Monte Carlo Calculation of the Energy Deposition in the Transformational Challenge Reactor

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INTRODUCTION

Accurate calculation of the recoverable (non-neutrinos) energy deposited in a nuclear facility requires the estimate of: the kinetic energy of fission fragments, the kinetic energy of prompt and delayed neutrons, the kinetic energy of prompt and delayed gammas, and the energy released by delayed betas. The MCNP Monte Carlo code [1] does not have the capability to tally the delayed gammas and betas energy deposition, therefore the calculation must rely on a few approximations, as discussed in detail in the next Section. The Serpent Monte Carlo code [2] evaluates the energy deposition in a more sophisticated approach that aims at reducing approximations and relies on the Kinetic Energy Released per unit Mass (KERMA) factors rather than the Q-value used by MCNP, as discussed in the Section after next. This summary aims at comparing the energy deposition results obtained by the aforementioned Monte Carlo codes for designing the Transformational Challenge Reactor (TCR), a microreactor designed, built, and operated using a rapid advanced manufacturing approach [3] .

MCNP CALCULATION METHODOLOGY

The MCNP code can calculate the energy deposition by two separate criticality (k-code) coupled (neutron and photon transport) simulations [4, 5]. In the first simulation, three different tallies are used:

1. the F6 neutron tally (F6n) scores the kinetic energy of neutrons and fission products in all cells (with fission products kinetic energy contributing only to the fuel cells);
2. the F6 photon tally (F6p) scores the energy from fission prompt gammas and gammas released from non-fission (e.g., γ capture) neutron incident reactions in all cells;
3. the F7 neutron (F7n) tally scores the kinetic energy of neutrons, fission products, and prompt gammas deposited in the fuel cells.

The third tally is used to estimate the energy released from the beta decay of fission products. More precisely, it is assumed that the latter parameter is equal to 6.5 MeV/fission (the U-235 value) and follows the spatial distribution of the F7n neutron tally. In the second MCNP simulation, only one F6 photon tally is used ($F6p_{prompt}$). This tally scores the photon energy deposition in all cells from fission prompt gammas. In the second simulation, all gammas coming from non-fission neutron incident reactions are suppressed by using the following MCNP card [6]:

```
pikmt   92234 1 18001 1
        92235 1 18001 1
        92236 1 18001 1
        92238 1 18001 1
```

With the above card only prompt gammas coming from fission reactions are produced and tracked. In criticality mode, MCNP6.2 does not model the production of delayed gammas from fission reactions. Consequently, the delayed gamma energy is assumed to be equal to 6.33 MeV/fission (the U-235 value) and the delayed gamma spatial distribution is assumed to follow that of prompt gammas, as given by the $F6p_{prompt}$ tally of the second MCNP simulation. Finally, the power (in Watt units) deposited in a (U-235) fuel cell volume can be calculated by Eq. (1).

$$\begin{aligned} &power = \\ &= \left(\nu \frac{F6n}{k_{eff}} + \nu \frac{F6p}{k_{eff}} + 6.5 \frac{F7n}{\sum_{fuel} F7n} + 6.33 \frac{F6p_{prompt}}{\sum_{all} F6p_{prompt}}\right) \frac{P}{Q} = \\ &= neutrons\ \ and\ fission\ products\ kinetic\ energy \\ &+ prompt\ gammas\ energy + beta\ decay\ energy \\ &+ delayed\ gammas\ energy \end{aligned} \tag{1}$$

In the above equation, ν is the number of fission neutrons (2.438), P is the system power (e.g., 3 MW for the Transformational Challenge Reactor [7]), the Σ_{fuel} and Σ_{all} are summatories over the fuel cells and all cells, respectively, and Q is the fuel Q-value (in MeV units). For U-235, the latter can be calculated by Eq. (2).

