Development of an On-The-Fly Doppler Broadening Module in McCARD

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1. Introduction

Continuous-energy Monte Carlo (MC) neutron transport calculations are generally performed with Doppler-broadened cross sections generated for the specific problem temperatures. However this traditional cross section treatments make the MC whole core transport analysis with temperature profiles difficult if not unrealizable because of a huge memory size requirement to store the cross section data at many different temperatures.

In order to overcome this problem, various on-the-fly Doppler-broadening (DB) methods [1-5] have been developed and tested recently. We have implemented two DB kernels such as SIGMA1 [6,7] and Leal-Hwang DB (LHDB) [8,9] in the Seoul National University MC code, McCARD [10] to generate the Doppler-broadened cross sections in runtime. In this paper, we apply the LHDB method with an initial temperature higher than 0 K and compare the computation efficiency with the SIGMA1 method for a PWR pin cell problem.

2. Imbedded Doppler Broadening Methods

2.1 SIGMA1 kernel broadening method

Assuming the velocity of the nuclei in the medium is given by the Maxwell distribution, the well-known DB equation describes the Doppler-broadened cross section at temperature T, $\sigma(v,T)$, from those at lower temperature T', $\sigma(V,T')$ as [7]

$$\sigma(v,T) = \sigma^*(v,T) - \sigma^*(-v,T), \tag{1}$$

where

$$\sigma^*(v,T) = \frac{\alpha^{1/2}}{\pi^{1/2}v^2}\int_0^\infty \sigma(V,T')V^2 e^{-\alpha(V-v)^2}dV, \tag{2}$$

$$\alpha = \frac{M}{mk(T-T')} \quad (T > T'). \tag{3}$$

m and M are masses of neutron and the target nuclei, respectively. v is the square root of the neutron energy E while V is that associated with the temperature T'. k is the Boltzmann constant.

When $\sigma(V,T')$ are given by a table of cross section versus energy, with linear-linear interpolation in energy and cross section between tabulated values, the SIGMA1 kernel broadening method [6] calculates exact value of $\sigma^*(v,T)$ using the function $H_n(a,b)$, which is defined by

$$H_n(a,b) = \frac{1}{\sqrt{\pi}}\int_a^b x^n e^{-x^2}dx\,. \tag{4}$$

It is notable that the calculation of H_n is time-consuming because of the error function or Taylor series computations.

2.2 Leal-Hwang Doppler broadening method

In LHDB method [8,9], the Doppler-broadened cross section is treated as the solution of a partial differential equation written as

$$\frac{\partial}{\partial\Theta}F(v,\Theta) = \frac{\partial^2}{\partial v^2}F(v,\Theta); \tag{5}$$

$$F(v,\Theta) = v^2\sigma(v^2,T), \tag{6}$$

$$\Theta = \frac{mk(T-T')}{4M}. \tag{7}$$

By the finite difference method with the step sizes, Δv and $\Delta\Theta$, Leal and Hwang [8] proposed the solution to Eq. (5) as

$$F_i^j = \frac{1}{6}F_{i-1}^{j-1} + \frac{2}{3}F_i^{j-1} + \frac{1}{6}F_{i+1}^{j-1}; \tag{8}$$

$$F_i^j \equiv F(v_i,\Theta_j), \tag{9}$$

where i and j are indices of v and $\Delta\Theta$ points, respectively.

Then F_i^j at the j-th temperature index corresponding to the target temperature T can be calculated by successively applying Eq. (8) until the cross sections at the initial temperature T', $F_i^0\left(=v_i^2\sigma(v_i,T')\right)$.

To enhance the accuracy in this study, the cross section between tabulated energy points at the initial temperature T' is approximated by the quadratic function except the cross sections in thermal energies where the power function is used.

3. Validation

The Doppler-broadened cross sections of ^{238}U at 600 K generated by the developed modules are compared with those by NJOY [7]. Figure 1 shows the relative differences between the point-wise cross sections calculated by the McCARD SIGMA1 module and NJOY [7]. From the figure, we can see that the developed module predicts very well within the maximum relative difference of 0.00014%.

Figures 2 and 3 compare the point-wise cross sections calculated by the LHDB module using the initial cross sections at 0 K and 300K, respectively,

with reference. From the figures, we can observe that the LHDB using the 300 K initial cross sections can reliably generate the 600K cross sections except those near unresolved resonance energies while the LHDB using the 0 K data shows big differences in lots of resonance regions.

