Self-Consistent Energy Normalization for Quasistatic Reactor Calculations

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Introduction

- Reactor feedback calculations require neutron flux distributions that are normalized to the specific power level of the reactor.
- Detailed power normalization methods rely on nuclide-specific energy release data in ENDF-format.
  - ENDF MT 458 (energy release per fission) and MT 300 (KERMA)
- Nuclear data is used to estimate the rate of energy release within the reactor.
  - At steady-state: energy deposition rate = energy release rate
  - Non-critical systems use quasistatic approximation to force a steady-state solution.
    - Neutron production rate is artificially modified by a factor $1/k_{eff}$.
    - Production adjustment results in a significant effect on energy deposition.
    - Conservation of energy release/deposition is not satisfied under this approximation.

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Background

- In 2013, Griesheimer and Stedry proposed a generalized framework for detailed energy deposition during radiation transport.
  - Four different levels of energy deposition fidelity were proposed
    - 1: Constant eV per Fission
    - 2: Constant indirect energy release
    - 3: Local photon deposition
    - 4: Fully coupled neutron/photon transport
  - Modes 3 and 4 include explicit neutron energy transport.
  - In these modes, an "energy rebalance factor" $(\tau = k_{\text{eff}})$ was used to balance neutron energy release and deposition for non-critical systems.

- In 2019, Serpent adopted a similar framework for detailed energy deposition treatments.

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Overview of Current Work

- Extensive testing of the 2013 energy deposition framework showed unexpected results for some cases.
  - Calculations produced negative indirect energy release rates for some fast-spectrum systems.
- Original energy rebalance factor definition ($\tau = k_{\text{eff}}$) is <u>not</u> exact
  - Original definition does not account for the incident energy of neutrons causing fission.
  - Additional questions uncovered regarding the application of the energy rebalance factor to exothermic (non-fission) reactions.
- This work establishes a self-consistent method for calculating energy deposition in non-critical systems
  - Complete (exact) definition for the energy rebalance factor.

Energy Balance Formulation

- Begin with the premise that energy release must equal energy deposition + leakage for a reactor in steady-state (or quasi-static conditions).

$$\mathrm{E}_{\mathrm{n,birth}} + \mathrm{Q}_{\mathrm{indirect}} + \mathrm{Q}_{\mathrm{fission}} = \left(\mathrm{E}^{\mathrm{total}}_{\mathrm{n,fission}} + \mathrm{E}^{\mathrm{total}}_{\mathrm{n,indirect}} \right) + \mathrm{E}_{\mathrm{n,leakage}}$$

  - Q and E values represent total energy release and transfer, respectively, integrated over space and energy for specified reaction types.
- Break the master energy balance equation into "local" and "non-local" energy deposition terms to represent the effects of secondary radiation transport.

$$\mathrm{E}_{\mathrm{n,birth}} + \mathrm{Q}_{\mathrm{indirect}} + \mathrm{Q}_{\mathrm{fission}} = \left(\mathrm{E}^{\mathrm{local}}_{\mathrm{n,fission}} + \mathrm{E}^{\mathrm{neutron}}_{\mathrm{n,fission}} + \mathrm{E}^{\mathrm{neutrino}}_{\mathrm{n,fission}} + \mathrm{E}^{\gamma}_{\mathrm{n,fission}} \right) + \left(\mathrm{E}^{\mathrm{local}}_{\mathrm{n,indirect}} + \mathrm{E}^{\gamma}_{\mathrm{n,indirect}} \right) + \mathrm{E}_{\mathrm{n,leakage}}$$

  - Variable superscripts denote energy form following reaction.
  - Auxiliary energy balance relationships for photons and neutrinos are illustrated on the next slide.