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$$Q = \nu \frac{\sum_{all} F6n}{k_{eff}} + \nu \frac{\sum_{all} F6p}{k_{eff}} + 6.5 + 6.33 =$$

$$= 172.41 + 17.41 + 6.5 + 6.33 = 202.65\ MeV \qquad (2)$$

All the tallies used in the MCNP simulations are integrated over the cell volumes using the *sd* card with all entries set to one. In Equation 1, the third addend on the right side is equal to zero if the cell contains no fuel. The beta decay energy is confined in the fuel cells because fission products travel less than 10 μm. Consequently, the power deposition in a cell that does not contain any fuel has been calculated by Eq. (3).

$$power = \left(\nu \frac{F6n}{k_{eff}} + \nu \frac{F6p}{k_{eff}} + 6.33 \frac{F6p_{prompt}}{\sum_{all} F6p_{prompt}}\right)\frac{P}{Q} \qquad (3)$$

SERPENT CALCULATION METHODOLOGY

The Serpent most accurate methodology [8] to calculate the energy deposition assumes that the energy deposited per fission reaction *f* for (fissioned) nuclide *i* ($E_{i,f}$) is given by Eq. 4.

$$E_{i,f} = \overline{KE}_i^{FP} + E_i^{\beta} \qquad (4)$$

In Eq. 4, the first term on the right hand side $\overline{KE}_i^{FP}$ is the average (prompt) kinetic energy of fission products and the second one E_i^{β} is the energy of delayed betas for nuclide *i*. The neutron and prompt gamma heating for reactions other than fission is calculated using KERMA factors. More precisely, the energy deposited per non-fission reaction *x* for nuclide *i* ($E_{i,j}$) is given by Eq. 5.

$$E_{i,x} = \rho_i k_{i,x}(E)\Phi(E) \qquad (5)$$

In Eq. 5, ρ_i is the atomic density of nuclide i, $k_{i,x}(E)$ is the KERMA factor for non-fission reaction *x* and nuclide *i* at incident neutron/prompt photon energy *E*, and $\Phi(E)$ is the scalar neutron/prompt photon flux for neutron/prompt photon energy *E*. With the direct method, NJOY calculates the KERMA factor $k_{i,x}(E)$ according to Eq. (6).

$$k_{i,x}(E) = \sum_m \overline{KE}_{i,x}^m \sigma_{i,x}(E) \qquad (6)$$

In Eq. 6, $\overline{KE}_{i,x}^m$ is the average kinetic energy of the *m* secondary particle born in the (*i*,*x*) reaction, $\sigma_{i,x}(E)$ is the microscopic cross section of the (*i*,*x*) reaction at incident neutron/prompt photon energy *E*, and the summatory [8] is carried out over all charged products of the (*i*,*x*) reaction including the recoil nucleus *i*. Consequently, NJOY computes the KERMA factor $k_{i,x}(E)$ according to Eq. 7.

$$k_{i,x}(E) = \left(E + Q_{i,x} - \overline{KE}_{i,x}^n - \overline{KE}_{i,x}^{pp}\right)\sigma_{i,x}(E) \qquad (7)$$

In Eq. 7, *E* is the incident neutron/prompt photon energy, $Q_{i,x}$ is the mass difference Q-value for target nucleus *i* and reaction *x*, $\overline{KE}_{i,x}^n$ is the average kinetic energy of secondary neutrons for target nucleus *i* and reaction *x*, and $\overline{KE}_{i,x}^{pp}$ is the average kinetic energy of secondary (prompt) photons for target nucleus *i* and reaction *x*. In summary, Serpent uses Eq. 5 for calculating the energy deposition from a non-fission reaction *x* and Eq. 4 for calculating the energy deposition from a fission reaction *f*. In Serpent, the energy deposited by delayed gammas (which is not included in Eqs. 4 and 5) is added to the energy deposited by prompt gammas using the scaling factor *f* defined in Eq. 8.

$$f = \frac{\bar{E}_{i,f}^{dp} + \bar{E}_{i,f}^{pp}}{\bar{E}_{i,f}^{pp}} \qquad (8)$$

In Eq. 8, $\bar{E}_{i,f}^{dp}$ and $\bar{E}_{i,f}^{np}$ are the delayed and prompt gamma energy released per fission reaction for nuclide *i*, respectively. These data can be retrieved in the MT458 section of ENDF nuclear data libraries [8].

