The Improved Subgroup Method Considering Resonance Elastic Scattering Effect and Resonance Interference Effect

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1. Introduction

The subgroup method is widely used in nuclear reactor neutronic codes such as DeCART[1] and MPACT[2] for its geometrical flexibility and higher accuracy compared with the conventional equivalence theory. There are mainly two steps in the subgroup method: (1) The probability tables are generated from the resonance integral (RI) tables. (2) The subgroup fixed source problems are solved by mature multi-group transport solvers such as method of characteristics (MOC). The RI tables are typically obtained by solving slowing down problems over a range of background cross sections using hyper-fine energy group method or Monte Carlo (MC) method. This introduces two problems into the subgroup method: ignorance of resonance elastic scattering effect and resonance interference effect.

In the hyper-fine energy group method, the asymptotic scattering kernel is applied to obtain the scattering source, which ignores the up-scattering of neutron in the epithermal energy range. In the MC method, the elastic scattering cross sections are assumed to be constant at zero temperatures in the free gas model, which is invalid for heavy nuclides that have resonance peaks. As a consequence, both the eigenvalue and the fuel temperature coefficient (FTC) are overestimated, which is the so-called resonance elastic scattering effect[3,4]. In this paper, to introduce the Doppler broadened scattering kernel into the multi-group deterministic method, the MC code OpenMC[5] modified via Doppler broadening rejection correction (DBRC)[6], which was proved to be able to consider both the elastic resonance and thermal agitation of target, is used to generate RI tables.

To generate the RI tables, the neutron slowing down equation was solved for infinite homogeneous problems mixed by a resonance nuclide and a background nuclide. The interference of the resonance peaks between different nuclides is ignored in the RI tables, which leads to the resonance interference effect. Conventionally, the background iteration scheme[7] is used to correct the effect. In this scheme, when performing resonance calculation of one resonance nuclide, all of other resonance nuclides are considered to be background nuclides with constant cross sections. Iteration is carried out to guarantee the convergence of background cross sections and self-shielding cross section. However, this scheme consumes much computation time and suffers from low accuracy. The conditional probability method proposed by Takeda[8] and the mutual resonance shielding model by Hébert[9] improve the accuracy of subgroup method to some extent. But these methods are still not applicable to problems of multiple resonance nuclides. Another approach that promising to address the resonance interference effect is the resonance interference factor (RIF) scheme[10]. RIFs can be tabulated or calculated on-the-fly[11,12]. The tabulated approach is time-saving but not applicable to problems with more than two resonance nuclides, while the on-the-fly approach consumes much more computation time due to solution of hyper-fine energy group or continuous energy slowing down equations on-the-fly. Therefore, this paper improves the conventional RIF scheme and proposes a new scheme named fast RIF to treat the resonance interference effect.

2. Theory

2.1 Subgroup method

The subgroups are defined according to the magnitude of the cross sections. The energy of a subgroup is

$$\Delta E_{g,i} \in \left\{ E \mid \sigma_{g,i} < \sigma(E) \le \sigma_{g,i+1} \right\} \tag{1}$$

where

g=group index and

i=subgroup index.

For each subgroup, the subgroup cross sections and the subgroup probabilities, which constitute the probability tables, are defined as

$$\sigma_{x,g,i} = \frac{\int_{\Delta E_{g,i}} \sigma_x(E)\phi(E)dE}{\int_{\Delta E_{g,i}} \phi(E)dE} \tag{2}$$

$$p_{g,i} = \frac{\Delta E_{g,i}}{\Delta E_g} \tag{3}$$

where

x=the type of the cross sections.

Integrating the continuous energy Boltzmann equation on a subgroup yields the subgroup fixed source problem (SFSP)

$$\begin{aligned} &\Omega\nabla\phi_{g,i}(\vec{r},\Omega) + \Sigma_{t,g,i}(\vec{r})\phi_{g,i}(\vec{r},\Omega) = \\ &Q_{s,g,i}(\vec{r},\Omega) + Q_{f,g,i}(\vec{r},\Omega) \end{aligned} \tag{4}$$

where

$\phi_{g,i}$ =the subgroup flux,

$Q_{s,g,i}$ =the subgroup scattering source and

$Q_{f,g,i}$ =the subgroup fission source.

Eq.(4) is solved by multi-group transport solver MMOC[13]. After obtaining the subgroup flux, the effective self-shielding cross sections can be obtained

$$\sigma_{x,g}^{eff}(r)=\frac{\int_{4\pi}\sum_i \sigma_{x,g,i}(r)\phi_{g,i}(r,\Omega)d\Omega}{\int_{4\pi}\sum_i \phi_{g,i}(r,\Omega)d\Omega} \tag{5}$$

2.2 Resonance elastic scattering correction

2.2.1 The asymptotic scattering kernel

Neutron slowing down equation of a homogeneous system can be written as

$$\sum_k \Sigma_{t,k}(E)\phi(E)= \sum_k \int_0^\infty \Sigma_{s,k}(E)\, f_k(E'\to E)\phi(E')dE' \tag{6}$$

where

k=nuclide index and

f_k =elastic scattering kernel.

