Application of the Method of Characteristics to Slowing Down Calculation for an Explicit Geometrical Effect

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1. Introduction

The conventional resonance treatment in the transport lattice codes requires resonance integral tables in which resonance integrals are tabulated as a function of the background cross sections to be a measure of dilution. Typically self-shielded resonance cross sections in the resonance integral table are generated by performing slowing down calculations with point-wise cross sections defined on an ultra fine energy grid for 1-dimensional cylindrical pin cells. Collision probability, interface current (ICM) and discrete ordinate methods have been used for the 1-dimensional cylindrical slowing down calculations. These resonance integral tables are to be used in estimating the self-shielded resonance cross sections for the rectangular or hexagonal pin cells, which results in a reactivity difference due to the geometrical effect on the effective resonance cross sections. In order to improve this problem, the method of characteristics (MOC)^[1] has been applied to the slowing down calculations for 2-dimensional square pin cells. The geometrical effect on the reactivity has been quantitatively analyzed by using the Monte Carlo code MCNP^[2] and the transport lattice code KARMA^[3]. The method of characteristics has been implemented into the MERIT^[4] code developed at KAERI for slowing down calculations.

2. Methods and Results

2.1 Slowing down calculation

The typical energy range in a resonance nuclide for the resolved resonance is $0.5 \text{eV} \sim 10 \text{ keV}$ where no fission source and no inelstic scattering can be assumed. Slowing down equation can be used in obtaining the self-shielded cross sections with a potential scattering cross section (σ_p), a resonance scattering cross section ($\sigma_{rs}(u)$) and a resonance absorption cross section ($\sigma_{ra}(u)$). Slowing down equation for region *k* can be written as follows:

$$\hat{\Omega} \cdot \nabla \psi_k + \sum_i \Sigma_{i,i}^k(u) \psi_k(u, \hat{\Omega}) = \sum_i \int_{u-\Delta_i}^u \Sigma_{i,i}^k(u') \phi_k(u') \frac{\exp(u'-u)}{1-\alpha_i} du',$$
(1)

where

$$\begin{split} & \Sigma_{i,x} = N_i \sigma_{i,x}, \\ & \Sigma_{i,s}^k(u) = \Sigma_{i,p}^k + \Sigma_{i,rs}^k(u), \\ & \Sigma_{i,i}^k(u) = \Sigma_{i,s}^k(u) + \Sigma_{i,ru}^k(u), \\ & \alpha_i = (A_i - 1)^2 / (A_i + 1)^2, \\ & \Delta_i = -\ln(\alpha_i). \end{split}$$

Eq. (1) for a square pin cell is solved by MOC in this study.

2.2 Quantitative analysis for the geometrical and the boundary condition effects

The MCNP calculations were performed to see the geometrical and boundary condition effects on the multiplication factors for three problems with different boundary shapes and conditions. White (SW) and reflecting (SR) boundary conditions were used for the square pin cell problems, and only white boundary condition was used for the circular pin cell problem (CW).

Sensitivity calculations were performed for the typical fuel pins of the pressurized water reactor (PWR) for which circular and square pin configurations are shown in Figure 1 and geometry and composition data are shown in Table 1. In order to consider various dilutions three different configurations were used in which the second one is for the typical PWR pin, the first one for low dilution and the last one for high dilution. When performing the three different MCNP calculations, 190group scalar fluxes, microscopic absorption, fission and elastic scattering cross sections and the number of neutrons released per fission were tallied for ²³⁵U and ²³⁸U in each case. The 190 energy group structure is identical to that of HELIOS^[5]. The MCNP results could provide accurate self-shielded resonance cross sections. The geometrical and the boundary condition effects on the reactivity were analyzed quantitatively with the following two procedures.

Since self-shielding effect is dependent upon the geometrical shape and the boundary condition, the resultant multi-group resonance cross sections are different from each other. The microscopic cross sections of ²³⁵U and ²³⁸U edited from three MCNP outputs were used directly in the KARMA calculations in which square pin models with reflecting boundary conditions were used. The KARMA calculations were performed to see the

influence of the various effective resonance cross sections due to the boundary shapes and the boundary conditions upon the reactivity. In the second step the 190-group macroscopic cross sections were edited for each material region from the KARMA calculations with reflecting boundary condition for three cases defined on Table 1 and used for the 190-group MCNP calculations.

