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Reaction rate tally and depletion calculation with on-the-fly temperature treatment

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A B S T R A C T

Monte Carlo method can provide high fidelity neutronic analyses of different types of nuclear reactors, because of its advantages of the flexible geometry modeling and the use of continuous-energy nuclear cross sections. MC codes can also couple with depletion solver and thermal-hydraulics codes simultaneously for the "transport-burnup-thermal-hydraulics" coupled calculations. In this paper, the target motion sampling (TMS) method was developed in RMC code to consider the Doppler broadening effect in resolved resonance energy region, and the on-the-fly interpolation of thermal scattering data was developed to consider the thermal scattering and bound effect in the thermal energy region. Moreover, TMS method was applied to reaction rate tally and depletion calculation for power generation feedback and nuclide density evolutions. This is the first time that a Monte Carlo code is developed for on-the-fly temperature treatment in MC depletion calculations. The results show that TMS method and on-the-fly interpolation of thermal scattering have high efficiency and accuracy in the cases of PWR assembly calculation. With TMS method, the reaction rate can be tallied with temperature feedback. Temperature feedback in each burnup step can also be considered, allowing for the high fidelity "transport-burnup-thermal-hydraulics" coupled calculation.

1. Introduction

Monte Carlo (MC) method can provide high fidelity neutronic analyses of different nuclear reactors, owing to its advantages of the flexible geometry modeling and the use of continuous-energy nuclear cross sections (XS). MC codes have coupled with different solvers for multi-physics calculations. In order to perform burnup calculations, MC codes are externally or internally coupled with a point depletion solver to figure out the nuclide densities in fuel during the depletion. It can also be coupled with thermal-hydraulics (TH) codes to obtain thermal–hydraulic feedback (Liu et al., 2015). When the burnup and TH feedbacks were taken into account simultaneously, it is known as "transport-burnup-thermal-hydraulics" multi-physics coupling, which is very important for realistic reactors simulations and benchmarks calculations such as MIT BEAVRS benchmark (Horelik and Herman, 2012).

From thermal reactors such as PWR and HTGR, two main temperature effects should be considered. First is the effect of thermal motion from target nucleus in resolved resonance energy, which is known as Doppler effect. Second is the thermal scattering and bound effect in thermal energy.

The traditional approach of pre-generated cross sections (Yu et al., 2015) has difficulty of memory footprint for detailed temperature modeling in multi-physics calculations. Recently, on-the-fly (OTF) technique have been proposed in order to reduce the memory usage for both resolved resonance energy (Cullen and Weisbin, 1976; Becker et al., 2009; Yesilyurt et al., 2012; Yang et al., 2015; Forget et al., 2014) and thermal energy (Pavlou and Ji, 2014). For resolved resonance energy, the target motion sampling (TMS) method (Viitanen and Leppänen, 2012) was considered as one of the most promising methods.

In this paper, the TMS method was developed in RMC code (Wang et al., 2015) based on the ray tracking for resolved resonance energy. The pre-generated technique was proposed and applied to accelerate the calculation of TMS method. For thermal energy, the on-the-fly interpolation of thermal scattering data was developed to consider the thermal scattering and bound effect.

Moreover, the reaction rate tally was developed in TMS method especially for power generation feedback. With reaction rate tally, the MC depletion calculation can also be developed to consider nuclides densities evolutions with temperature feedback. It should

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be noticed that it is the first attempt to applied on-the-fly temperature treatment to MC depletion calculation for Monte Carlo codes.

The results show that TMS method and on-the-fly interpolation of thermal scattering have high efficiency and accuracy in the cases of PWR assembly. With TMS method, the reaction rate tally can be tallied with temperature feedback. Temperature feedback in every burnup step can also be considered, so as to do the high fidelity "transport-burnup-thermal-hydraulics" coupling calculation.

The remainder of this paper is organized as follows. Section 2 introduces the methodology, including burnup capability of RMC, TMS method, on-the-fly interpolation of thermal scattering data, reaction rate tally and depletion calculation with on-the-fly temperature treatment. In Section 3, the developed TMS method with reaction rate tally and depletion calculation and on-the-fly interpolation of thermal scattering data were verified by cases of PWR and HTGR. Finally, the conclusions are presented in Section 4.

2. Computational method

2.1. Burnup capability of RMC

RMC is developed with an embedded depletion module aimed at performing burnup calculations of large-scale problems with high efficiency. Several measures have been taken to strengthen the burnup capabilities of RMC.

- A new depletion module called DEPTH is developed and implemented. The DEPTH module is able to handle detailed depletion chains containing thousands of isotopes at an extremely fast speed with accuracy owing to its advanced matrix exponential solvers including the rational approximation methods and the Laguerre polynomial approximation method. Numerical results of several depletion cases have shown that the DEPTH module is more accurate and efficient than the formerly embedded depletion module (She et al., 2013).
- The energy-bin method and the cell-mapping method are implemented to speed up the transport calculations with large numbers of nuclides and tally cells (She et al., 2013).
- Auto expansion of burnable cells and materials in lattice structure (She et al., 2013).
- The batch tally method and the parallelized depletion module have been utilized to better handle cases with massive amounts of burnup regions in parallel calculations (She et al., 2013).
- Data decomposition technologies of reducing memory requirements for large-scale parallel MC burnup calculations (She et al., 2014).