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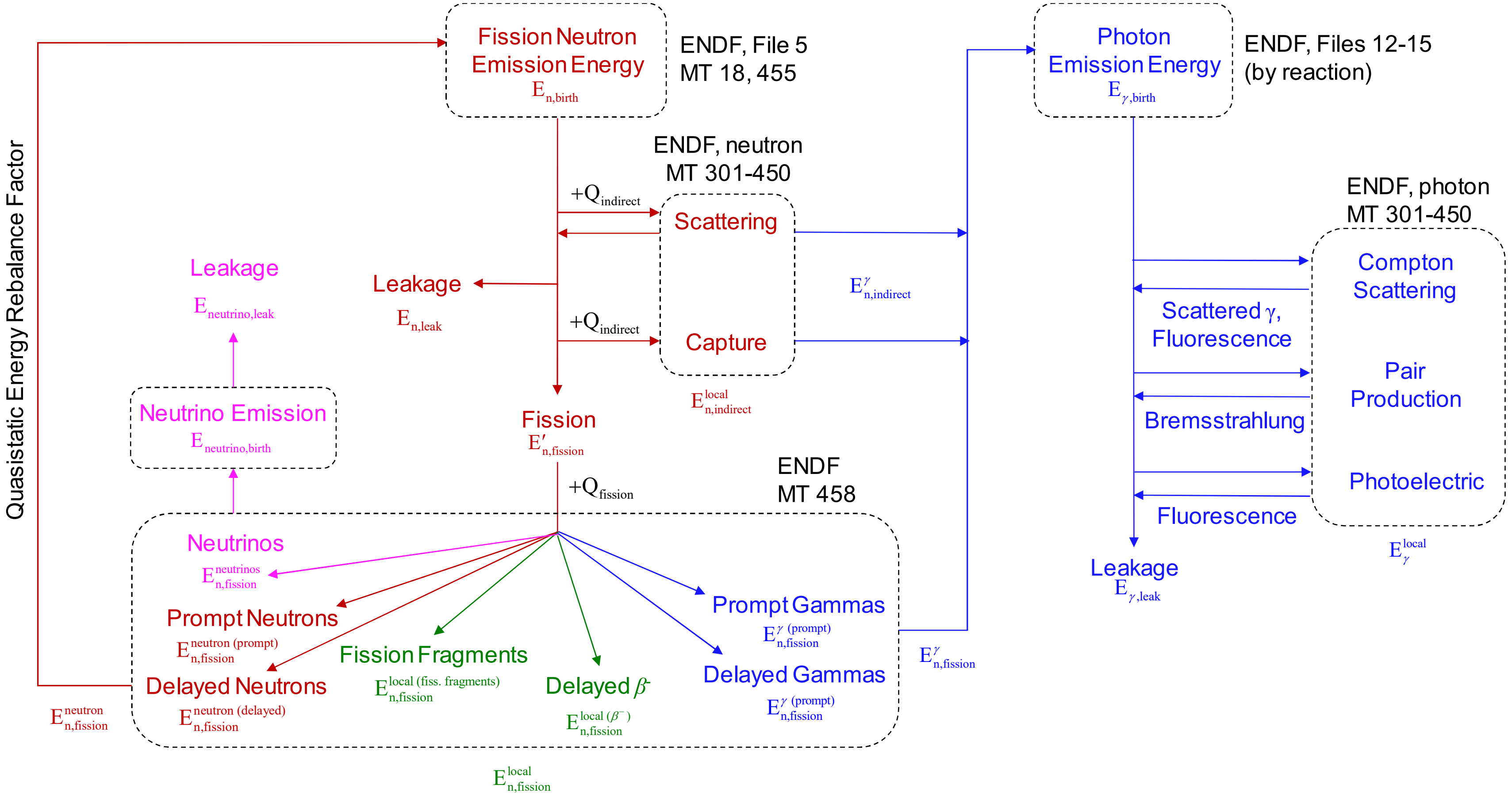
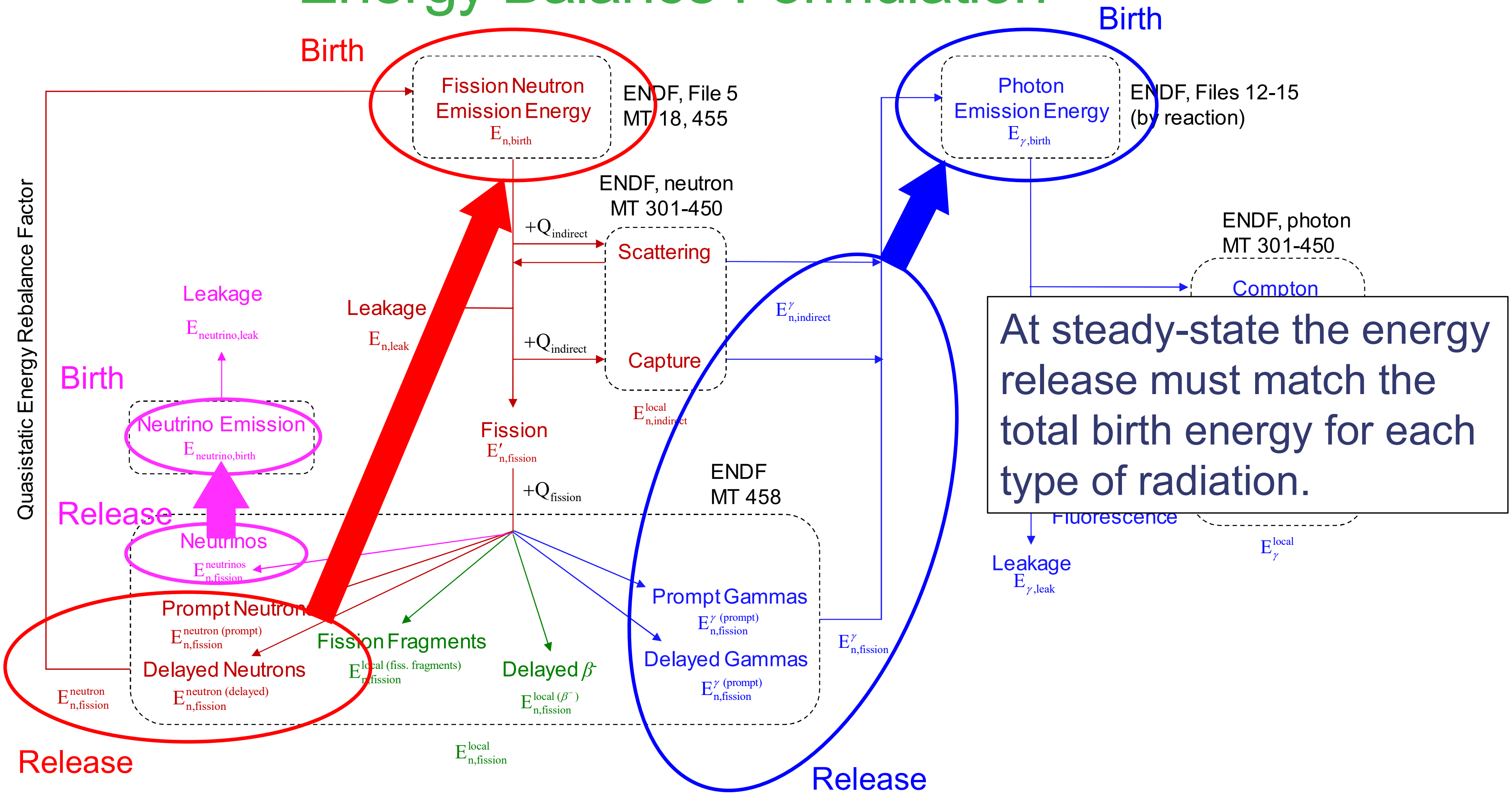
Energy Balance Formulation



Energy Balance Formulation



At steady-state the energy release must match the total birth energy for each type of radiation.