Table 2 provides the computational results for the continuous MCNP, the 190-group KARMA and the 190-group MCNP calculations for three difference cases. The results of the MCNP calculation with the continuous cross sections shows that the reactivity differences for the typical PWR pin (Case-B) are 222 pcm for SR vs. CW, 130 pcm for SR vs. SW and 92 pcm for SW vs. CW, respectively. It can be said that the geometrical effect on the reactivity is 92 pcm and the boundary condition effect is 130 pcm, respectively. The computational results of Case-A show much bigger reactivity differences compared to those of Case-B and Case-C. In other words, as dilution in the problem increases, the geometrical and the boundary condition effects on the reactivity decrease.



Fig. 1. Circular and square pin cells

Table 1	Geometry	v and	com	position

Region		Temp.(K)	Radius (pitch)(cm)	Density(g/cm ³)
Fuel (UO ₂)		700	0.4025	10.4
Clad (²⁷ A	l)	600	0.4759	2.7
Moderator (H ₂ O)	Α	600	0.7120 (1.2620)	0.13
	В		0.7120 (1.2620)	0.65
	С		1.2762 (2.2621)	0.65

Table 2 Effect of the geometrical boundary and the boundary condition on the multiplication factor

Case	Code	$\Delta \rho$ (pcm)			Effect
	Code	SR-CW	SR-SW	SW-CW	Effect
А	MCNP ^[a]	441	332	109	Overall
	KARMA ^[b]	156	133	23	Resonance
	MCNP-MG ^[c]	262	163	99	Geometry+B.C.
	Sum[b+c]	418	296	122	Overall
В	MCNP ^[a]	222	130	92	Overall
	KARMA ^[b]	100	50	50	Resonance
	MCNP-MG ^[c]	117	59	58	Geometry+B.C.
	Sum[b+c]	217	109	108	Overall
С	MCNP ^[a]	-18	-7	-12	Overall
	KARMA ^[b]	10	12	-2	Resonance
	MCNP-MG ^[c]	-39	3	-42	Geometry+B.C.
	Sum[b+c]	-29	15	-44	Overall

2.3 Explicit geometry consideration in slowing down calculation

Effective resonance cross sections were estimated by using MOC in slowing down calculations. Table 3 provides the analysis results. There were also significant improvements on the reactivity differences and the multigroup cross sections compared to the MERIT ICM calculations for all cases. However, there is still 111 pcm reactivity difference between the MCNP and the MERIT MOC calculations for Case-A. However, Case-A includes 80% void in moderator and is a severe condition which can be rarely happened in the reactor core operation.

Table 3 A comparison of the reactivity and maximum cross section differences

Case	Method	Δρ	Max. XS diff. (%)			
		(pcm)	σ_a^{u235}	$\nu \sigma_{f}^{u235}$	σ_a^{u238}	
А	ICM ^a	294	1.95	1.07	2.46	
	MOC ^b	111	1.29	0.73	1.37	
В	ICM ^a	216	1.44	1.07	3.90	
	MOC ^b	38	0.61	0.52	1.79	
С	ICM ^a	33	1.13	0.93	2.70	
	MOC ^b	5	0.86	0.72	1.96	

^a 3/1/1 subdivision and 1000000 energy groups

^b 2/8/0.02 ray option for polar/azimuthal/ray spacing, 8/1/4 subdivision and 1000000 energy groups

3. Conclusion

The computation results show that the reactivity differences and the discrepancies of the effective resonance cross sections due to the geometrical inconsistency and numerical method could be significantly improved by using the method of characteristics.

REFERENCES

[1] J.R. Askew, "The Current UK Position on Uranium-238 Resonance Capture. In: Seminar on ²³⁸U Resonance Capture Held at National Neutron Cross Section Center," Brookhaven National Laboratory Upton, New York, USA, March 18-20, 1975, BNL-NCS-50451 (ENDF-217) (1975)

[2] J. F. Breismeister, et al., "MCNP - A General Monte Carlo N-Particle Transport Code, Version 4B," LA-12625-M (2009)

[3] Kang-Seog Kim, et al., "Transport Lattice Code KARMA 1.1," Transactions of KNS Autumn Meeting, Gyeongju, Korea, Oct. 29-30, 2009.

[4] Kang-Seog Kim, et al., "Improvements on MERIT 1.1 and SUBDATA 1.1 and a New Procedure for Resonance Integral Adjustment," Transactions of KNS Autumn Meeting, Gyeongju, Korea, Oct. 29-30, 2009.

[5] R.J.J. Stamm'ler, et al., "HELIOS Methods," Studsvik Scandpower (2009)