Unresolved Resonance Treatment Using Probability Table in the iMC code

Inyup Kim[a], Tae-suk Oh[a], Yonghee Kim[a*]
Department of Nuclear and Quantum Engineering, Korea Advanced Institute of Science and Technology,
Daehak-ro 291, Yusung-gu, Daejoen, Republic of Korea 34141
**Corresponding author: yongheekim@kaist.ac.kr*

1. Introduction

Cross-section of reactions depends on an incident neutron's energy. Due to the quantum state of the target nuclide, some energy points cause resonance. The resonance cause resonance peaks and valleys of the cross-sections. Because of the resonance, energy self-shielding occurs. Proper consideration of the resonance of each reaction is crucial for accurate reactor analysis. The resonance region is an energy region where the resonance occurs.

The resonance region can be subdivided into two regions, resolved and unresolved resonance regions. The resonance is fully tabulated in the cross-section data libraries in the resolved resonance region. In the Monte Carlo transport, neutron energy is directly simulated. Thus, simply using the recorded resonance peaks in the resolved resonance region will accurately handle the resonance. However, the unresolved resonance region requires further consideration since the peaks are too close. Due to the self-shielding effect, proper treatment is essential, especially in fast reactors.

iMC code is a continuous energy Monte Carlo transport code developed in KAIST [1]. The iMC code supports several reactor analysis-related features, including reactor depletion capability, multiphysics coupled calculation, and variance reduction schemes. In this study, the unresolved resonance region treatment based on the probability table was implemented in the iMC code and validated.

2. Method

3.1. Probability Table method

Resonance is a phenomenon that occurs when an incident neutron energy matches with the target nuclide's energy level. Then, the reaction probability between the neutron and the nuclide increases significantly. The resolved resonance region is an energy region where the resonance peaks are observable. Otherwise, some resonances cannot be tabulated since they are not further enough to be resolved. The energy region containing these resonances is called the unresolved resonance region. Since the gap between nuclides' energy levels becomes narrower in higher energy, the unresolved resonance region is a relatively higher energy part of the resonance region.

In practical neutron cross-section libraries, the cross-sections in the unresolved resonance region are tabulated smoothly. Simply using the cross-section without any

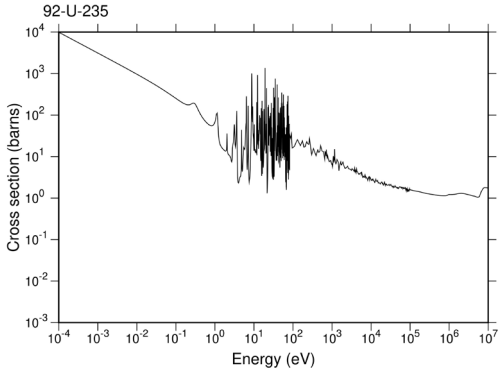

Figure 1. Fission cross-section of U-235 from ENDF-B/VII.1, processed by NJOY2012

treatment ignores the impact of the energy self-shielding caused by the resonance. Therefore, the resonances in the unresolved resonance region require additional treatments. The consequences are negligible in thermal reactors. On the other hand, fast reactors are more affected by the unresolved resonance regions.

TABLE I. Unresolved Resonance Region for some important fissile

Isotope	Unresolved Resonance Region	
	Lower bound	Upper bound
U-235	2.25 keV	25 keV
U-238	20 keV	149 keV
Pu-239	2.5 keV	30 keV

The probability table method is one of the methods proposed to consider the unresolved resonance. An idea of the probability table is to simplify the overlapped resonances by sampling cross-sections. The method chooses the column on the probability table based on the random number generated and tabulated cumulative distribution function (CDF). After the column is determined, its corresponding cross-sections are used.