Quasistatic Energy Balance Formulation

- At steady-state, energy equations for each radiation type are coupled by balancing energy release and energy emission.

$$\mathrm{E}_{\mathrm{n,birth}} = \mathrm{E}^{\mathrm{neutron}}_{\mathrm{n,fission}}, \qquad \mathrm{E}_{\mathrm{neutrino,birth}} = \mathrm{E}^{\mathrm{neutrino}}_{\mathrm{n,fission}}, \qquad \text{and} \qquad \mathrm{E}_{\gamma,\mathrm{birth}} = \mathrm{E}^{\gamma}_{\mathrm{n,fission}} + \mathrm{E}^{\gamma}_{\mathrm{n,indirect}}$$

- Neutron energy balance is not preserved under the quasi-static approximation (i.e., $1/k_{\mathrm{eff}}$ factor applied to ν).

$$\mathrm{E}_{\mathrm{n,birth}} = \left\langle \bar{E}_{\mathrm{n}}\left(E'_{\mathrm{n}}\right)\frac{1}{k_{\mathrm{eff}}}\nu\Sigma_{\mathrm{f}}\left(\vec{r},E'_{\mathrm{n}}\right)\phi_{\mathrm{n}}\left(\vec{r},E'_{\mathrm{n}}\right)\right\rangle_{E'_{\mathrm{n}},\vec{r}} \neq \mathrm{E}^{\mathrm{neutron}}_{\mathrm{n,fission}} = \left\langle h^{\mathrm{neutron}}_{\mathrm{n,fission}}\left(E'_{\mathrm{n}}\right)\Sigma_{\mathrm{f}}\left(\vec{r},E'_{\mathrm{n}}\right)\phi_{\mathrm{n}}\left(\vec{r},E'_{\mathrm{n}}\right)\right\rangle_{E'_{\mathrm{n}},\vec{r}}$$

where

E'_{n}	Incident energy of neutron causing fission
$\bar{E}_{\mathrm{n}}\left(E'_{\mathrm{n}}\right)$	Avg. fission neutron birth energy
$h^{\mathrm{neutron}}_{\mathrm{n,fission}}\left(E'_{\mathrm{n}}\right)$	Avg. energy released as neutrons during fission.

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Quasistatic Energy Rebalance Factor

- Compensate for quasistatic energy deposition imbalance by adjusting the neutron weight for energy deposition and leakage reactions.
  - **Transport Energy**: True energy of neutron used for xs lookups
  - **Deposition Energy**: Adjusted neutron energy used for deposition/leakage
  - **Energy Rebalance Factor (τ_n)**: Ratio of Deposition to Transport Energy

- To enforce balance between neutron energy release/deposition, define:

$$\tau_{\mathrm{n}} = \frac{\mathrm{E}_{\mathrm{n,fission}}^{\mathrm{neutron}}}{\mathrm{E}_{\mathrm{n,birth}}} = \frac{\left\langle h_{\mathrm{n,fission}}^{\mathrm{neutron}}\left(\tau_{\mathrm{n}}, E_{\mathrm{n}}'\right)\Sigma_{\mathrm{f}}\left(\vec{r}, E_{\mathrm{n}}'\right)\phi_{\mathrm{n}}\left(\vec{r}, E_{\mathrm{n}}'\right)\right\rangle_{E_{\mathrm{n}}',\vec{r}}}{\dfrac{1}{k_{\mathrm{eff}}}\left\langle \int_0^\infty \bar{E}_{\mathrm{n}}\left(E_{\mathrm{n}}'\right)\nu\Sigma_{\mathrm{f}}\left(\vec{r}, E_{\mathrm{n}}'\right)\phi_{\mathrm{n}}\left(\vec{r}, E_{\mathrm{n}}'\right)\right\rangle_{E_{\mathrm{n}}',\vec{r}}}.$$

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Note the implicit definition: $\tau_{\mathrm{n}} = f\left(\tau_{\mathrm{n}}\right)$

Neutron Energy Release Per Fission

- The 2013 definition for the energy rebalance factor assumed that

Fission neutron energy release per neutron

$$\frac{h_{\mathrm{n,fission}}^{\mathrm{neutron}}\left(E_{\mathrm{n}}'\right)}{\nu} = \bar{E}_{\mathrm{n}}\left(E_{\mathrm{n}}'\right)$$

Average fission neutron birth energy

- This assumption yields $\tau_{\mathrm{n}} = k_{\mathrm{eff}}$, but the assumption is **not correct**

- Per ENDF, $h_{\mathrm{n,fission}}^{\mathrm{neutron}}\left(E_{\mathrm{n}}'\right)$ includes the energy of the neutron causing fission.

$$h_{\mathrm{n,fission}}^{\mathrm{neutron}}\left(\tau_{\mathrm{n}}, E_{\mathrm{n}}'\right) = h_{\mathrm{n,fission}}^{\mathrm{neutron}}\left(1, E_{\mathrm{n}}'\right) + E_{\mathrm{n}}'\left(\tau_{\mathrm{n}} - 1\right).$$

- Note that E_{n}' is the neutron deposition energy, which leads to the dependence of $h_{\mathrm{n,fission}}^{\mathrm{neutron}}\left(\tau_{\mathrm{n}}, E_{\mathrm{n}}'\right)$ on the rebalance factor τ_{n}.

