ON-THE-FLY INTERPOLATION OF CONTINUOUS TEMPERATURE-DEPENDENT THERMAL NEUTRON SCATTERING DATA IN RMC CODE

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ABSTRACT

Thermal neutron scattering data have an important influence on the high-fidelity neutronics calculation of thermal reactors. Due to the limited storage capabilities of computers, a discrete ACE representation of the secondary neutron energy and angular distribution has been used for Monte Carlo calculation since the early 1980s. The use of this discrete representation does not produce noticeable effects in the integral calculations such as keff eigenvalues, but can produce noticeable deficiencies for differential calculations. A new continuous representation of the thermal neutron scattering data was created in 2006, but was not widely known. Recently, the continuous representation of the thermal neutron scattering ACE data based on ENDF/B-VIII.0 library was officially released and was available for all users. The new representation shows great difference compared with the discrete one. In order to utilize the more physical and rigorous representation data for high fidelity neutronic-thermohydraulic coupling calculation, the on-the-fly treatment capability was proposed and implemented in RMC code. The two-dimensional linear-linear interpolation method was used to calculate the inelastic scattering cross sections and the secondary neutron energies and angles. The on-the-fly treatment capability was tested by a pressurized water reactor assembly. Results show that the on-the-fly treatment capability has high accuracy, and can be used to consider the temperature feedback in the neutronic-thermohydraulic coupling calculations. However, the efficiency of the on-the-fly treatment still need to be improved in the near future.

KEYWORDS: interpolation, continuous thermal neutron scattering data, on-the-fly, RMC

1. INTRODUCTION

Thermal neutron scattering data have an important influence on the high-fidelity neutronics calculation of thermal reactors. Since the energy of the thermal neutrons is very low (generally lower than 10eV), neutron scattering processes are easily affected by the chemical binding of the target to other nuclides in a material or crystalline structure effects in the interaction with target materials. Meanwhile, neutron scattering events can occur resulting in a gain or loss in energy during the scattering process. All these effects complicate the description and processing of thermal scattering information. Therefore, large amount of computer memory is need to store all the detailed thermal neutron scattering data. A discrete ACE representation of the secondary neutron spectrum and angular distribution processed by NJOY [1]

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has been used for Monte Carlo calculation since the early 1980s due to the limited storage capabilities of computers [2]. The use of the discrete representation does not produce noticeable effects in integral calculations such as keff eigenvalues [3], but can produce unphysical phenomena [2] and noticeable deficiencies for differential calculations [4].

To overcome the inherent deficiencies of the discrete representation, a new continuous ACE representation for the thermal neutron scattering data was firstly created by Los Alamos National Laboratory in 2007 [5]. Continuous representation thermal neutron scattering data based on ENDF/B-VII.0 [6] and ENDF/B-VII.1 [7] data libraries were released and available online whereafter, but were not widely known. In the lasted ENDF/B-VIII.0 [8] data libraries, only the continuous ACE representation of the thermal neutron scattering data were provided by Los Alamos National Laboratory (LANL).

In order to utilize the more physical and rigorous representation thermal neutron scattering data for high fidelity neutronics calculations, the continuous thermal neutron scattering data processing capability in Reactor Monte Carlo code RMC [9] has been developed and was introduced in our previous work[10]. In this paper, the on-the-fly treatment capability for the continuous representation thermal neutron scattering data was developed to consider the temperature feedback effect in the neutronic-thermohydraulic coupling calculations. The second part of this paper gives a brief introduction to the continuous thermal neutron scattering data, the third part presents the detailed interpolation method for the on-the-fly treatment capability, the test cases and results are given in the fourth part, and a conclusion was drawn in the final part.