In cross sections generation codes such as NJOY[14], the target is assumed to be at rest and the elastic scattering kernel can be written as

$$f_k(E'\to E)=\frac{1}{(1-\alpha_k)E'} \tag{7}$$

where

$\alpha_k=(A_k-1)^2/(A_k+1)^2$ and

A_k =ratio of the mass of the target to a neutron.

Eq.(7) is the asymptotic scattering kernel.

2.2.2 The conventional free gas model

The MC method usually employs the free gas model to consider the thermal agitation of the target at elastic collision[15]. Once the velocity of the target is sampled, the velocity of the out-coming neutron can be determined. The probability density function of the target velocity is

$$P(V,\mu|v_n)=\frac{\sigma_s(v_r,0)v_r P(V)}{2\sigma_s^{eff}(v_n,T)v_n} \tag{8}$$

where

V=the speed of the target,

μ =the cosine of the azimuth angle,

v_n =the speed of the neutron,

v_r =the relative speed,

T =temperature,

$P(V)$ =Maxwell-Boltzmann distribution,

$\sigma_s(v_r,0)$ =elastic scattering cross section at relative speed at zero temperature and

$\sigma_s^{\text{eff}}(v_n,T)$ =the effective elastic scattering cross section.

Assuming that $\sigma_s(v_r,0)$ doesn't fluctuate with energy, Eq.(8) can be written as

$$P(V,\mu|v_n)=C\left\{\frac{v_r}{v_n+V}\right\}\{P_1 f_1(V)+P_2 f_2(V)\} \tag{9}$$

where

$$C=\frac{\left(2+\sqrt{\pi}\beta v_n\right)\sigma_s(v_r,0)}{2\sigma_s^{\text{eff}}(v_n,T)\sqrt{\pi}\beta v_n},$$

$$P_1=\frac{1}{1+\frac{\sqrt{\pi}\beta v_n}{2}},$$

$$P_2=1-P_1,$$

$$f_1(V)=2\beta^4V^3e^{-\beta^2V^2},$$

$$f_2(V)=\frac{4\beta^3}{\sqrt{\pi}}V^2e^{-\beta^2V^2},$$

$$\beta=\sqrt{\frac{AM_n}{2kT}},$$

M_n =mass of a neutron and

k=Boltzmann constant.

2.2.3 The Doppler broadening rejection correction

In the DBRC method, the modified probability density function can be written as

$$P(V,\mu|v_n)= C'\left\{\frac{\sigma_s(v_r,0)}{\sigma_s^{\max}(v_\xi,0)}\right\}\left\{\frac{v_r}{v_n+V}\right\}\{P_1 f_1(V)+P_2 f_2(V)\} \tag{10}$$

where

$$C'=\frac{\left(2+\sqrt{\pi}\beta v_n\right)\sigma_s^{\max}(v_\xi,0)}{2\sigma_s^{\text{eff}}(v_n,T)\sqrt{\pi}\beta v_n},$$

$$v_\xi\in\left[v_n-\frac{4}{\sqrt{\alpha}},v_n+\frac{4}{\sqrt{\alpha}}\right],$$

$$\alpha=\frac{M_t}{2kT}$$ and

$\sigma_s^{\max}(v_\xi,0)$ =the maximum value of the elastic scattering cross sections within a range of the dimensionless speed of v_ξ.

2.3 Resonance interference effect correction

2.3.1 Background iteration scheme

The computation flow of the background iteration scheme is as follows

- Take resonance nuclide *k* as the present resonant isotope with all the others being assumed to be without resonance peaks. Calculate the macroscopic subgroup cross sections of the medium as follows

$$\Sigma_{x,g,i}=N_k\sigma_{x,k,g,i}+\sum_{k'\neq k}N_{k'}\sigma_{x,k',g} \tag{11}$$

- For nuclides without intrinsic resonance peaks, the microscopic cross sections $\sigma_{x,k',g}$ are directly read

from the multi-group nuclear data library. For resonant nuclides assumed to be without resonance peaks, the microscopic cross sections are updated iteratively by starting with a guess at the beginning. Perform subgroup resonance calculation for current nuclide.

- Repeat the above two steps for each of the resonance nuclides.
- Start another resonance nuclide sweep until a convergence of the self-shielding cross sections can be reached.

2.3.2 Fast resonance interference factor scheme

The calculation flow of fast RIF is as follows

- For each energy group, the dominant resonance nuclide is chosen according to the magnitude of $RS_{k,g} = N_k \mathrm{RI}_{t,k,g}^{\max} / \mathrm{RI}_{t,k,g}^{\min}$ where $\mathrm{RI}_{t,k,g}^{\max}$ and $\mathrm{RI}_{t,k,g}^{\min}$ are respectively the maximum and minimum total RI of group *g* in the RI table of isotope *k*. The quotient of these two represents the severity of the resonance in the microscopic scale, while the $RS_{k,g}$ represents the severity in the macroscopic scale.
- Perform subgroup resonance calculation for the dominant resonant nuclide, with all the other resonant nuclides are considered as background nuclides.
- The heterogeneous system is converted to an equivalent homogeneous system according to self-shielding cross section conservation of the dominant resonant nuclide. The equivalent macroscopic dilution cross section is given by

$$\Sigma_{0,g} = \sigma_{0,g} N_{\mathrm{dom}} - \sum_{k' \neq \mathrm{dom}} \sigma_{p,k'} N_{k'} \qquad (12)$$

where $\sigma_{0,g}$ is the equivalent microscopic dilution cross section. The subscript "dom" stands for the dominant resonant nuclide.