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Corrected Energy Rebalance Factor

- Substituting definition for $h_{\mathrm{n,fission}}^{\mathrm{neutron}}\left(\tau_{\mathrm{n}}, E_{\mathrm{n}}'\right)$ into the implicit energy rebalance formula and solving for τ_{n} gives

$$\boxed{\tau_{\mathrm{n}} = \frac{\left\langle h_{\mathrm{n,fission}}^{\mathrm{neutron}}\left(E_{\mathrm{n}}'\right)\Sigma_{\mathrm{f}}\left(\vec{r}, E_{\mathrm{n}}'\right)\phi_{\mathrm{n}}\left(\vec{r}, E_{\mathrm{n}}'\right)\right\rangle_{E_{\mathrm{n}}', \vec{r}} - \left\langle E_{\mathrm{n}}'\Sigma_{\mathrm{f}}\left(\vec{r}, E_{\mathrm{n}}'\right)\phi_{\mathrm{n}}\left(\vec{r}, E_{\mathrm{n}}'\right)\right\rangle_{E_{\mathrm{n}}', \vec{r}}}{\dfrac{1}{k_{\mathrm{eff}}}\left\langle \int_{0}^{\infty} \overline{E}_{\mathrm{n}}\left(E_{\mathrm{n}}'\right)\nu\Sigma_{\mathrm{f}}\left(\vec{r}, E_{\mathrm{n}}'\right)\phi_{\mathrm{n}}\left(\vec{r}, E_{\mathrm{n}}'\right)\right\rangle_{E_{\mathrm{n}}', \vec{r}} - \left\langle E_{\mathrm{n}}'\Sigma_{\mathrm{f}}\left(\vec{r}, E_{\mathrm{n}}'\right)\phi_{\mathrm{n}}\left(\vec{r}, E_{\mathrm{n}}'\right)\right\rangle_{E_{\mathrm{n}}', \vec{r}}}}$$

- Note that τ_{n} approaches k_{eff} if E_{n}' is small
  - For thermal-spectrum reactors this is a reasonable assumption.
  - Not accurate for reactors where a significant fraction of fissions are caused by above-thermal neutrons.

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Corrected Energy Rebalance Factor

- Substituting definition for $h_{\mathrm{n,fission}}^{\mathrm{neutron}}\left(\tau_{\mathrm{n}}, E_{\mathrm{n}}'\right)$ into the implicit energy rebalance formula and solving for τ_{n} gives

Total energy of neutrons causing fission events

Fission energy released as neutrons

$$\boxed{\tau_{\mathrm{n}} = \frac{\left\langle h_{\mathrm{n,fission}}^{\mathrm{neutron}}\left(E_{\mathrm{n}}'\right)\Sigma_{\mathrm{f}}\left(\vec{r},E_{\mathrm{n}}'\right)\phi_{\mathrm{n}}\left(\vec{r},E_{\mathrm{n}}'\right)\right\rangle_{E_{\mathrm{n}}',\vec{r}} - \left\langle E_{\mathrm{n}}'\Sigma_{\mathrm{f}}\left(\vec{r},E_{\mathrm{n}}'\right)\phi_{\mathrm{n}}\left(\vec{r},E_{\mathrm{n}}'\right)\right\rangle_{E_{\mathrm{n}}',\vec{r}}}{\frac{1}{k_{\mathrm{eff}}}\left\langle\int_0^{\infty}\bar{E}_{\mathrm{n}}\left(E_{\mathrm{n}}'\right)\nu\Sigma_{\mathrm{f}}\left(\vec{r},E_{\mathrm{n}}'\right)\phi_{\mathrm{n}}\left(\vec{r},E_{\mathrm{n}}'\right)\right\rangle_{E_{\mathrm{n}}',\vec{r}} - \left\langle E_{\mathrm{n}}'\Sigma_{\mathrm{f}}\left(\vec{r},E_{\mathrm{n}}'\right)\phi_{\mathrm{n}}\left(\vec{r},E_{\mathrm{n}}'\right)\right\rangle_{E_{\mathrm{n}}',\vec{r}}}}$$

Total birth energy of fission neutrons

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Quasistatic Energy Balance Revisited

- Enforcing balance between neutron energy release and deposition allows simplification of the master energy balance equation.

$$\cancel{\mathrm{E}_{\mathrm{n,birth}}} + \mathrm{Q}_{\mathrm{indirect}} + \mathrm{Q}_{\mathrm{fission}} = \left(\mathrm{E}^{\mathrm{local}}_{\mathrm{n,fission}} + \cancel{\mathrm{E}^{\mathrm{neutron}}_{\mathrm{n,fission}}} + \mathrm{E}^{\mathrm{neutrino}}_{\mathrm{n,fission}} + \mathrm{E}^{\gamma}_{\mathrm{n,fission}}\right) + \left(\mathrm{E}^{\mathrm{local}}_{\mathrm{n,indirect}} + \mathrm{E}^{\gamma}_{\mathrm{n,indirect}}\right) + \mathrm{E}_{\mathrm{n,leakage}}$$

- Illustrates that neutron energy present in a (quasi)static system remains constant over time.

- Note that Q_{fission} and Q_{indirect} energy release rates are preserved on a per reaction basis, regardless of k_{eff}.
  - However, the total energy release rate will change with respect to k_{eff}, due to changes in the capture/fission rate.