2. CONTINUOUS THERMAL NEUTRON SCATTERING DATA

Currently, the continuous ACE representation was designed for both the elastic and the inelastic scattering. In order to generate the continuous representation thermal neutron scattering data, the *aceth* module in NJOY program has been modified to convert the secondary energy distributions from *thermr* into probability density functions (PDFs) and cumulative density functions (CDFs) form, PDFs and CDFs are packed into the big inelastic array of the ACE format thermal scattering data. If the users want to obtain the continuous representation ACE data, the weighting option (iwt flag) in card 9 of the ACER module in the NJOY input file should be set to 2 (tabulated). The memory consumption for the continuous ACE representation thermal neutron scattering data is about 10 times larger than the traditional discrete one.

The continuous representation for the inelastic scattering data contains a table of incident energies, a table of inelastic cross sections, a table of pointers to the start of each distribution, a table of the number of points in each distribution, and the secondary energy and angle distributions. Two extra data blocks as well as PDFs/CDFs for the secondary energy distributions are added to the continuous representation compared to the traditional discrete one. A detailed introduction to the format of the continuous representation for the inelastic thermal scattering data can refer to our previous work [10].

3. ON-THE-FLY TREATMENT CAPABILITY

Since the inelastic scattering exists in all the thermal materials and plays a key role in the processing of thermal scattering, the present on-the-fly treatment capability mainly focus on the inelastic scattering. The linear-linear interpolation strategy was adopted to calculate the scattering cross sections and the secondary energies and angles. It should be emphasized that the number of grids for the incident energy and secondary energy changes differently with the increase of temperature, the corresponding processing methods were therefore developed for the inelastic scattering cross sections and the secondary energies in this paper.

3.1. On-the-fly treatment of cross sections

For the continuous representation inelastic scattering data, the number of the incident energy grids remains unchanged with the increase of temperature. Therefore, the general two-dimensional linear-linear interpolation method was adopted to calculate the cross sections at target temperature and target energy as shown in Fig 1. E_1 and E_2 are the incident neutron energy grids correspond to the target energy E_t. T_1 and T_2 are the temperature grids correspond to the target temperature T_t. The inelastic scattering cross sections at target energy E_t is calculated at different temperatures firstly, and then the temperature interpolation is performed to calculate the cross section at target temperature T_t.
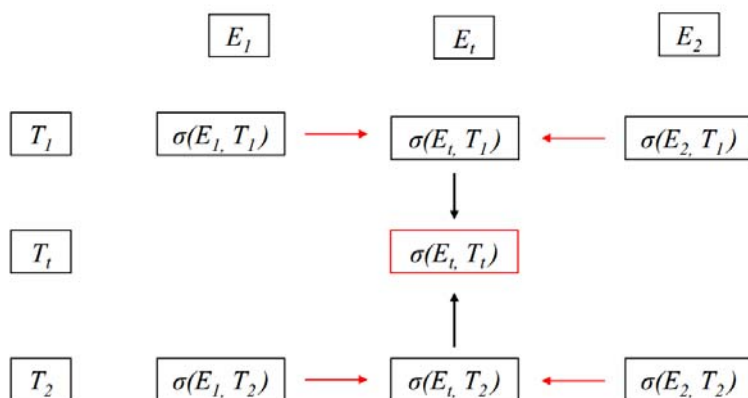

Figure 1. Two-dimensional linear-linear interpolation for the inelastic scattering cross section

3.2. On-the-fly treatment of secondary energies and angles

The number of the secondary energy points correspond to incident neutron energies are various from each other at different temperatures for the continuous representation inelastic scattering data. We take light water as an example, the number of the secondary energies correspond to the different incident neutron energies is shown in Fig. 2, and no regular changes are found.
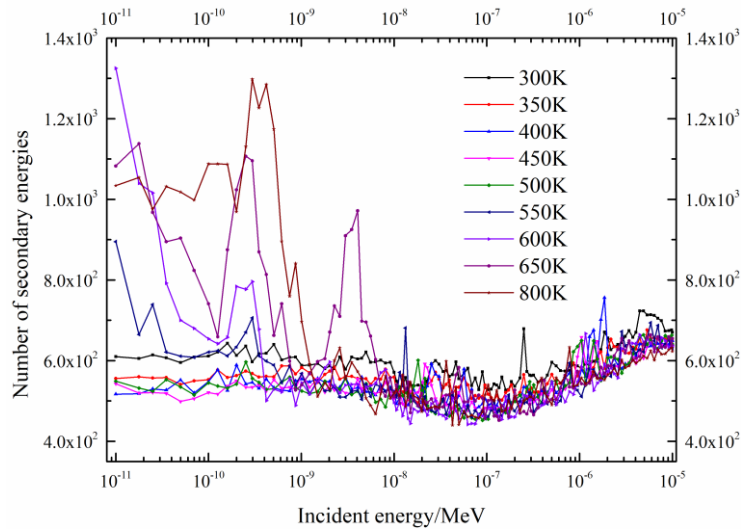
Figure 2. The number of secondary energies corresponding to incident energies for light water inelastic scattering