Therefore in the McCARD on-the-fly DB calculations, the LHDB option is accompanied with the SIGMA1 method which is applied when the initial cross sections are in the unresolved resonance region.

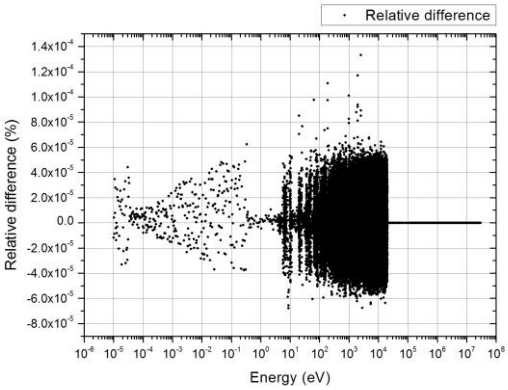

Fig. 1. Relative difference of the ^{238}U cross sections at 600K calculated by the McCARD SIGMA1 module

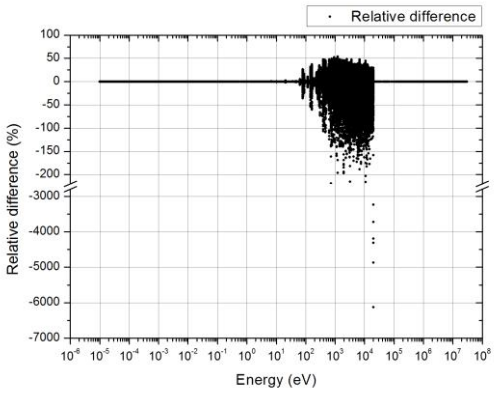

Fig. 2. Relative difference of the ^{238}U cross sections at 600K calculated by the McCARD LHDB module using 0K data

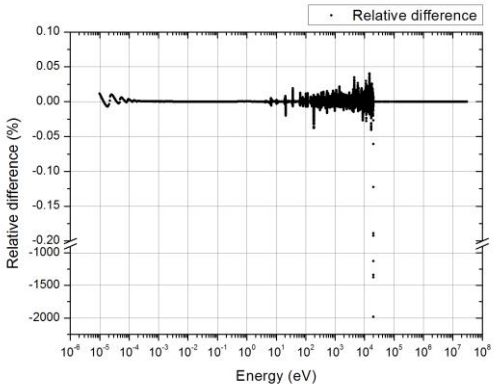

Fig. 3. Relative difference of the ^{238}U cross sections at 600K calculated by the McCARD LHDB module using 300K data

4. Application Results

The McCARD eigenvalue calculations without and with on-the-fly DB calculations using the SIGMA1 and LHDB kernels are conducted for a UO_2 pin cell problem, shown in Fig. 4. The temperatures of fuel, cladding, and coolant are set to 900 K, 600 K, 600 K, respectively, while their initial cross sections for LHDB are taken from 600 K, 300 K, and 300 K respectively. The MC eigenvalue calculations are conducted with 50 inactive and 200 active cycles on 10,000 histories per cycle.

Table 1 compares k_{eff} and computation times of three McCARD runs. In the table, the reference denotes the MC calculation using the cross sections given at the problem temperatures. From the table, we can see that the k_{eff}'s are agree with the reference within 95% confidence intervals and the LHDB option is about five times slower than the reference calculations.

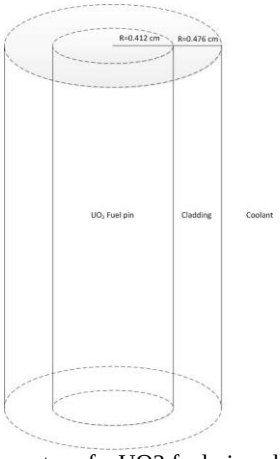

Fig. 4. Geometry of a UO2 fuel pin cell problem

Table 1. Comparison of k_{eff} and computation times of the McCARD on-the-fly DB calculations

	Ref.	SIGMA1	LHDB
k_{eff}	1.42318 (42)	1.42331 (44)	1.42243 (43)
Time(s)	19.0	295.0	100.0

5. Conclusion

In McCARD, the SIGMA1 and LHDB kernels are implemented and tested for the on-the-fly DB calculations. In order to enhance the accuracy and efficiency of LHDB, we apply the LHDB method using an initial temperature higher than 0 K and the SIGMA1 method near the unresolved resonance range.

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