Local Heating Edits

- The energy rebalance factor, τ_n, is applied to neutron leakage and all reactions involving energy deposition or transfer.
- For indirect (non-fission) reactions the modification is given by:

$$\mathrm{E}_{\mathrm{n,indirect}}^{\mathrm{total}} = \left\langle \phi_\mathrm{n}\left(\vec{r}, E'_\mathrm{n}\right) \sum_{i}^{\mathrm{nucs}} \sum_{j}^{\mathrm{rxns}} \left(\tau_\mathrm{n} E'_\mathrm{n} + Q_{i,j}\left(E'_\mathrm{n}\right) - \tau_\mathrm{n} \bar{E}_{\mathrm{n},i,j}\left(E'_\mathrm{n}\right) \right) \Sigma_{i,j}\left(\vec{r}, E'_\mathrm{n}\right) \right\rangle_{E'_\mathrm{n}, \vec{r}}$$

  - Note that the rebalance factor is *not* applied to the reaction Q-values.

- In ENDF, energy deposition is represented by the KERMA pseudoreaction cross section, which is defined as:

$$K_{\mathrm{n,indirect}}^{\mathrm{total}}\left(E'_\mathrm{n}\right) = \sum_{i}^{\mathrm{nucs}} \sum_{j}^{\mathrm{rxns}} \left(E'_\mathrm{n} + Q_{i,j}\left(E'_\mathrm{n}\right) - \bar{E}_{\mathrm{n},i,j}\left(E'_\mathrm{n}\right) \right) \Sigma_{i,j}\left(\vec{r}, E'_\mathrm{n}\right),$$

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  - No

NOTICE:

$$\mathrm{E}_{\mathrm{n,indirect}}^{\mathrm{total}} \neq \left\langle \phi_\mathrm{n}\left(\vec{r},E'_\mathrm{n}\right) \tau_\mathrm{n} K_{\mathrm{n,indirect}}^{\mathrm{total}}\left(E'_\mathrm{n}\right) \right\rangle_{E'_\mathrm{n},\vec{r}}$$

The R.H.S **incorrectly** applies the τ_n factor to *all* reaction Q-values!

- In EN action
  cross

$$K_{\mathrm{n,indirect}}^{\mathrm{total}}\left(E'_\mathrm{n}\right) = \sum_{i}^{\mathrm{nucs}} \sum_{j}^{\mathrm{rxns}} \left(E'_\mathrm{n} + Q_{i,j}\left(E'_\mathrm{n}\right) - \bar{E}_{\mathrm{n},i,j}\left(E'_\mathrm{n}\right) \right) \Sigma_{i,j}\left(\vec{r},E'_\mathrm{n}\right),$$

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KERMA Inconsistency

- In KERMA data there is no way to know how the incident neutron energy is apportioned among deposition and secondary neutrons exiting the reaction.

- Many codes assume that KERMA deposition is scaled by τ_n :

$$\mathrm{E}^{\mathrm{total}}_{\mathrm{n,indirect}} \approx \left\langle \phi_\mathrm{n}\left(\vec{r}, E'_\mathrm{n}\right) \tau_\mathrm{n} K^{\mathrm{total}}_{\mathrm{n,indirect}}\left(E'_\mathrm{n}\right) \right\rangle_{E'_\mathrm{n}, \vec{r}}$$

- This approximation unphysically applies τ_n to all (non-fission) reaction Q-values.
  - Violates philosophy of preserving reaction Q-values.
  - Typically a small effect – indirect energy release accounts for <1% of reactor power.

- Resolving inconsistency will require changes to KERMA calculation and ENDF format.
  - Adopt a common KERMA format that explicitly accounts for incident neutron energy, similar to the format of the ENDF MT 458 fission energy release data.

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Numerical Results

- An analytical reference model was used to quantify the effects of the quasistatic approximation on energy release/deposition.
  - Monoenergetic 2.0 MeV neutrons in an infinite, homogeneous mixture of two nuclides.
  - Fuel – Purely fissioning, $\sigma_t = \sigma_f = 1.0$, $\nu = 2.0$ n/fiss., $Q_{\text{fission}} = 200$ MeV/fiss.
  - Poison – Purely absorbing, $\sigma_t = \sigma_a = 1.0$, $Q_{\text{absorption}} = 1.0$ MeV/abs.
  - Number density of fuel N_f is constant at 1.0 atoms/(barn·cm)
  - Number density of poison N_f was adjusted from 0.5 to 1.5 atoms/(barn·cm).

Fission energy release by category for fictitious, purely-fissioning fuel nuclide.

Category	**Nominal Energy Rel. ($h(0)$) [MeV/fiss]**	**Energy-Dependent Energy Rel. ($h(E')$) [MeV/fiss]**
Fission Fragments (h^{FR})	169.0	$h^{\text{FR}}(0)$
Prompt Neutrons† (h^{neutron})	1.386	$h^{\text{neutron}}(0) + 1.307 \times E' \times (\tau_n - 1)$
Prompt Gammas† (h^{γ})	12.15	$h^{\gamma}(0) - 0.075 \times E'$
Beta Particles (h^{β})	7.15	$h^{\beta}(0) - 0.075 \times E'$
Neutrinos (h^{neutrino})	10.2	$h^{\text{neutrino}}(0) - 0.010 \times E'$

†Delayed neutron and photon release is assumed to be equal to zero.

Numerical Results

- Analytical solutions for k_{eff} and energy release/deposition as a function of poison number density.

$$k_{\text{eff}} = \frac{N_{\text{F}} \nu \sigma_{\text{f}}}{N_{\text{F}} \sigma_{\text{f}} + N_{\text{P}} \sigma_{\text{a}}} = \frac{2}{1 + N_{\text{P}}}.$$

$$\frac{\text{E}_{\text{n,deposited}}^{\text{total}}}{\text{fission}} = 190 + N_{\text{P}} \frac{\text{MeV}}{\text{fission}}.$$

- Theoretical behavior of three energy renormalization schemes considered
  - No correction ($\tau = 1$), approximate correction ($\tau = k_{\text{eff}}$), exact correction
  - Effects of scaled KERMA values also considered.