Since the secondary energy grids change with the increase of temperature, a treatment method similar to that of the inelastic scattering cross section was adopted. Once the temperature grids for the target temperature is determined, the secondary neutron energy corresponding to the determined incident energy is calculate for the temperature grids using the method introduced in our previous work [10]. The secondary neutron energies and angles are then calculate using the temperature interpolation method. Detailed calculation method is presented as shown below.

First, find the closest temperature grids T_1 and T_2 for the interpolation of the target temperature T_t.

Second, for a given incident neutron energy E_{in}, search the corresponding location of the energy in the energy tables at temperature T_1 and T_2, and calculate the energy fraction r_i, where i = 1, 2, and correspond to T_1 and T_2. $E_{i,j}$ and $E_{i,j+1}$ are the energy grids in the incident energy table.

$$E_{i,j} < E_{in} < E_{i,j+1} \tag{1}$$

$$E_{in} = E_{i,j} + r_i (E_{i,j+1} - E_{i,j}) \tag{2}$$

Third, chose the closest energy as the "incident energy", if $r_i > 0.5$, $E_{i,j}$ is chosen as the "incident energy", otherwise, $E_{i,j+1}$ is chosen as the "incident energy".

Fourth, sample random number ξ_1, search the CDFs to determine the outgoing energy grid. $c_{i,l,k}$ and $c_{i,l,k+1}$ are the CDFs corresponding to the "incident energy". It should be emphasized that the same random number must be used for temperature T_1 and T_2.

$$c_{i,l,k} < \xi_1 < c_{i,l,k+1} \tag{3}$$

Fifth, calculate the outgoing energy E_i' and the interpolation fraction fr_i for the outgoing angle. $E_{i,l,k}$ and $E_{i,l,k+1}$ are the sampled outgoing energy grids corresponding to ξ_1. $p_{i,l,k}$ and $p_{i,l,k+1}$ are the PDFs .

$$E_i^{'} = E_{i,l,k} + \frac{\left|\sqrt{p_{i,l,k}^2 + 2\left(\xi_1 - c_{i,l,k}\right)\dfrac{p_{i,l,k+1} - p_{i,l,k}}{E_{i,l,k+1} - E_{i,l,k}}} - p_{i,l,k}\right|}{\dfrac{p_{i,l,k+1} - p_{i,l,k}}{E_{i,l,k+1} - E_{i,l,k}}} \tag{4}$$

$$fr_i = \frac{E_i^{'} - E_{i,l,k}}{E_{i,l,k+1} - E_{i,l,k}} \tag{5}$$

Sixth, sample the random number ξ_2, and search the location of the outgoing angle grid. *NIL* is the inelastic dimensional parameter.

$$Loc = \text{int}\left[\left(NIL - 1\right) * \xi_2\right] \tag{6}$$

Seventh, project the outgoing energy up or down, and calculate the final secondary energy. The down projection scheme is given in Eq. (7). The up projection share a similar format to that of the down projection, and the subscript needs to be adjusted to i + 1.

$$E_i^{out} = \begin{cases} E_i^{'} \dfrac{2E_{in} - E_{i,j}}{E_{i,j}}, E_i^{'} > 0.5E_{i,j} \\ E_i^{'} + E_{in} - E_{i,j}, E_i^{'} \leq 0.5E_{i,j} \end{cases} \tag{7}$$