- The slowing down problem (SDP) of the constructed homogeneous system is solved with hyper-fine energy group method and the effective self-shielding cross sections of all the resonant nuclides are obtained.

3. Numerical results

The ACE format library used by OpenMC and multi-group library are generated by NJOY based on ENDF/B-Ⅶ.0, while the RI tables are generated by OpenMC. The Corrections are implemented on a subgroup method code SUGAR[16].

3.1 Verification of the Doppler broadened elastic scattering kernel

The Mosteller Doppler defect benchmark[17] is analyzed with both SUGAR and the modified OpenMC. The difference of eigenvalues for the UO_2 pin cell problems at HZP and HFP between the conventional scattering kernel and the Doppler broadened scattering kernel are given in Fig. 1 and Fig. 2. The Doppler broadened scattering kernel is implemented into MVP[18] with weight correction method (WCM), MCNP6[19] with DBRC and TRIPOLI[20] with both. It can be drawn that results provided by SUGAR are consistent with the other. For the UO_2 pin cell, the asymptotic scattering kernel overestimates the eigenvalues by 30 pcm to 140 pcm at HZP and 80 pcm to 230 pcm at HFP.

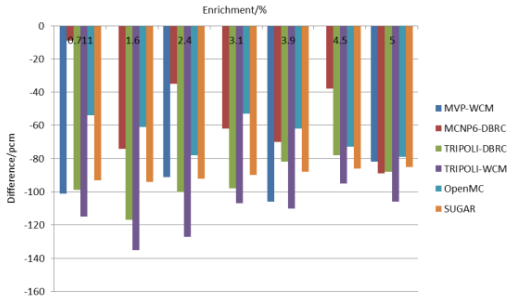

Fig. 1.Impact of resonance elastic scattering on k_∞ for UO_2 pin cell problems at HZP of Mosteller benchmark

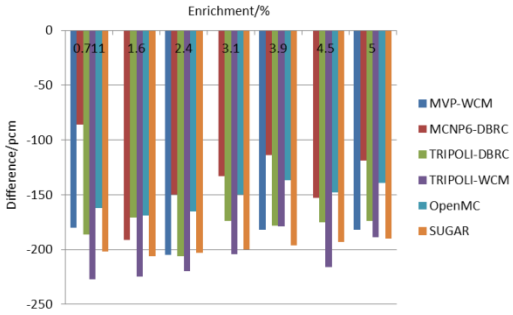

Fig. 2.Impact of resonance elastic scattering on k_∞ for UO_2 pin cell problems at HFP of Mosteller benchmark

3.2 Comparison of different resonance interference correction schemes

The Mosteller MOX benchmark problems at HZP are analyzed by different resonance interference correction schemes. Scheme 1 applies the background iteration scheme, while scheme 2 applies the fast RIF scheme. Both schemes use the subgroup probability tables considering resonance elastic scattering effect.

Table Ⅰ shows the error of k_∞ of different schemes. The reference k_∞ is calculated by OpenMC with DBRC method. It can be found that scheme 2 provide higher precision than scheme 1.

Table Ⅱ compares the number of SFSPs and SDPs to be solved by these two schemes and the time of the resonance calculation. The speed up of scheme 2 to scheme 1 is ~4.56.

Table Ⅰ. Comparison of k_∞ errors between background iteration scheme and fast RIF scheme

PuO_2 content / %	Error of k_∞ /%

	Scheme 1	Scheme 2
1	-0.17	-0.17
2	-0.20	-0.17
4	-0.23	-0.18
6	-0.26	-0.19
8	-0.28	-0.19

Table Ⅱ. Comparison of time for resonance calculation between background iteration scheme and fast RIF scheme

Scheme	SFSP/n	SDP/n	Time for resonance calculation/s
Scheme 1	564	0	108.03
Scheme 2	47	3	23.69

4. Conclusions

The subgroup method is improved in two aspects. Firstly, the resonance elastic scattering effect is considered. The Mosteller benchmark problems are analyzed with the modified OpenMC code and SUGAR code. The results shows that the Doppler broadened scattering kernel decreases k_∞ 30~140 pcm at HZP and 80~230 pcm in HFP for LWR pin cell problems.

Secondly, the fast RIF scheme is proposed to treat the resonance interference effect. It obtains higher precision than the background iteration scheme. Its speed up to the background iteration scheme is ~4.56 for MOX pin cell problems.

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