TCR ANALYSES

The MCNP model of the TCR created at ORNL has been automatically converted to a Serpent model by a Python script developed at ANL. The Python script ensures that all geometry and materials specifications are the same in both Monte Carlo codes inputs. Serpent version 2.1.32 and MCNP version 6.2 have been used with the ENDF/B-VIII.0 and ENDF/B-VII.1. Only the ENDF/B-VIII.0 nuclear data library contains S(α,β) data for hydrogen and yttrium bound in yttrium hydride. Serpent has the capability to read and use the ACE files shipped with MCNP. When both Monte Carlo code use the same ACE files based on the ENDF/B-VIII.0 nuclear data library (as shipped with MCNP version 6.2), the effective multiplication factor k_{eff} calculated by Serpent and MCNP is 1.03612±2E-5 and 1.03632±5E-5, respectively.

As discussed in the previous Section, the calculation of the energy deposition by Serpent requires enhanced ACE files with additional data. These enhanced ACE files have been provided by the Serpent development team for the ENDF/B-VII.1 nuclear data library, which does not have any S(α,β) data for hydrogen and yttrium bound in yttrium hydride. Consequently, the Serpent simulation calculating the energy deposition is based on the ENDF/B-VII.1 enhanced ACE files from Serpent development team and the S(α,β) data from the ENDF/B-VIII.0 library shipped with MCNP version 6.2. Similarly, the MCNP simulation calculating the energy deposition is based on the ENDF/B-VII.1 ACE files and the S(α,β) data from the ENDF/B-VIII.0 library, with all data coming from the files shipped with MCNP version 6.2.

Figure 1 shows the total energy deposition, including both neutron and gamma contributions, calculated by Serpent in the first fuel layer (located at the bottom of the core) and the fourth fuel layer (located in the middle of the core). The fuel zone of the core is segmented in eight axial layers. Obviously, the energy deposition peaks at the center of the core and drops at the central hexagon. The latter does not contain any fuel since it allocates the channel for the central safety rod. The relative difference between Serpent and MCNP results is shown in Fig. 2 and is generally below 0.5 and 1% for neutrons and photons in the fuel zone (blue hexagons in Fig. 2). In other zones (non-blue hexagons in Fig. 2), this difference increases up to a few percent.

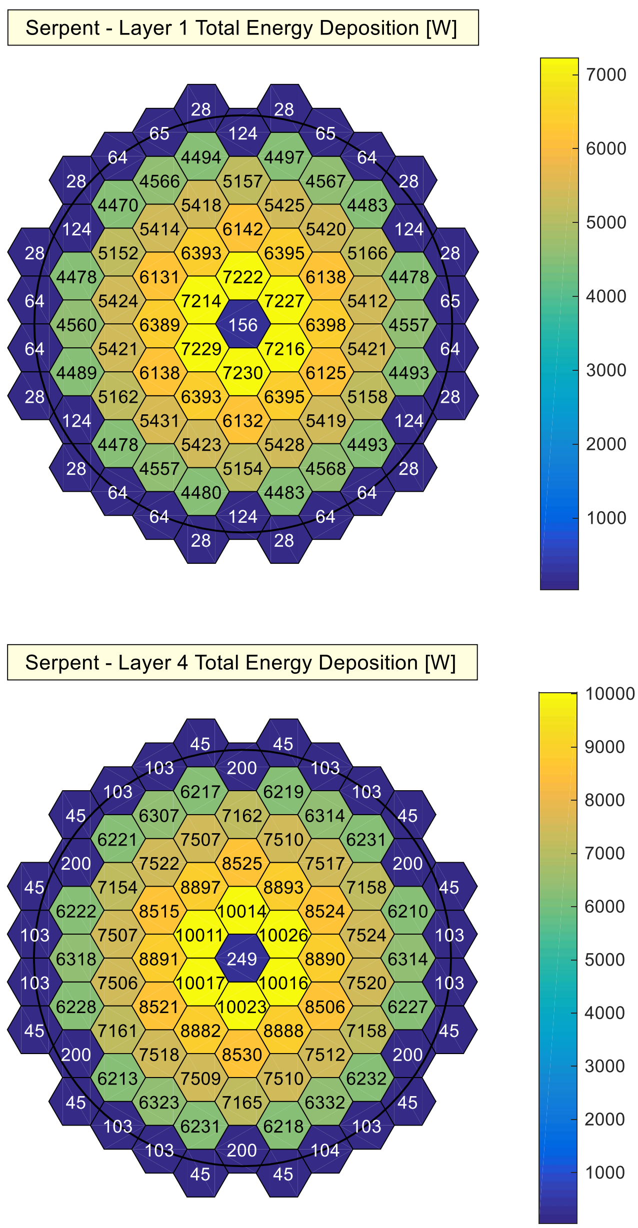

Fig. 1. Total energy deposition calculated by Serpent in the first (top plot) and fourth (bottom plot) fuel layers.