Eighth, the linear-linear interpolation method is used to calculate the secondary neutron energy at the target temperature.

$$E_t^{out} = E_1^{out} + \frac{T_t - T_1}{T_2 - T_1}\left(E_2^{out} - E_1^{out}\right) \tag{8}$$

Ninth, sample a random number ξ_3, and calculate the outgoing angle μ_i^{out}, $\mu_{i,l,k,Loc}$ is the outgoing angle grid corresponding to the outgoing energy. The detailed calculation of d is complicate and can refer to our previous work [10].

$$\mu_i^{out} = \mu_{i,l,k,j} + fr_i * (\mu_{i,l,k+1,Loc} - \mu_{i,l,k,Loc}) + d * (2\xi_3 - 1) \tag{9}$$

Finally, the linear-linear interpolation method is used to calculate the secondary angle at the target temperature.

$$\mu_t^{out} = \mu_1^{out} + \frac{T_t - T_1}{T_2 - T_1}\left(\mu_2^{out} - \mu_1^{out}\right) \tag{10}$$

4.   RESULTS AND ANALYSES

A traditional 17× 17 pressurized water reactor (PWR) assembly is used to test the accuracy and the efficiency of the on-the-fly interpolation strategy, the sketch of the assembly is shown in Fig.3. The assembly has three materials including fuel (^{235}U, ^{238}U, ^{16}O), gas gap (^{16}O) and light water (^{1}H, ^{16}O). The continuous representation thermal neutron scattering data generated by Los Alamos National Laboratory [11] were downloaded and used to consider the thermal scattering effect. And the ENDF/B-VIII.0 based neutron ACE files were generated by using NJOY2016 [12]. The temperature of the light water is set to 500K, while the fuel and the gas gap are at room temperature.

Four cases adopting the thermal neutron scattering ACE files at different temperatures were performed:

(1) accurate light water S(α,β) at 500K;

(2) on-the-fly treatment using S(α,β) at both 450K and 550K;

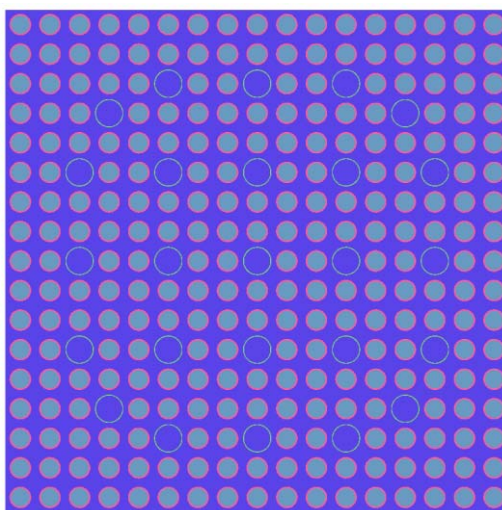(3) S(α,β) at 450K;

(4) S(α,β) at 550K;

Figure 3. The sketch of the PWR assembly

All calculations were performed using the develop branch of RMC with the on-the-fly treatment for continuous representation thermal scattering data capability implemented. Calculations were performed under the Ubuntu 18.04 system utilizing 6 cores (Intel® Core(TM) i7-7700 CPU @3.60GHz). All cases were run in the criticality mode, using 100 inactive cycles, 400 additional active cycles, and 100000 neutrons per cycle, resulting in the standard deviation lower than 10pcm for kinf eigenvalues. It should be noted that the calculation time given in Table I is single core calculation time.

