625 3 52
-7275000.0 -7653000.00          0         23          1         27 625 3 52
```

$$K = (E_n + Q - \overline{E_n{'}})\,\sigma(E)$$

3α emission

Q = -7.275E+6

E_n (eV)	$\overline{E_n{'}}$ (eV)	$\overline{E_R}$ (eV)	σ (b)	KERMA (eVb)
9.00E+6	7.12E+5	8.29E+6	7.00E-3	7.09E+3
1.00E+7	1.61E+6	8.39E+6	1.55E-2	1.72E+4
1.10E+7	2.51E+6	8.49E+6	2.36E-2	2.87E+4
1.20E+7	3.41E+6	8.59E+6	2.88E-2	3.79E+4

Table 2: ^{12}C MT52 values of outgoing neutron and KERMA as calculated by heatr

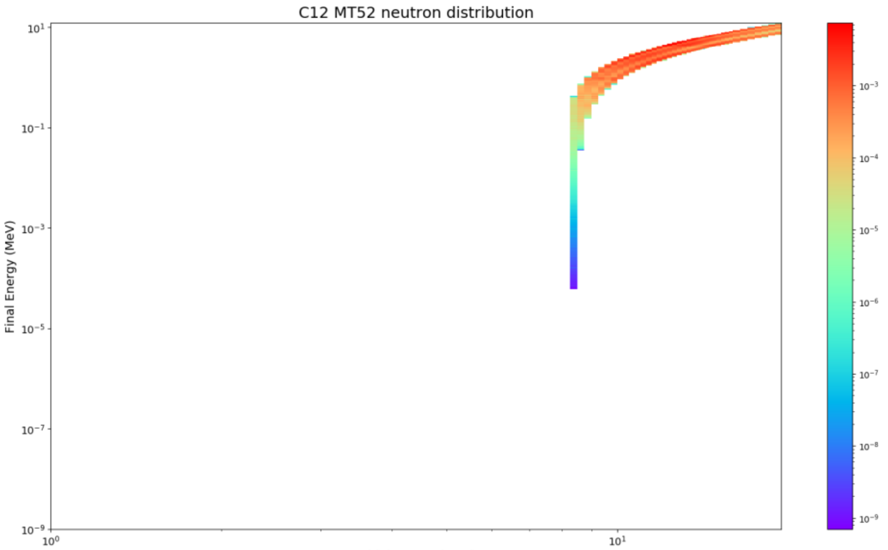

Figure 2: ^{12}C *(n,n')* 3α values of outgoing neutron distribution (MT52)

Available KERMA is reduced from loss of mass energy in the $^{12}C^*$ -> 3α breakup

All good!

$^{118}Ag_{m1}$ – Cross sections

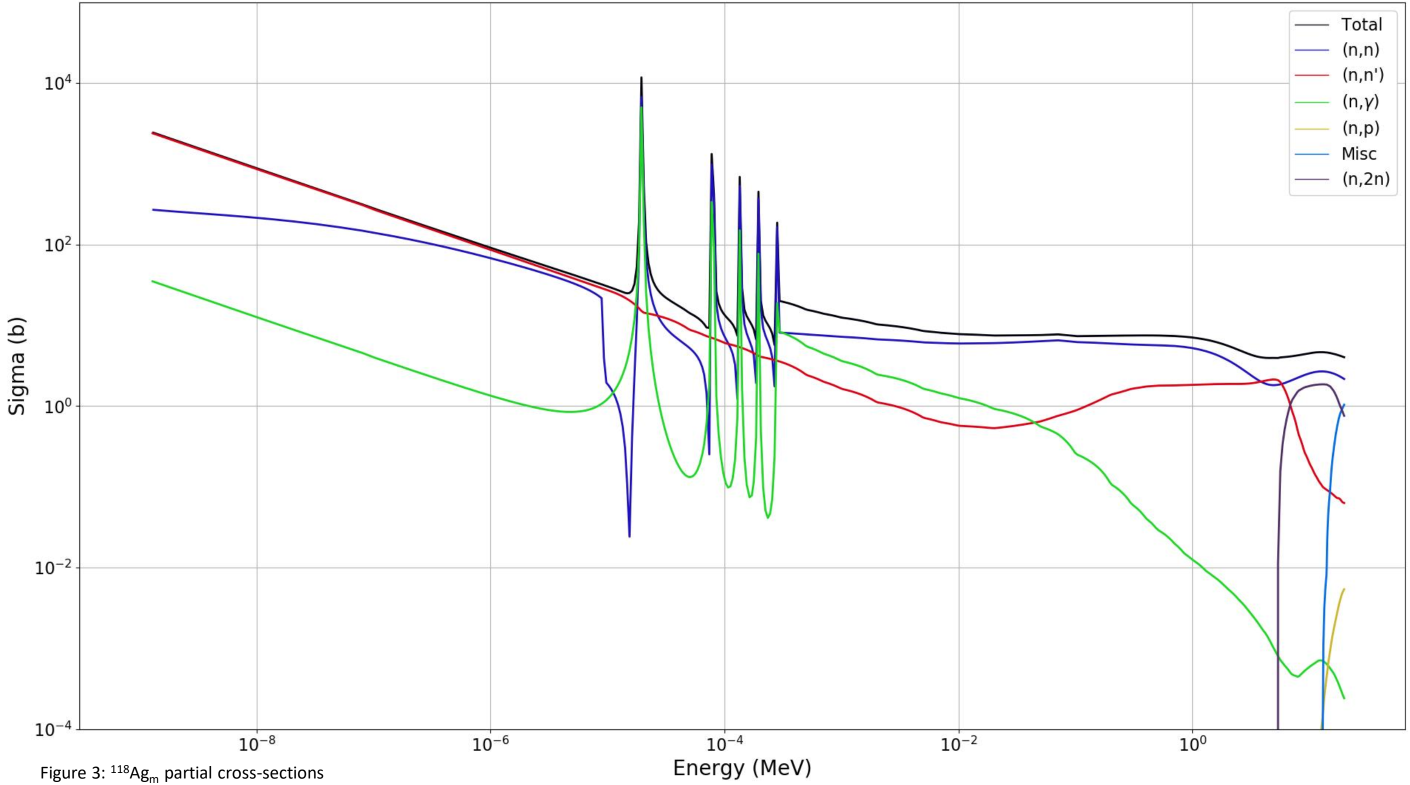

Figure 3: $^{118}Ag_m$ partial cross-sections

(n,n’) significant at low energies

Reactions that will ‘knock’ the metastable back down to the ground state.

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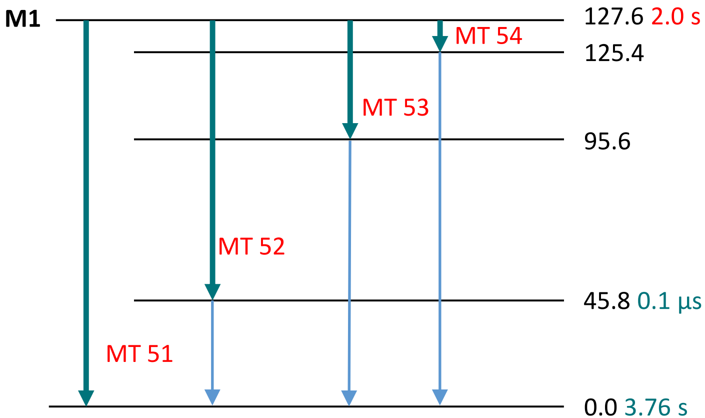

$^{118}Ag_{m1}$ - inelastic

- Example case $^{118}Ag_{m1}$ 127.63 keV
- Inelastics knock the metastable down to ground state via another level

```
47118.0000 116.901600          0          0          0          04759 3 51
127630.00  127630.000          0          0          1       2384759 3 51

47118.0000 116.901600          0          0          0          04759 3 52
127630.00  81839.9900          0          0          1       2384759 3 52

47118.0000 116.901600          0          0          0          04759 3 53
127630.00  32019.9900          0          0          1       2384759 3 53

47118.0000 116.901600          0          0          0          04759 3 54
127630.00  2199.99200          0          0          1       2384759 3 54
```

All gamma emission

Metastable energy level being stored in QM but not used in KERMA calculation, **is set to zero**!

$^{118}Ag_{m1}$- inelastic MT 51 – $\overline{E_n}$

$$R = A\sqrt{1 - \frac{(A+1)S}{AE_n}} \quad S = -Q$$

- For inelastic reactions on a ground state, QI is negative, *S* is forced positive. For a metastable inelastic to a lower energy, QI is positive forcing *S* **negative**.
- How does R change with E_n:
  - Ground state: R=0 –> A(1) from $E_{threshold}$
  - Metastable: R= Inf. -> A(1) from E_n=0
- This results in the outgoing neutron to have a minimum energy based on the value of QI.