2.2. Target motion sampling (TMS)

TMS method is a new on-the-fly temperature treatment which takes the thermal motion of target nuclei into account explicitly to model arbitrary temperatures with only 0 K continuous-energy cross sections (Viitanen and Leppänen, 2012). TMS method can be separated in the following steps:

(1) Sample free flight distance l. ξ is a random number between 0 and 1. Σ_{maj} is the majorant cross sections. For ray tracking in RMC, Σ_{maj} is the temperature dependent majorant macroscopic cross sections of the material in which neutron locates.

$$l = -\frac{1}{\Sigma_{\mathrm{maj}}}\ln(\xi) \tag{1}$$

The temperature dependent majorant macroscopic cross sections of material is the sum of the temperature dependent majorant cross sections of nuclides $\Sigma_{\mathrm{maj,n}}$. $g(E,\ T_{\max},\ A_n)$ is the correction factor, and $T_{\max}$ is the maximum temperature of nuclide. A_n is the weight ratio of nuclide n to the neutron mass.

$$\Sigma_{\mathrm{maj,n}} = g(E, T_{\max}, A_n) \max_{E_\xi \in [(\sqrt{E}-\alpha)^2, (\sqrt{E}+\alpha)^2)} \Sigma^0_{tot,n}(E_\xi) \tag{2}$$

$$g(E,T,A_n) = \left(1 + \frac{1}{2\lambda_n(T)^2 E}\right)\mathrm{erf}(\lambda_n(T)\sqrt{E}) + \frac{e^{-\lambda_n(T)^2 E}}{\sqrt{\pi}\lambda_n(T)\sqrt{E}} \tag{3}$$

$$\alpha = \frac{4}{\lambda_n(T)}, \qquad \lambda_n(T) = \sqrt{\frac{A_n}{kT}} \tag{4}$$

(2) Sample collision nuclide

$$P_n = \frac{\Sigma_{\mathrm{maj,n}}(E)}{\Sigma_{\mathrm{maj}}(E)} = \frac{\Sigma_{\mathrm{maj,n}}(E)}{\sum_n \Sigma_{\mathrm{maj,n}}(E)} \tag{5}$$

(3) Sample target nuclide velocity from Maxwell–Boltzmann (MB) distribution $f_{MB}(V_t)$. V_t is the target nuclide velocity, v is the velocity of neutron, and v' is the relative velocity between target nuclide and neutron, corresponding to the relative energy E'. μ is the cosine of angle between the directions of target and neutron.

$$f(V_t,\mu) = \frac{v'}{2v} f_{MB}(V_t), \qquad v' = \sqrt{v^2 + V_t^2 - 2vV_t\mu} \tag{6}$$

(4) Rejection sampling. If Eq. (7) is met, the collision is accepted. Otherwise, the collision is rejected and the algorithm should return to step 1.

$$\xi < \frac{g_n(E,T,A_n)\Sigma^0_{tot,n}(E')}{\Sigma_{\mathrm{maj,n}}(E)} \tag{7}$$

$\Sigma^0_{tot,n}$ is total cross section of nuclide n at temperature $T = 0$ K.

(5) Sample reaction type. Here, r is a reaction type.

$$P_r = \frac{\Sigma^0_{r,n}(E')}{\Sigma^0_{tot,n}(E')} \tag{8}$$

More detailed explanations of TMS method can be referred to paper of Viitanen and Leppänen (2012).

2.3. Pre-calculated TMS

If the temperature dependent majorant cross sections of nuclides $\Sigma_{\mathrm{maj,n}}$ is calculated during the transport calculation as in Eq. (2), it will be will time consuming. The pre-generated technique was used to accelerate the calculation of majorant cross sections in TMS method. The procedure is illustrated as following:

(1) Before the transport calculation, the temperature dependent majorant cross sections are calculated for all the energy grids of each nuclides based on Eq. (2). Different from the original TMS method, the temperature dependent majorant cross sections are not calculated for the exact energy of neutrons, during the neutrons' flights, but pre-calculated for the energy grids of each nuclide in the library.
(2) During the transport calculation, if the majorant cross sections of nuclide n is needed, search the neutron energy E in the energy grids of this nuclide n, to find out the adjacent energy grids, i.e. $E_1 < E < E_2$.
(3) Compare the pre-generated $\Sigma_{\mathrm{maj,n}}(E_1)$ and $\Sigma_{\mathrm{maj,n}}(E_2)$, find out the larger one i.e. max $\{\Sigma_{\mathrm{maj,n}}(E_1), \Sigma_{\mathrm{maj,n}}(E_2)\}$.
(4) Finally, $\Sigma_{\mathrm{maj,n}}(E)$= max $\{\Sigma_{\mathrm{maj,n}}(E_1), \Sigma_{\mathrm{maj,n}}(E_2)\}$.