Table I. Comparison of kinf eigenvalues and efficiency

	kinf	Std/pcm	Δk/pcm	Time/min
S(α,β) at 500K	1.415712	0.000075	/	18.6100
On-the-fly treatment	1.415631	0.000071	8.1	26.0620
S(α,β) at 450K	1.416268	0.000076	55.6	18.2872
S(α,β) at 550K	1.414673	0.000082	-103.9	18.5930

It can be observed from Table I that the kinf value based on the on-the-fly treatment agrees with that based on the accurate light water S(α,β) at 500K within 1 sigma. While, the kinf discrepancies are all larger than 50pcm for S(α,β) at 450K and 550K, which is huge compared with a standard deviation lower than 10pcm. For the time consumption, about 40% increase is found for the on-the-fly treatment compared with that of the accurate thermal scattering data.
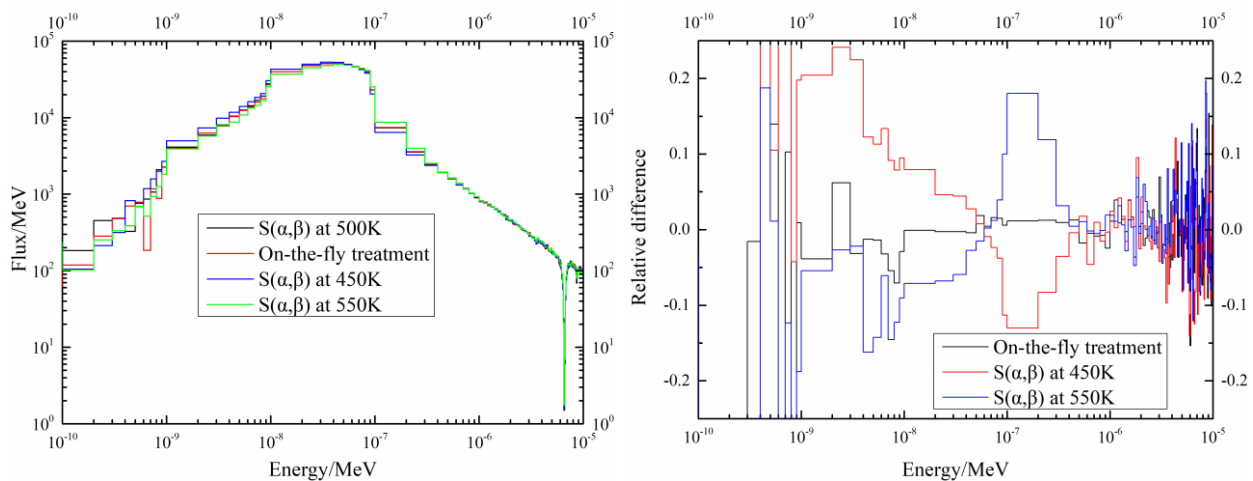

Figure 4. Comparison of energy spectra

Since the maximum energy for thermal treatment is 10eV for light water, the energy spectra below 10eV are compared for the four calculation cases in Fig.4. It is found from the spectra that the relative errors between the on-the-fly treatment and the accurate light water S(α,β) at 500K are within 5% for most energy regions, relatively large discrepancies appear at energy regions where the neutron flux are very low and the statistical uncertainties are very large.

The calculation results in Table I and Fig.4 demonstrate that the current on-the-fly treatment for the continuous thermal neutron scattering data capability has high accuracy, and can be used to consider the temperature feedback in the neutronic-thermohydraulic coupling calculations. However, the efficiency of the on-the-fly treatment still needs to be improved in the near future.

5. CONCLUSIONS

In this paper, the on-the-fly treatment capability for the continuous representation thermal neutron scattering data has been proposed and implemented in the RMC code. The two-dimensional linear-linear interpolation method was used to calculate the inelastic scattering cross sections and the secondary neutron energies and angles. The on-the-fly treatment capability was tested by a pressurized water reactor assembly. The integral kinf eigenvalues, the efficiency and the energy spectra of the on-the-fly treatment capacity were compared with these of the accurate thermal scattering data at target temperature.

Comparison results show that the on-the-fly treatment capability has high accuracy, and can be used to consider the temperature feedback in the high fidelity neutronic-thermohydraulic coupling calculations. However, the efficiency of the on-the-fly treatment still needs to be improved in the near future. Therefore, our future work mainly focus on the improvement of the efficiency and the implementation of the on-the-fly treatment for the elastic thermal scattering.

ACKNOWLEDGMENTS

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