E_n (eV)	$\overline{E_n{}'}$ (eV)
1.00E-5	1.27E+5
1.00E-2	1.27E+5
1.00E+1	1.27E+5
1.00E+4	1.36E+5
1.00E+7	9.96E+6

Table 3: $^{118}Ag_m$ MT51 values of outgoing neutron as calculated by heatr

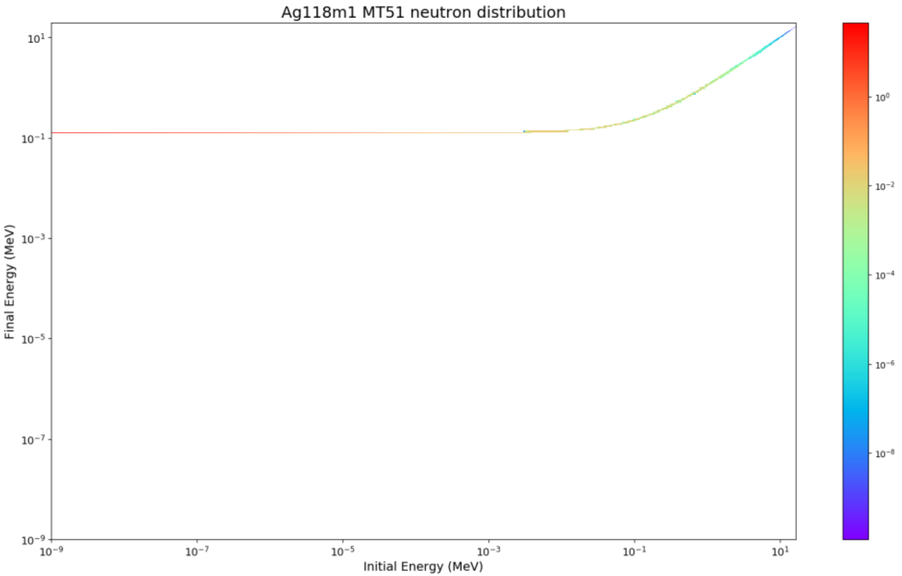

Figure 4: $^{118}Ag_m$*(n,n')* ^{118}Ag values of outgoing neutron distribution (MT51)

$^{118}Ag_{m1}$- inelastic MT 51 – $\overline{E_R}$

- With $\overline{E_n}' > E_n$, $\overline{E_R}$ is forced negative.
- Since reaction is gamma producing, the Q=+127630 is discarded and set to Q=0
- Negative KERMA is calculated with a not insignificant magnitude; this can be greater than the contribution from all other reactions combined.

E_n (eV)	$\overline{E_n}'$ (eV)	$\overline{E_R}$ (eV)	σ (b)	KERMA (eVb)
1.00E-5	1.27E+5	- 1.27E+5	5.13E+2	-6.49E+7
1.00E-2	1.27E+5	- 1.27E+5	1.62E+1	-2.06E+7
1.00E+1	1.27E+5	- 1.27E+5	5.12E-1	-6.49E+4
1.00E+4	1.36E+5	- 1.26E+5	1.80E-2	-2.27E+3
1.00E+7	9.96E+6	4.16E+4	1.93E-7	8.04E-3

Table 4: $^{118}Ag_m$ MT51 values of outgoing neutron and KERMA as calculated by heatr

$^{118}Ag_{m1}$ - inelastic MT 51 – fix?

- If Q keeps the value of +127630 as given in the file (as if it were a charged particle LR), this value can be added to $\overline{E_R}$.
- All values for KERMA now positive, energy liberated from the initial excited state at the start of the reaction

+Q to get

E_n (eV)	$\overline{E_n}'$ (eV)	Old $\overline{E_R}$ (eV)	New $\overline{E_R}$ (eV)	σ (b)	Old KERMA (eVb)	New KERMA (eVb)
1.00E-5	1.27E+5	- 1.27E+5	1.08E+3	5.13E+2	-6.49E+7	5.55E+5
1.00E-2	1.27E+5	- 1.27E+5	7.90E+2	1.62E+1	-2.06E+7	1.28E+4
1.00E+1	1.27E+5	- 1.27E+5	1.03E+3	5.12E-1	-6.49E+4	5.27E+2
1.00E+4	1.36E+5	- 1.26E+5	1.25E+3	1.80E-2	-2.27E+3	2.24E+1
1.00E+7	9.96E+6	4.16E+4	1.69E+5	1.93E-7	8.04E-3	3.27E-2

Table 5: $^{118}Ag_m$ MT51 values of outgoing neutron and KERMA as calculated by heatr, with adjustment of including Q-value

Summary

- Two questions have arisen through this investigation:

- Is the current implementation of R correct for metastables to calculate $\overline{E_n{}'}$?
    - Approximately all the metastable energy is being given to the outgoing neutron as a result of how the positive Q value interacts with the calculation of R.

$$R = A\sqrt{1 - \frac{(A+1)S}{AE_n}} \quad S = -Q$$

- Is the negative KERMA that is being calculated physical, or should the metastable energy that is being 'lost' be included in the calculation of KERMA – I believe it should.
    - Unlikely that `heatr` was written to consider metastables!