- Theoretical results validated by calculating energy deposition with the MC21 Monte Carlo transport solver.
  - 100 batches (10 discard) of 10,000 histories
  - Manually created nuclear data library.
  - Scaled KERMA values only.

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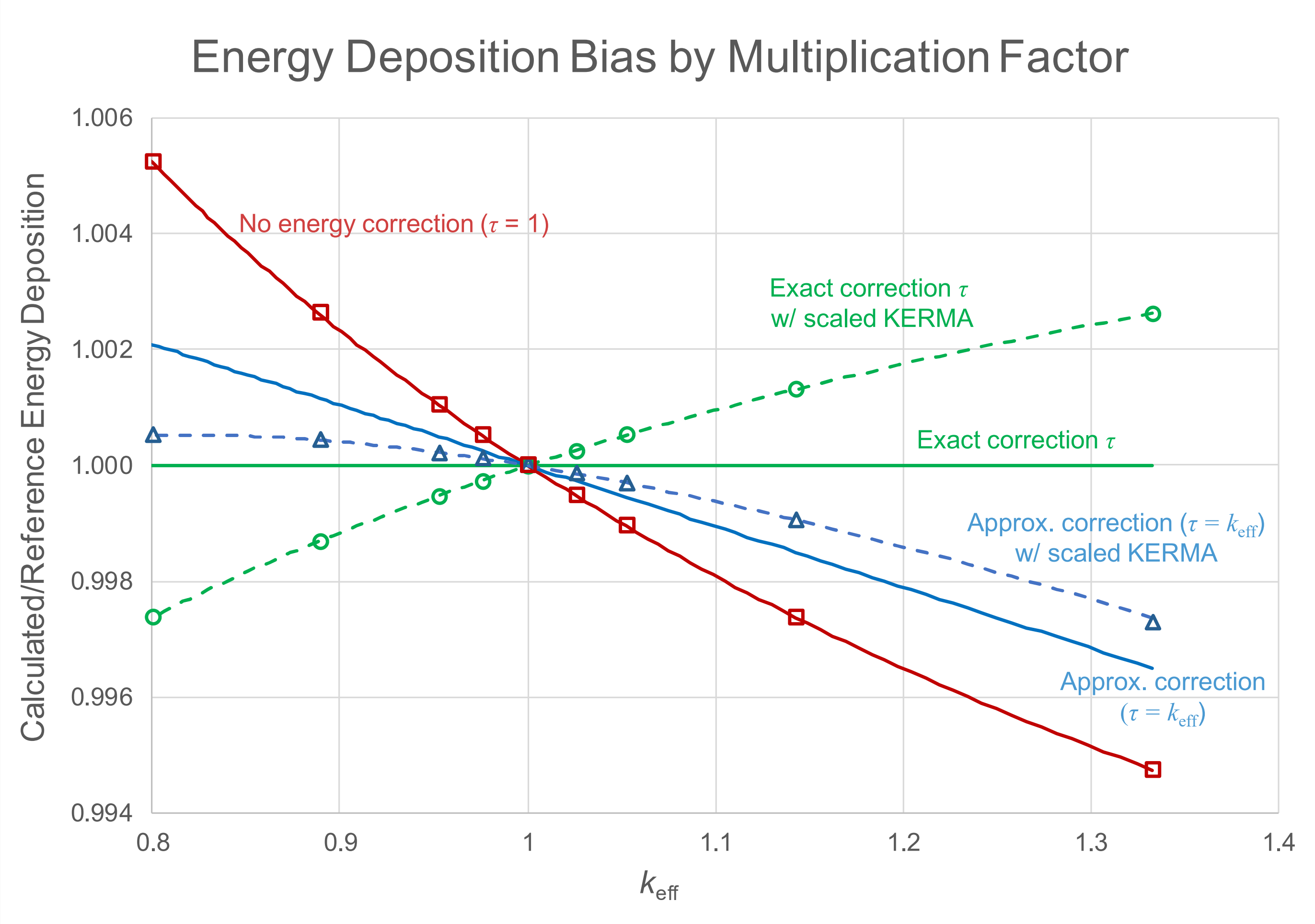
Energy Deposition Bias

Plot illustrates the ratio between computed energy deposition (for each correction factor) and the analytical reference solution for energy deposition.