3.2. Implementation in the iMC code

iMC code utilizes ACE-formatted cross-section libraries [2]. In the ACE format, the probability table contains CDF values and their corresponding total, elastic, fission, (n,γ) cross-sections, and neutron heating number. The probability table is tabulated for designated energy points and some nuclides. According to the ACE format, four flags exist, including interpolation parameter (linear or log-log) or factors flag. If the factors flag is turned on, the tabulated values are relative. These

options are all considered in the iMC code and successfully implemented.

The particle's traveling distance in the Monte Carlo code requires a cross-section. Figure 2 denotes the procedure to obtain macroscopic cross-sections with the probability table.

Before the probability method is applied, the iMC code checks whether the particle energy is within the broad unresolved resonance range. In this case, the broad range can be defined as the energy region where at least one isotope is in unresolved resonance. Therefore, this method needs to collect the maxima and minima of each isotope's unresolved resonance region. The procedure prevents the code from double-checking for the unresolved resonance range and enhances efficiency. If the cross-section evaluation is unionized-grid based, the method is crucial for optimization.

First, the cross-sections are directly obtained from the cross-section library. In this case, unresolved resonance regions are denoted as a smooth cross-section. The cross-section value is used if the target nuclide does not have the probability table data.

Otherwise, since the probability table is tabulated for some energy points, the incident neutron energy will be located in an energy grid. Thus, the energy grid of the incident neutron and upper/lower bound is found. Following calculations are done with probability tables at these two energy points.

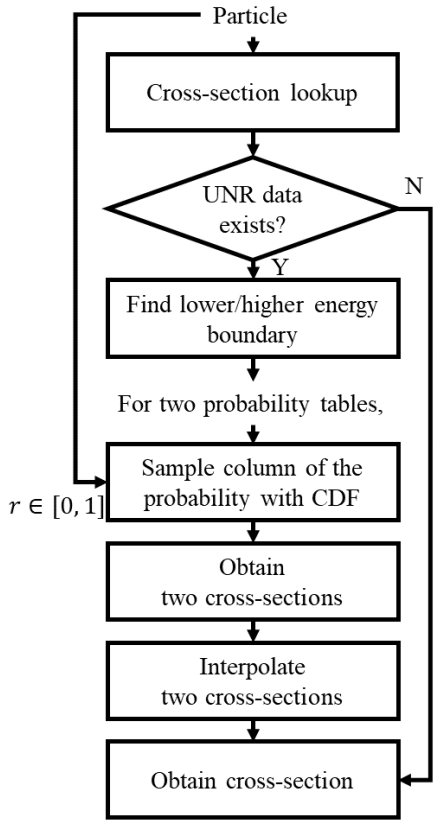

Figure 2. Workflow of unresolved resonance treatment in the iMC code

For both probability tables, columns of the probability tables are sampled based on the uniform random number and tabulated CDF values. Suppose that the probability table of a single energy point has a size of (Number of columns) × (Number of cross-sections provided+1). Assume that the random number r is given in [0,1]. Then, let CDF exists as Eq. 1. According to the definition of the CDF, note that the values are monotonically increasing.

$$\mathrm{CDF_i} \in [0,1] \; \forall \; i = 1 \ldots M \tag{1}$$

Then, column n is selected, which satisfies

$$\mathrm{CDF_n} > r > \mathrm{CDF_{n-1}} \tag{2}$$

Note that the CDF value may differ in the two tables. However, the random number cannot be generated at each cross-section calculation. Otherwise, the cross-section value varies even in the same condition. For instance, a material's macroscopic cross-section may differ from the macroscopic cross-section's summation. If so, colliding nuclide cannot be adequately sampled. Therefore, iMC generates the random number after the collision to retain a correlation.

