Temperature-Dependent Resonance Treatment in the Direct Resonance Integral Method

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1. Introduction

Resonance treatment is the most important part in the deterministic transport lattice calculation associated with the prediction accuracy. Mostly resonance transport calculations are performed for various problems involving the uniform temperature distribution in the fuel region. However, recently it is required to perform transport lattice calculations involving non-uniform temperature distribution, which include the whole core problems considering thermal feedback effect. New methods have been developed for the temperature-dependent resonance treatment when using the subgroup method.[1,2] The transport lattice code KARMA[3] developed at KAERI adopts two different methods for the resonance treatments which are the subgroup method and the direct resonance integral (RI) method[4]. In this study the temperature-dependent resonance treatment method in Ref. [2] has been implemented and tested for the KARMA subgroup method, and the similar method has been developed for the direct RI method in KARMA. The reference solutions were obtained by performing the Monte Carlo calculations by using MCNP[5] with the ENDF/B-VI R8 continuous cross sections.

2. Methods and Results

2.1 Fixed source resonance calculation

In a heterogeneous system, the self-shielded resonance cross sections are estimated from the self-shielded scalar fluxes obtained by the following fixed source transport equation.

$$\hat{\Omega}\cdot\nabla\psi_{g,m}+\sum_i(\Sigma^m_{i,a,g}+\lambda_{i,g}\Sigma^m_{i,p})\psi_{g,m}(\hat{\Omega})=\sum_i\lambda_{i,g}\Sigma^m_{i,p}\ , \quad (1)$$

where subscript *m* denotes a problem case with different absorption cross section levels at energy group *g*. In eq. (1), $\Sigma_{i,a,g}$ and $\Sigma_{i,p}$ denote macroscopic absorption and potential cross sections of nuclide *i*, respectively, and $\lambda_{i,g}$ intermediate resonance parameter. Eq. (1) can be used for both the subgroup method and the direct RI method without any modification.

Eq. (1) should be modified for the resonance transport calculations involving non-uniform temperature distribution in which the macroscopic absorption cross sections should include the temperature distribution as follows:

$$\begin{aligned}\Sigma^m_{i,a,g}&=N_i\sigma^m_{i,a,g}(T_{ave.})\frac{\sigma^m_{i,a,g}(T)}{\sigma^m_{i,a,g}(T_{ave.})}\ ,\\&=N_i\sigma^m_{i,a,g}(T_{ave.})\,f_{i,a,g}(T)\end{aligned} \quad (2)$$

where T and $T_{ave.}$ are local and volume-averaged temperatures, respectively.

While the function *f(T)* was approximated by using the subgroup weights in Ref. [1], the function was approximated by the following equation.

$$f_{i,a,g}(T)=\frac{R_{i,a,g}(T,\sigma_p)}{R_{i,a,g}(T_{ave.},\sigma_p)}\cdot\frac{\sigma_p-R_{i,a,g}(T_{ave.},\sigma_p)}{\sigma_p-R_{i,a,g}(T,\sigma_p)}\ , \quad (3)$$

where

$$\sigma_p=\frac{\sum_{j=all}N_j\lambda_{j,g}\sigma_{j,p}}{N_i}\ , \quad (4)$$

N_i is the particle number density of nuclide *i*, and $R_{i,a,g}$ resonance integral.

2.2 Resonance Interference and Resonance Integrals

Resonance interference in the subgroup method is considered as follows:

$$\sigma_{ia}=\frac{1}{N_i}\frac{\sum_n w_{ni}\frac{\Sigma_{ian}\Sigma_{ibn}}{\Sigma_{ian}+\Sigma_{ix}+\Sigma_{ibn}}}{1-\sum_{j=all}\sum_n w_{jn}\frac{\Sigma_{jan}+\Sigma_{jx}}{\Sigma_{jan}+\Sigma_{jx}+\Sigma_{jbn}}}\ , \quad (5)$$

where Σ_{jx} is a total summation of other resonant nuclides. Since Σ_{jx} depend on Σ_{ia}, iterations are required. The iteration procedure is as follows:

$$\Sigma^{(0)}_{ix}\rightarrow\Sigma^{(0)}_{ia}\rightarrow\Sigma^{(1)}_{ix}\rightarrow\Sigma^{(1)}_{ia}\rightarrow\Sigma^{(2)}_{ix}\rightarrow\Sigma^{(2)}_{ia}\rightarrow\ . \quad (6)$$

Resonance interference in the direct RI method is considered as follows:

$$\sigma_{ia}=R_{ia}(\sigma_{ibx})\frac{\Sigma_{ib}+\Sigma_{ix}+\Sigma_{ia}}{\Sigma_{ib}+\Sigma_{ix}}\ , \quad (7)$$

where

$$\sigma_{ibx}=\frac{\Sigma_{ib}+\Sigma_{ix}}{N_i}\ . \quad (8)$$

The iteration procedure is performed by eq. (6).