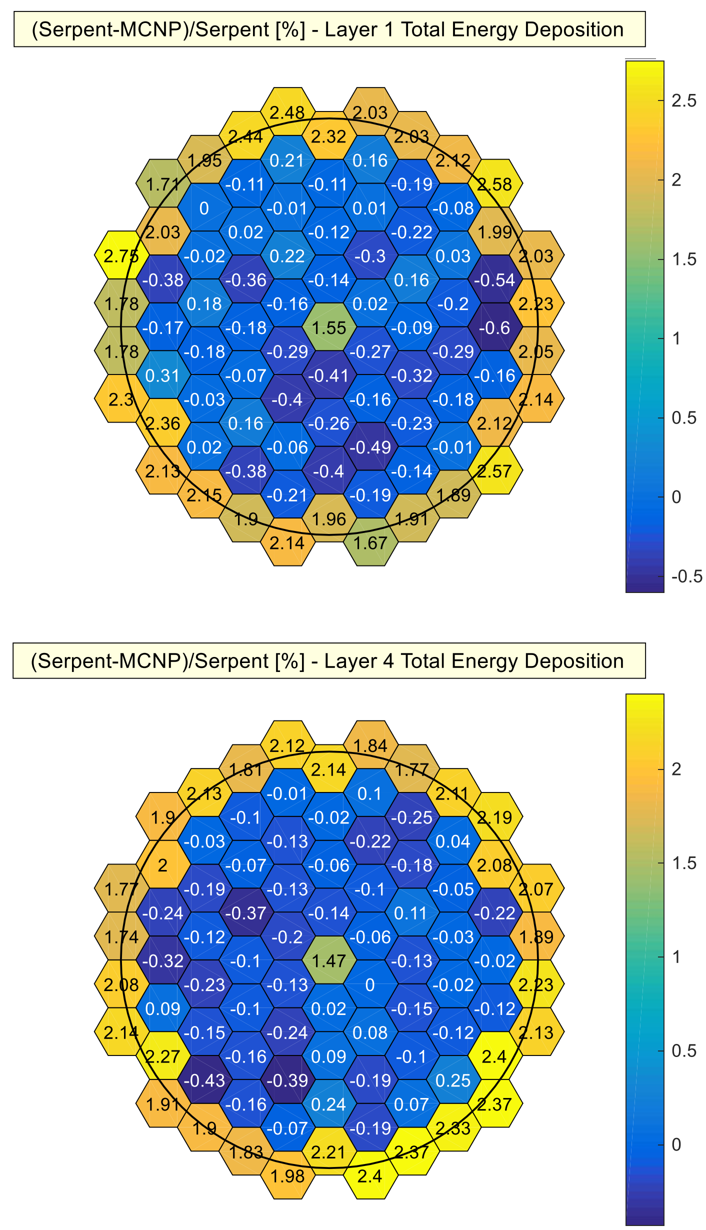

Fig. 2. Relative difference between Serpent and MCNP total energy deposition in the first (top plot) and fourth (bottom plot) fuel layers.

CONCLUSIONS

The TCR design effort leverages high-fidelity reactor physics tools and thermofluidic and thermomechanical multiphysics simulations for design and analysis. Within this context, the calculation of the energy deposition is of paramount importance because it strongly impacts thermal-fluid dynamics and structural mechanics analyses. This work shows that independent computational models based on two different Monte Carlo codes, Serpent and MCNP, provide very similar results (within 2% relative error). The Serpent calculation is based on KERMA factors and requires a single simulation and a single tally card, whereas the MCNP simulation is based on the fission Q-value and requires two simulations and four tally cards. Both codes assume that delayed gammas have the spatial distribution of prompt gammas.

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