Two sets of cross-sections are obtained from the sampling for their energy points. Cross-section of the incident neutron can be estimated with interpolation between them. The interpolation method can be linear or log-log interpolations depending on the interpolation flag recorded on the cross-section library. Suppose that the cross-section σ_0 and σ_1 are obtained from the probability tables. For the corresponding two energy points, $\mathrm{E_0}$ and $\mathrm{E_1}$. (without loss of generality,$\mathrm{E_0} < E_1$), linear interpolation can be done as Eq.(3).

$$\bar{\sigma} = \sigma_0 + (\sigma_1 - \sigma_0)\frac{E - E_0}{E_1 - E_0} \tag{3}$$

while log-log interpolation can be expressed as below.

$$\ln \bar{\sigma} = \ln \sigma_0 + \ln(\sigma_1 - \sigma_0) \times \left(\frac{\ln E - \ln E_0}{\ln E_1 - \ln E_0}\right) \tag{4}$$

Furthermore, a cross-section without a probability table may need to be multiplied depending on the 'factors' flag. The flag is applied to the cross-section prior to the interpolation step.

$$\sigma = \sigma_{\mathrm{smooth}} \times R \tag{5}$$

where σ_{smooth} denotes a tabulated smooth cross-section of the unresolved resonance range, and R represents the value retrieved from the probability table.

This research does not consider the Doppler broadening of the unresolved resonance, but the study aims to implement the probability table method accurately. The future version of the iMC code will support the feature.

3. Numerical Calculation

This section suggests and solves two benchmark problems to test the validity of the iMC code's unresolved resonance treatment. The validity of the resonance will be tested by observing the effective multiplication factor, neutron flux, and burnup behavior.

The serpent code is a well-validated Monte Carlo transport code developed in VTT [3]. This section will compare several quantities obtained from the iMC calculation to the Serpent. As a cross-section library, ENDF-B/VII.0 in ACE format was utilized in both codes.

3.1 Jezebel benchmark

The first problem is Jezebel (PU-MET-FAST-001), a simple Plutonium sphere mixed with Gallium. The detailed specification of the reactor is tabulated in Table II. Regarding compositions of the material, atomic fractions are listed in Table III. The effective multiplication factor k_{eff} and neutron spectrum are tallied in this benchmark.

Both calculations are done with 1 million histories per cycle. Twenty inactive cycles and 500 active cycles were utilized. The resulting standard deviations vary from 3 to 5 pcm.

TABLE II. Jezebel benchmark specification

Radius	6.3849 cm
Temperature	300 K

TABLE III. Jezebel fuel composition

Nuclide	Atomic density [#/cm^3]
Pu-239	3.7047E+22
Pu-240	1.7512E+21
Pu-241	1.1674E+20
Natural Gallium	1.3752E+21

First, the effective multiplication factor k_{eff} was compared. Table IV records the keff value in four cases; calculation with and without unresolved resonance

Figure 3. Flowchart of obtaining macroscopic cross-section with consideration of the unresolved resonance treatment. According to the values, the difference between results with and without unresolved resonance treatment shows a difference of about 20 pcm in both codes. Moreover, the difference between iMC and Serpent is within the confidence interval of the difference. Despite the small impact of the unresolved resonance treatment, iMC shows good agreement with the Serpent result, implying a successful implementation of the probability table method.

TABLE IV. Jezebel k_{eff} comparison

k_{eff}	Without URR	With URR
iMC	1.000020 ± 3.8	0.999866 ± 3.6
Serpent	0.999908 ± 4.4	0.999788 ± 4.5

Next, the neutron energy spectrums are tallied. EURLIB 100-group energy bin is selected to tally the neutron energy spectrum. Figure 3. denotes the spectrum and their relative differences. Note that the x-axis is the log-scaled axis. According to the plot, the neutron spectrum agrees below 0.5% for the neutron energy region higher than 100 keV. Although the relative difference in lower energy regions is high, the difference stems from relatively lower spectrum values. Unresolved resonance is applied for lower energy regions within 10 ~ 100 keV. The spectrum clearly shows that their difference is marginal. Thus, the spectrum also shows that the unresolved resonance treatment of the iMC is accurate.