Resonance interference formulae of eqs. (3) and (5) cannot consider the real resonance interference exactly, which causes an error in estimating the self-shielded cross sections. Therefore, resonance integrals should be adjusted to conserve reaction rates by using the following equation.

$$\tilde{R}_{ag}(\sigma_{bg}) = \frac{\Delta\sigma_{ag} + \sigma_{ag}(\sigma_{bg})}{1 + (\Delta\sigma_{ag} + \sigma_{ag}(\sigma_{bg}))/\sigma_{bg}}. \quad (9)$$

2.3 Calculation and results

Table 1 provides the composition and geometry for the sample problems, and Table 2 shows the temperature distributions for fuel, cladding and moderator regions. The reference solutions were obtained by the MCNP calculations with the ENDF/B-VI R8 continuous cross sections. Calculations were performed by using 100,000 particle histories and 50 inactive and 250 active cycles. The KARMA calculations were performed for the same problems with the ENDF/B-VI R8 based 47- and 190-group cross sections. The subgroup and the direct RI methods were used for the resonance treatment with and without special treatment for the temperature distributions.

Table 3 provides a comparison of the multiplication factors between the MCNP and the KARMA calculations with various options. There are significant improvements for Cases 4 and 6 with the subgroup method which include the non-uniform temperature distribution. However, the KARMA results by the direct RI method show good consistency with the MCNP ones always regardless of the incorporation of the temperature dependent resonance treatment. Table 4 shows the Doppler temperature coefficients. While there are some improvements when using the subgroup method with the temperature dependent resonance treatment, the direct RI method can predict the accurate DTC always regardless of the temperature dependent resonance treatment.

Table 1. Geometry and composition data for fuel pin

Region	Material	Density (g/cm^3)	Radius (cm)	U^{235} w/o
Fuel	UO_2	10.20	0.4100	4.0
Cladding	$Zr^{nat.}$	6.55	0.4165	-
Moderator	H_2O	0.7116	1.2600*	-

*Pin pitch

Table 2. Temperature distributions (K)

Region		Case					
		1	2	3	4	5	6
Fuel	1	296	450	900	1300	1350	2150
	2	296	450	900	1200	1350	1950
	3	296	450	900	1100	1350	1750
	4	296	450	900	1000	1350	1550
	5	296	450	900	900	1350	1350
	6	296	450	900	800	1350	1150
	7	296	450	900	700	1350	950
	8	296	450	900	600	1350	750
	9	296	450	900	500	1350	550
	Ave.	296	450	900	900	1350	1350
Cladding		296	450	450	450	450	450
Moderator		296	450	450	450	450	450

Table 3. A comparison of the multiplication factor

M	Case	$T_{ave.}$	MCNP k_{eff}	Reactivity diff. (pcm)			
				47-g		190-g	
				old	new	old	new
SG	1	296	1.39706	69	69	97	97
	2	450	1.38642	103	103	117	117
	3	900	1.36789	160	160	138	138
	4	900	1.36907	-114	-8	-59	51
	5	1350	1.35426	192	192	166	166
	6	1350	1.35571	-303	-105	-218	-25
RI	1	296	1.39706	-74	-74	-11	-11
	2	450	1.38642	-54	-54	-1	-1
	3	900	1.36789	-3	-3	2	2
	4	900	1.36907	-16	-29	-17	-33
	5	1350	1.35426	14	14	25	25
	6	1350	1.35571	-32	-49	-58	-77

Table 4. A comparison of the Doppler temperature coefficient (pcm/K)

M	Case	MCNP	47g		190	
			old	new	old	new
SG	2-4	2.03	1.55	1.78	1.64	1.89
	2-6	1.82	1.36	1.58	1.44	1.66
	4-6	1.60	1.18	1.38	1.25	1.43
RI	2-4	2.03	2.12	2.09	2.00	1.96
	2-6	1.82	1.84	1.82	1.75	1.73
	4-6	1.60	1.56	1.55	1.51	1.50

3. Conclusion

The direct RI method can predict Doppler temperature coefficients accurately with or without any special temperature dependent resonance treatment. This method can be a god candidate for the temperature dependent resonance treatment in the whole core transport calculations considering a thermal hydraulic feedback effect.

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