What is the problem

- At LLNL we were comparing our Monte Carlo code Mercury results to MCNP results
- Energy deposition agreed well when transporting neutrons only
- Energy deposition did not agreed well at low neutron (projectile) energy when gammas were added to transporting
- I concluded that the difference was due to the fact that FUDGE was implementing the formula for the primary gamma energy as specified in Chapters 12 and 13 in the ENDF manual and NJOY was not.
- I also was concluded that the formula in the ENDF manual is incorrect, and speculated that NJOY developers realized this and had implemented a more correct formula
- Basically, the formula in the ENDF manual ignores the recoil of the residual

Gamma energy?

- What in chapters 12 and 13 of the ENDF manual is calls the primary gamma energy is really the total available "kinetic energy" for the gamma and the "residual" in the center-of-mass frame

  - Kinetic energy for a photon is its energy (in my lingo)

  - In chapters 12 and 13, the gamma is either a primary or a discrete gamma
    - primary gamma via capture reaction

      projectile + target → primary_gamma + residual (e.g., n + O16 → γ + O17_e5)

    - Discrete gamma

      residual → discrete_gamma + residual (e.g., O17_e5 → γ + O17_e2)

      residual → discrete_gamma + residual (e.g., O17_e2 → γ + O17_e1)

Current ENDF statement

EG_k photon energy for LP=0 or 1 or Binding Energy for LP=2. For a continuous photon energy distribution, $EG_k \equiv 0.0$ should be used.

LP indicator of whether or not the particular photon is a primary:

LP=0 origin of photons is not designated or not known, and the photon energy is EG_k;

LP=1 for non-primary photons where the photon energy is again simply EG_k;

LP=2 for primary photons where the photon energy EG'$_k$ is given by

$$EG'_k = EG_k + \frac{AWR}{AWR+1} E_n.$$

- For LP = 0 or 1, I do not know if this is correct as it depends on what evaluators are doing. Is it the gamma energy? Or is it the transition energy (i.e., Q-value) for the decay?
- For LP = 2, EG_k is the binding energy (i.e., Q-value) and EG'_k is the total kinetic energy in the center-of-mass frame. Not the primary gamma energy.

Correct formulas

- Discrete energy: the center-of-mass relativistic and classical formula from the transition energy (i.e., $Q = m_i - m_f$)

$$E_\gamma = Q\left(1 - \frac{Q}{2\, m_\mathrm{i}\, c^2}\right)$$

- Primary energy: $Q = m_i - m_f = m_p + m_t - m_r$
  - Relativistic formula

$$E_\gamma = \frac{Q\ \left(2\,(m_1 + m_2) - Q/c^2\right) + 2\,K_1\,m_2}{2\sqrt{(m_1 + m_2)^2 + 2\,K_1\,m_2/c^2}}$$

  - Classical formula

$$E_\gamma = Q\ \left(1 - \frac{Q}{2(m_1 + m_2)\,c^2} - \frac{K_1\,m_2}{(m_1 + m_2)^2\,c^2}\right) + \frac{K_1\,m_2}{m_1 + m_2}$$

Changes to ENDF manual

- Replace the LP = 2 formula with both correct relativistic and classical formulas, and state that gamma energy defined in the center-of-mass frame.

$$E_\gamma = \frac{Q\ \left(2\,(m_1 + m_2) - Q/c^2\right) + 2\,K_1\,m_2}{2\sqrt{(m_1 + m_2)^2 + 2\,K_1\,m_2/c^2}}$$

$$E_\gamma = Q\ \left(1 - \frac{Q}{2(m_1 + m_2)\,c^2} - \frac{K_1\,m_2}{(m_1 + m_2)^2\,c^2}\right) + \frac{K_1\,m_2}{m_1 + m_2}$$

- Note, AWR is not correct mass to use, especially for non-neutron projectiles. In above formulas, m_1 is the projectile's mass. What to do?

$$\mathrm{EG}'_k = \mathrm{EG}_k + \frac{\mathrm{AWR}}{\mathrm{AWR} + 1}\ E_n$$

- Codes must convert center-of-mass energy to lab frame if desired.