New energy deposition treatment in Serpent 2

Serpent UGM 2018
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Outline

- Introduction
- New energy deposition modes
- Normalization and a new detector
- Energy rebalance factor
- Initial testing
- Future work
Introduction

- Accurate modelling of energy deposition in Monte Carlo transport calculations is a complex task
  - Energy deposition in a large number of different reactions
  - Energy release in reactions such as fission and radiative capture
  - Reactions can produce secondary particles
  - In transient simulations the time dependency of energy deposition must be taken into account (delayed fission heating etc.)

- Often some simple approximations are used
  - Typically all energy is deposited locally at the fission site
  - A conservative approximation concerning the fuel/cladding temperature

- More accurate models for high definition coupled calculations?
Introduction

- In [1] the spatial accuracy of energy deposition in steady state Monte Carlo transport calculations is discussed and different energy deposition treatments developed for Monte Carlo code MC21 are presented.
- Similar energy deposition treatments or modes are in development for Serpent 2.
- The new energy deposition modes require additional data not available in the standard ACE format files.
- The additional data is currently added to the end of ACE files when the files are created with NJOY.
- Cross section libraries with this additional data will be distributed at some point in the future.

New energy deposition modes

Mode 0
• Default mode used previously in Serpent 2
• All energy is deposited locally at fission sites
• Energy deposition per fission is calculated as

\[ E_d = \frac{Q_i}{Q_{235}} H_{235}, \]

where \( Q_i \) is the fission Q-value for nuclide i, \( Q_{235} \) is the fission Q-value for U\(_{235}\) and \( H_{235} = 202.27 \) MeV is an estimate for the energy deposition per fission in a light water reactor
• Spatially inaccurate, magnitude inaccurate
New energy deposition modes

Mode 1

• All energy is deposited locally at fission sites
• Energy deposition is calculated based on ENDF MT 458 data which gives components of energy release due to fission as a function of incident neutron energy
• Three ways to specify the energy dependency:
  - Thermal point evaluation (legacy format)
  - Polynomial evaluation
  - Tabular evaluation (introduced in ENDF/B-VIII)
New energy deposition modes

Mode 1

- Energy deposition per fission is calculated as

\[ E_d = E_{FR} + E_{NP} + E_{ND} + E_{GP} + \alpha(E_{GD} + E_B) + E_{capt}, \]

where \( E_{FR} \) is the kinetic energy of the fission products, \( E_{NP} \) the kinetic energy of the prompt neutrons, \( E_{ND} \) the kinetic energy of the delayed neutrons, \( E_{GP} \) the energy of the prompt gammas, \( \alpha (= 0 \text{ or } 1) \) coefficient for including delayed gamma and beta components, \( E_{GD} \) the energy of the delayed gammas, \( E_B \) the energy of the delayed betas and \( E_{capt} \) is an user-defined constant for additional energy released in capture reactions.

- Spatially inaccurate, magnitude OK if \( E_{capt} \) is OK
New energy deposition modes

Mode 2

• Neutron heating rate is calculated using special microscopic cross sections, expressed in eV·barns, referred as KERMA (Kinetic Energy Release in Materials) coefficients:

\[ H(E) = \sum_i \sum_j \rho_i k_{ij}(E) \phi(E), \]

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 scalar flux at \( E \).

• Fission energy deposition is calculated separately based on MT 458 data as

\[ E_d = EFR + EGP + \alpha(EGD + EB) \]

• Photon energy is deposited locally at emission sites

• Improved spatial accuracy and magnitude compared to modes 0 and 1 with minimal increase in the calculation time
New energy deposition modes

Mode 3

- Adds photon transport to mode 2
- Photons are created during the coupled neutron-photon transport calculation in reactions such as fission, inelastic scattering and radiative capture
- The energy of the delayed fission gammas is deposited with the same distribution as the prompt fission gammas
- Fission energy deposition is calculated as
  \[ E_d = EFR + \alpha(EB) \]
- Higher spatial accuracy and computational time compared to mode 2
Normalization and a new detector

- Energy deposition mode is selected using `set edep` option
- Affects also the normalization if normalization to total power (`set power`) is used
  - Normalization is done based on the total energy deposition in the problem geometry
  - Energy deposition mode defines how this deposition is calculated
- New detector (`dr -80`) to estimate the total energy deposition
  - Includes also different components of the energy deposition based on the energy deposition mode
  - No need to define separate detectors or response functions for the different components
  - As an example, in mode 3 the energy deposition is calculated in fission reactions, in non-fission reactions due to neutrons and also in photon interactions using an analog estimator
Energy rebalance factor (modes 2 and 3)

- In the criticality source mode the kinetic energy of the fission neutrons is not preserved between generations in a non-critical system
- Energy rebalance factor based on cycle-wise $k_{eff}$ can be used as a weighting factor for the energy deposition tallies to correct this imbalance
- The energy of the delayed gammas is deposited using a similar rebalance factor calculated as

$$f = \frac{E_{GD} + E_{GP}}{E_{GP}},$$

which is calculated for each generated prompt fission gamma
- Prompt and delayed gammas should have similar spectra to get accurate results
  - In [2] the results given by the above approximation are compared to results given by a gamma transport calculation with delayed gamma source
  - Some differences are observed but no significant change of spatial distribution of the deposited energy

Initial testing: VERA 2b

- In [3] energy deposition in several VERA benchmark problems is studied using MCNP5 and ENDF/B-VII.1
- VERA benchmark 2b:
  - A single Westinghouse 17x17 fuel assembly with 3.1 % enriched UO$_2$ fuel at beginning of life
  - 2D with reflecting boundary conditions
  - Empty guide tubes (and instrumentation tube)
- Energy deposition mode 3 with analog photon production mode
- 100 million active neutron histories were simulated
- Two runs with ENDF/B-VII.1 and ENDF/B-VIII

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<tr>
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<th>MCNP (ENDF/B-VII.1)</th>
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<th>Serpent (ENDF/B-VIII)</th>
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Initial testing: LFR

- 3D fuel assembly of a small lead cooled reactor with reflecting boundary conditions radially
- Fresh fuel
- Fuel material: UO$_2$ (19.9 %)
- Cladding material: D9
- Hex-can material: D9
- Height of the fuel column: 1.2 m
- 100 million active neutron histories were simulated
- Two runs with ENDF/B-VII.1 and ENDF/B-VIII
<table>
<thead>
<tr>
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Some observations

- Energy deposition per fission is clearly underestimated in mode 1 since $E_{\text{capt}}$ was set to 0.0 MeV
- Energy deposition per fission is overestimated in mode 0
  - The empirical constant $H_{235}$ is for light water reactors
  - Less capture reactions in a lead cooled reactor
  - Fission reaction rate and all other reaction rates are underestimated (Burnup calculations?)
- Energy deposition to fuel decreases with increasing accuracy in the energy deposition treatment
- The lead coolant is heated up by gammas
  - The effect is seen only in mode 3
- $E_d$ per fission is different in modes 2 and 3 with ENDF/B-VII.1
  - Prompt fission gammas are lumped together with gammas from other emission channels above 1.09 MeV incident neutron energy
  - Prompt gamma energy in MT 458 is probably not entirely consistent with the total energy of the gammas that are actually sampled
Future work

- Report the results
- New energy deposition modes should be tested in all of the optimization modes
- Burnup calculations?
- Energy deposition in transients
  - How to handle the delayed components?
Thank you! Questions? Suggestions?
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