Implementation of a Multigroup Cross-Section Generation Capability into McCARD

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1. Introduction

Monte Carlo (MC) particle transport codes [1,2] have been successfully used to precisely analyze various nuclear systems with the help of an increasing computing power. However their considerable computation time makes it impossible for the MC method to prevail over deterministic methods for a neutronics analysis like discrete ordinate transport codes or diffusion theory codes. On the other hand, the deterministic codes require reliable multigroup cross-sections which have been collapsed over an appropriate flux spectrum. Especially, macroscopic cross-sections in homogenized regions are needed for the few-group nodal diffusion calculations.

The purposes of this paper are to implement a multigroup cross-section generation capability into McCARD (Monte Carlo Code for Advanced Reactor Design and analysis) [2] and to compare its calculation results with commercial lattice codes. This work will enable the users to generate accurate multi-group cross-sections using a precise geometry model and continuous energy cross-section libraries.

2. Methods and Results

2.1 Fine Group Cross-Section Generation

The group-averaged microscopic cross-section for region m of volume V_m, isotope i, reaction x and energy group g, ΔE_g, is defined by

$$\sigma_{x,g}^{m,i} = \frac{\int_{V_m}\int_{\Delta E_g}\int_{4\pi}\sigma_x^i(E)\phi(\mathbf{r},E,\mathbf{\Omega})d\mathbf{\Omega}dEd\mathbf{r}}{\int_{V_m}\int_{\Delta E_g}\int_{4\pi}\phi(\mathbf{r},E,\mathbf{\Omega})d\mathbf{\Omega}dEd\mathbf{r}}, \quad (1)$$

where $\phi(\mathbf{r},E,\mathbf{\Omega})$ denotes the angular flux.

The numerator and denominator in Eq. (1) indicate a microscopic reaction rate and an average flux, respectively, in region m and energy group g. And using the MC track length estimators, they can be estimated by

$$\int_{V_m}\int_{\Delta E_g}\int_{4\pi}\sigma_x^i(E)\phi(\mathbf{r},E,\mathbf{\Omega})d\mathbf{\Omega}dEd\mathbf{r} = \left\langle w_l\sigma_x^i(E_l)T_l/V_m\right\rangle$$
$$\int_{V_m}\int_{\Delta E_g}\int_{4\pi}\phi(\mathbf{r},E,\mathbf{\Omega})d\mathbf{\Omega}dEd\mathbf{r} = \left\langle w_lT_l/V_m\right\rangle \ (E_g \le E_l < E_{g-1}) \quad (2)$$

$\langle x\rangle$ means the expected value of x. w_l, E_l, and T_l denote a weight, energy, and track length of neutron's l-th track.

Assuming that the regional reaction rate is independent of the regional flux, the relative error of the microscopic cross-section can be calculated by

$$err\left[\overline{\sigma_{x,g}^{m,i}}\right] = \sqrt{\left(err\left[\overline{w_l\sigma_x^i(E_l)T_l/V_m}\right]\right)^2 + \left(err\left[\overline{w_lT_l/V_m}\right]\right)^2} \quad (E_g \le E_l < E_{g-1}) \quad (3)$$

$err\left[\bar{x}\right]$ denotes the relative error of x defined by one estimated standard deviation of $\bar{x}$ over the estimated mean of x, $\bar{x}$.

The group-averaged macroscopic cross-section for a homogenized region of volume V defined as below can be calculated in the same way to estimate the microscopic cross-section.

$$\Sigma_{x,g} = \frac{\int_V\int_{\Delta E_g}\int_{4\pi}\Sigma_x(\mathbf{r},E)\phi(\mathbf{r},E,\mathbf{\Omega})d\mathbf{\Omega}dEd\mathbf{r}}{\int_V\int_{\Delta E_g}\int_{4\pi}\phi(\mathbf{r},E,\mathbf{\Omega})d\mathbf{\Omega}dEd\mathbf{r}} \quad (4)$$

$\Sigma_x(\mathbf{r},E)$ denotes the macroscopic cross-section of reaction x at location $\mathbf{r}$ and energy E.

Especially, the n-th coefficient of the Legendre expansion of the group-to-group scattering cross-section is written as [3]

$$\Sigma_{s,g'g}^n = \frac{\int_V\int_{\Delta E_g}\int_{\Delta E_{g'}}\Sigma_s^n(\mathbf{r},E'\to E)\phi^n(\mathbf{r},E')dE'dEd\mathbf{r}}{\int_V\int_{\Delta E_{g'}}\phi^n(\mathbf{r},E)dEd\mathbf{r}}. \quad (5)$$

$\Sigma_s^n(\mathbf{r},E'\to E)$ and $\phi^n(\mathbf{r},E)$ denote the n-th Legendre components of the double differential scattering cross-section and the angular flux, respectively.

$$\Sigma_s^n(\mathbf{r},E'\to E) = 2\pi\int_{-1}^{1}\Sigma_s(\mathbf{r},E'\to E,\mu_0)P_n(\mu_0)d\mu_0$$
$$\phi^n(\mathbf{r},E) = 2\pi\int_{-1}^{1}\phi(\mathbf{r},E,\mathbf{\Omega})P_n(\mu)d\mu \quad (6)$$

In the MC neutron simulations, it is extremely difficult to estimate the Legendre components of the angular flux beyond an order of 0 because the components will approach zero if the neutron flux is nearly isotropic in many applications. Assuming that the energy dependencies of the P_n fluxes are proportional to that of the P_0 flux, the following approximation is made [4]

$$\phi^n(\mathbf{r},E) \approx C_n\phi^0(\mathbf{r},E) = C_n\cdot\int_{4\pi}\phi(\mathbf{r},E,\mathbf{\Omega})d\mathbf{\Omega}. \quad (7)$$