Lines – Theoretical
Markers – MC21

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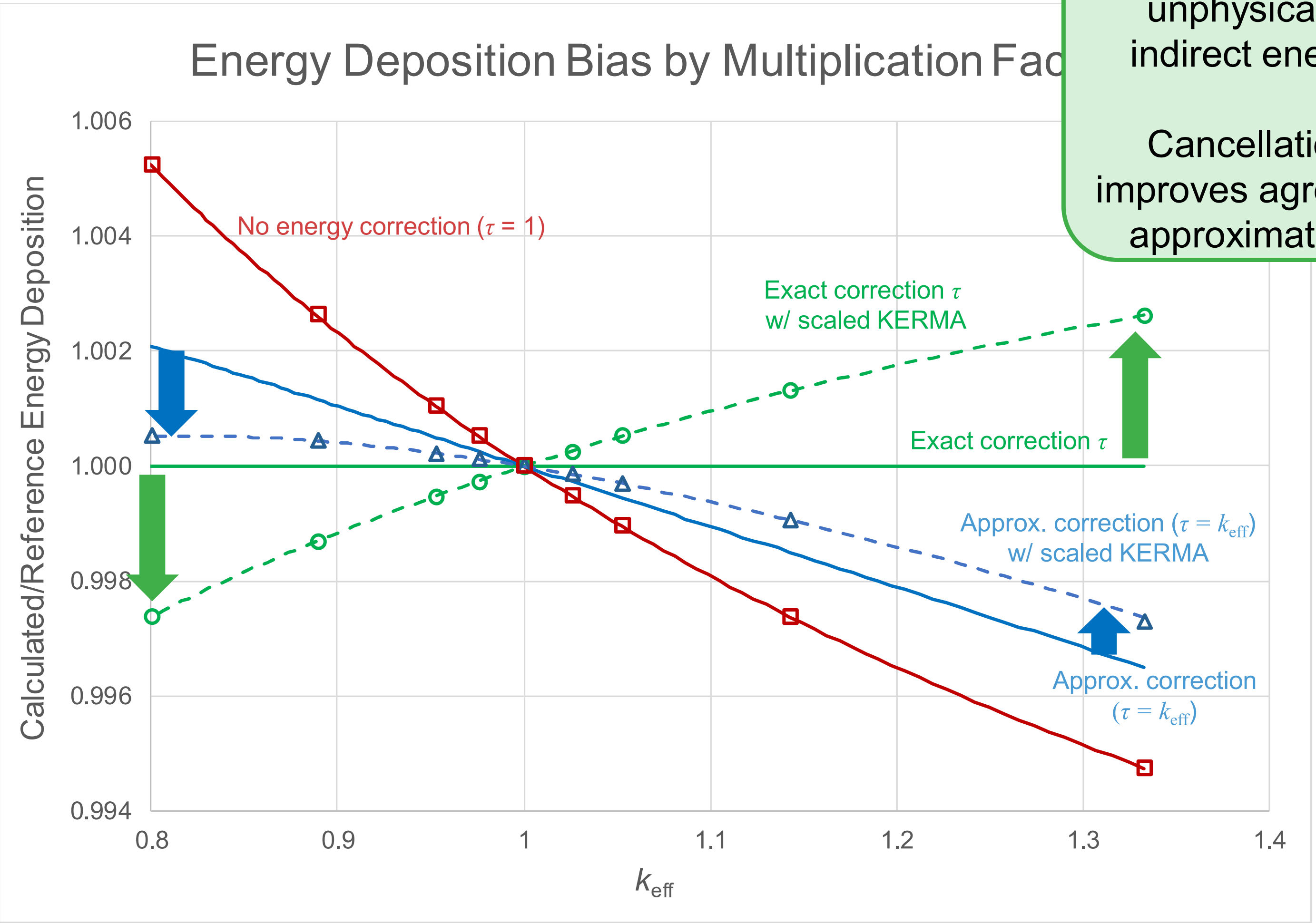


KERMA scaling unphysically changes indirect energy release.

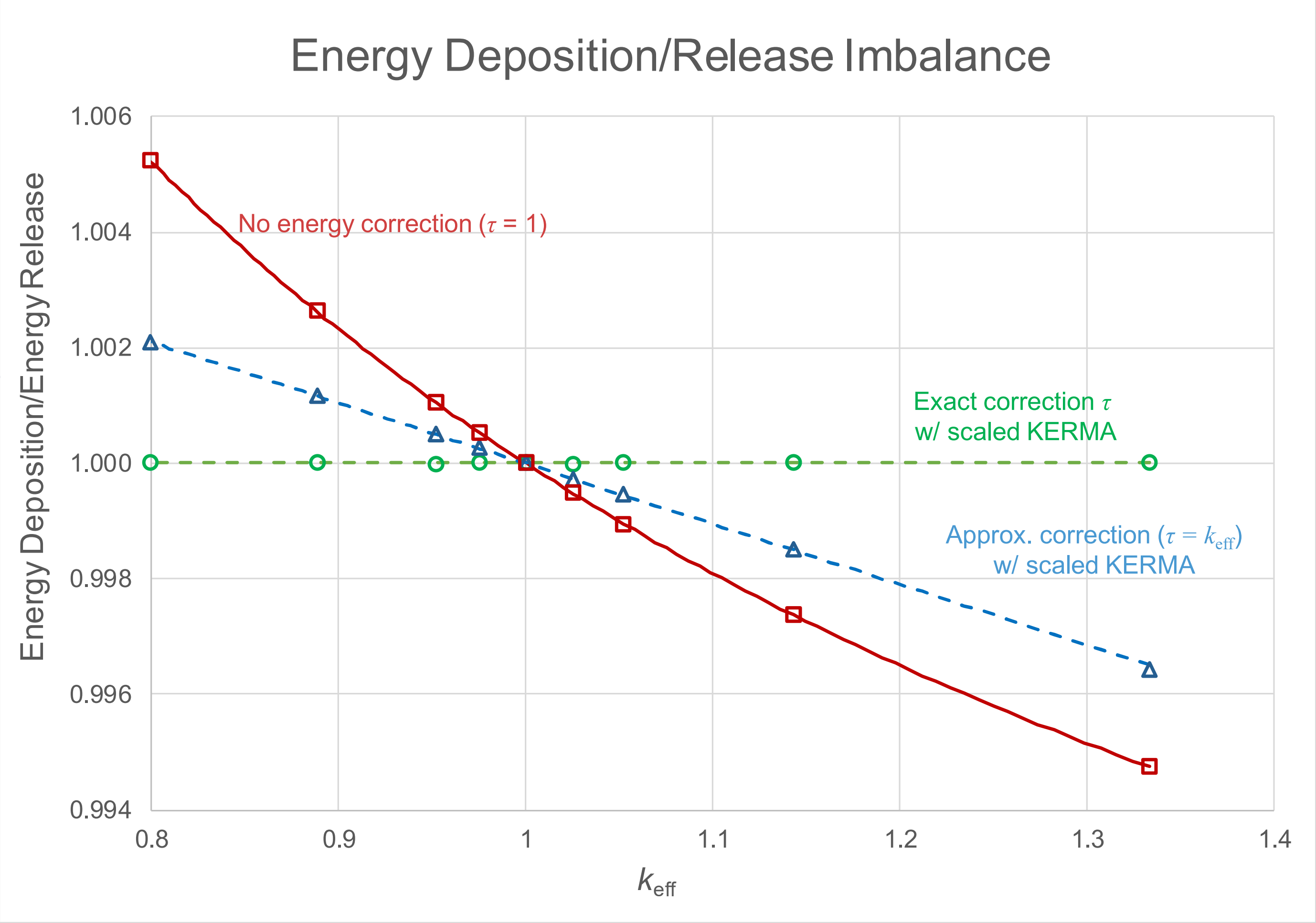
Cancellation of errors improves agreement for the approximate correction.