Then the P_n group-to-group scattering cross-section can be calculated by

$$\Sigma^n_{s,g'g} \cong \frac{\int_V \int_{\Delta E_g} \int_{\Delta E_{g'}} \Sigma^n_s(\mathbf{r}, E' \to E)\phi^0(\mathbf{r}, E')dE'dEd\mathbf{r}}{\int_V \int_{\Delta E_{g'}} \phi^0(\mathbf{r}, E)dEd\mathbf{r}} . \quad (8)$$

2.2 Few Group Cross-Section Generation

For a homogenized system, the criticality spectrum can be found by the following B_1 equations with fine group cross-sections [5]

$$\Sigma_{t,g}\phi_g \pm iBJ_g = \sum_{g'} \Sigma^0_{s,g'g}\phi_{g'} + \chi_g , \quad (9)$$

$$\pm iB\phi_g + 3\alpha_g(B)\Sigma_g J_g = 3\sum_{g'} \Sigma^1_{s,g'g} J_{g'} . \quad (10)$$

ϕ_g and J_g are defined by

$$\begin{aligned} \phi_g &= \int_V \int_{\Delta E_g} \int_{4\pi} \phi(\mathbf{r}, E, \mathbf{\Omega})d\mathbf{\Omega}dEd\mathbf{r} , \\ J_g &= \int_V \int_{\Delta E_g} \int_{4\pi} \mathbf{\Omega}\phi(\mathbf{r}, E, \mathbf{\Omega})d\mathbf{\Omega}dEd\mathbf{r} . \end{aligned} \quad (11)$$

B^2 denotes the buckling and $\alpha_g(B)$ is defined by

$$\alpha_g = \begin{cases} \frac{1}{3}x^2\left(\frac{\tan^{-1}(x)}{x - \tan^{-1}(x)}\right) & \text{for } x^2 = \left(\frac{B}{\Sigma_{t,g}}\right)^2 > 0 \\ \frac{1}{3}x^2\left(\frac{\ln\{(1+x)/(1-x)\}}{\ln\{(1+x)/(1-x)\} - 2x}\right) & \text{for } x^2 = -\left(\frac{B}{\Sigma_{t,g}}\right)^2 > 0 \end{cases} \quad (12)$$

The fission source of $\sum_{g'} \nu\Sigma_{f,g'}\phi_{g'}$ is normalized to k denoting the multiplication factor and χ_g is the fission spectrum of energy group g.

Then using $\phi_{B,g}$, $J_{B,g}$ and B_1 satisfying k=1, the group-wise diffusion coefficient can be calculated by

$$D_g = \frac{\pm iJ_{B,g}}{B_1\phi_{B,g}} . \quad (13)$$

Finally, the fine group macroscopic cross-section including D_g is condensed to a few-group cross-section as

$$\Sigma_G = \frac{\sum_{g\in G} \Sigma_g \phi_{B,g}}{\sum_{g\in G} \phi_{B,g}} . \quad (14)$$

2.3 Application Results

The macroscopic cross-sections to solve a two-group diffusion equation were generated using McCARD for a Westinghouse-type fuel assembly with 16 Gadolinia burnable poison rods. Table I shows a comparison with results from the lattice physics codes CASMO [6] and HELIOS [7]. From the table, we can see that the two group constants calculated by McCARD agree well with those from HELIOS.

Table I. Comparison of Two Group Constants

	McCARD		Rel. Diff. from McCARD (%)	
	xs	RSD* (%)	HELIOS	CASMO
B_1^2	2.37020E-03	-	1.14	0.58
D_1	1.47856E+00	0.09	-0.67	1.49
$\Sigma_{a,1}$	9.64119E-03	0.08	0.14	0.38
$\Sigma_{s,12}$	1.52717E-02	0.09	-0.27	1.58
$\nu\Sigma_{f,1}$	6.94361E-03	0.06	0.35	2.86
D_2	5.08171E-01	0.09	1.16	-6.45
$\Sigma_{a,2}$	9.54533E-02	0.11	-0.33	0.02
$\nu\Sigma_{f,2}$	1.35712E-01	0.10	-0.05	-0.77
k_{inf}(2gr)	1.15026	-	0.20	0.17
k_{inf}	1.14934	0.04	0.28	0.25

* RSD denotes the relative standard deviation.

3. Conclusions

We augmented the McCARD usability with a multigroup cross-section generation capability. This work will enable its users to directly generate multi-group cross-sections by the MC method.

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REFERENCES

[1] Advanced Monte Carlo Computer Programs for Radiation Transport, Section I, OECD Nuclear Energy Agency, 1995.
[2] H. J. Shim, C. H. Kim, et al., Monte Carlo Depletion Anaysis of a PWR with the MCNAP, M&C'99, Madrid, Spain, 1999.
[3] G. I. Bell and S. Glasstone, Nuclear Reactor Theory, Robert E. Krieger Publishing, Malabar, Florida, 1970.
[4] E. L. Redmond II, Multigroup Cross Section Generation via Monte Carlo Method, PhD Thesis, Massachusetts Institute of Technology, 1997.
[5] R. J. J. Stamm'ler and M. J. Abbate, Methods of Steady-State Reactor Physics in Nuclear Design, Academic Press, London, 1983.
[6] M. Edenius, and B. H. Forrsen, "CASMO-3 A Fuel Assembly Burnup Program User's Manual," Studsvik/NFA-89-3, Rev. 2, Studsvik AB, 1992.
[7] Helios Methods, Scandpower, 2003.