Lines – Theoretical
Markers – MC21

Energy Deposition/Release Imbalance

Plot illustrates the ratio of energy deposition to energy release for each correction factor.

Values other than 1.0 indicate an imbalance between energy release and deposition.



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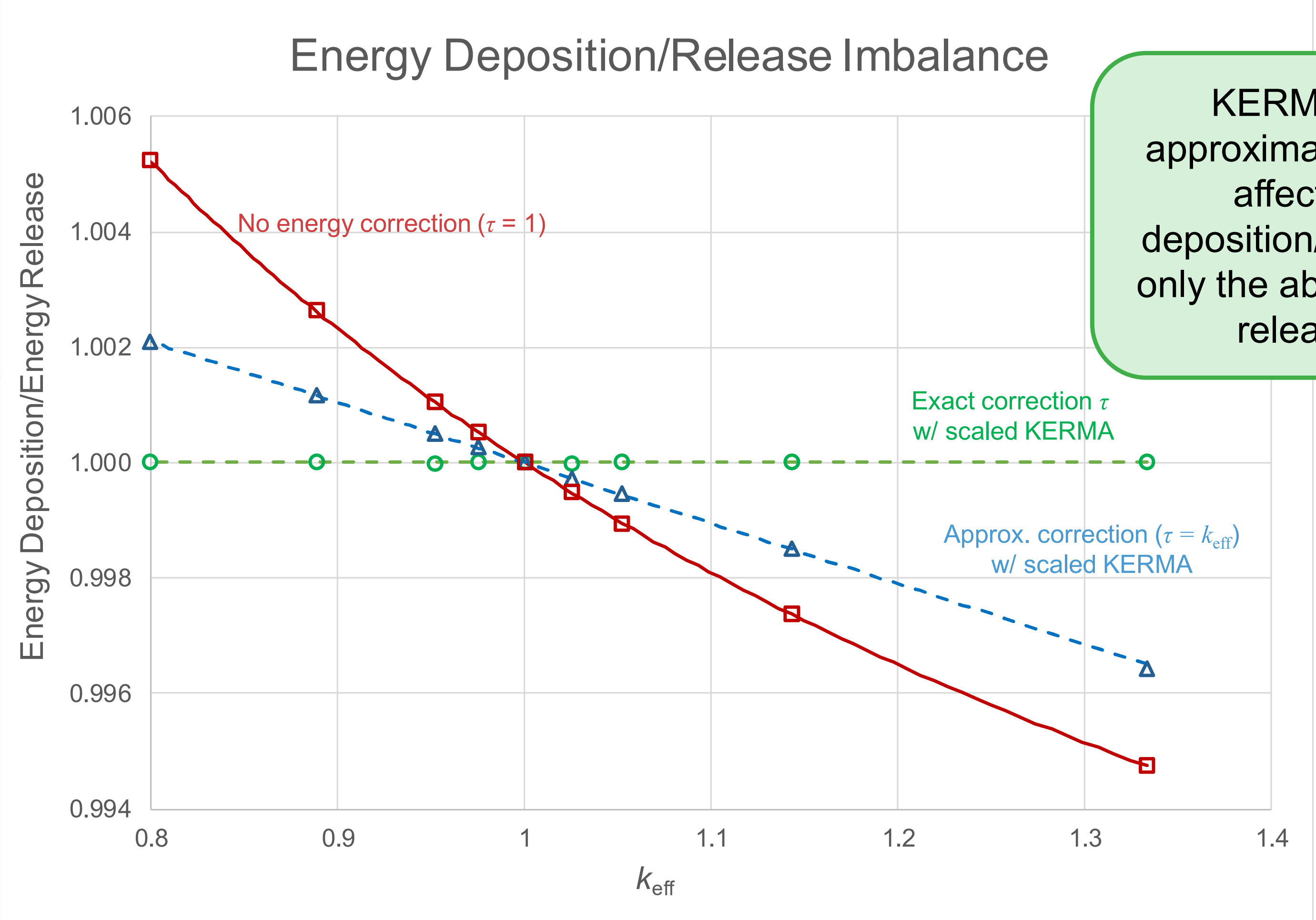

KERMA scaling approximation does not affect energy deposition/release ratio, only the absolute energy release rate.

Lines – Theoretical
Markers – MC21

Conclusions

- In non-critical fission systems, the use of the quasistatic approximation leads to an imbalance between energy release and deposition.

- In this work, we formally quantified this imbalance and derived an exact technique for enforcing energy release/deposition balance.
  - Technique involves applying an energy rebalance factor to local energy deposition, transfer, or leakage reactions.
  - Numerical results for an analytical energy deposition problem confirm the effectiveness of the technique.

- Limitations in the KERMA data format still prevents conservation of indirect energy release in most applications.
  - Consider improvements to KERMA data representation in ENDF.

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Questions?