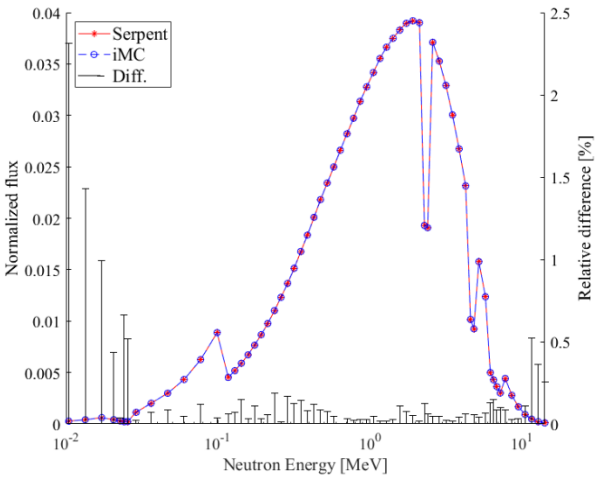

Figure 4. Neutron spectrum comparison

3.2 VERA-2B benchmark

The unresolved resonance treatment is applied to a larger problem. VERA-2B is a depletion benchmark problem provided by CASL [4]. The VERA benchmark is based on actual nuclear fuel and plant data of Watts Bar Nuclear Plant Unit 1. Among the VERA benchmark, the 2B model is at hot zero power. The temperature is set to be 600 K. Previously, iMC has evaluated VERA-2B calculation. Figure 4 is a cross-sectional view of the VERA-2B benchmark core.

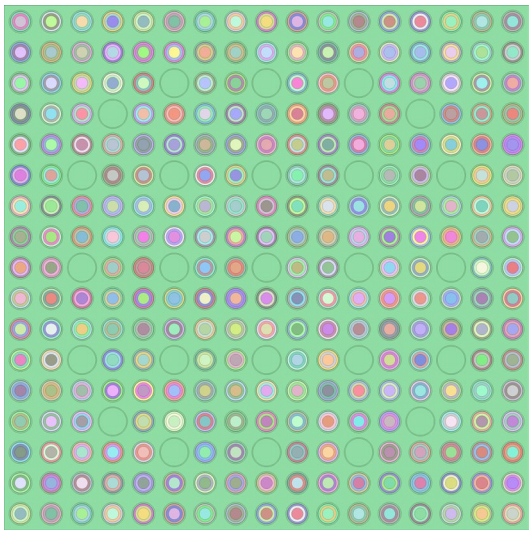

Figure 5. VERA-2B schematics

Figure 5. is a burnup-dependent multiplication factor from both iMC and Serpent code. For both codes, unresolved resonance treatments were applied. As shown through the whole depletion steps, the difference was within the 2σ (standard deviation).

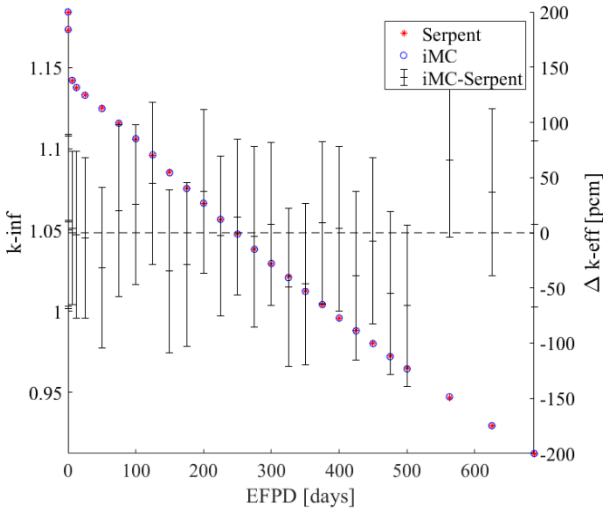

Figure 6. Burnup-dependent k_{eff} of the VERA-2B core. Error bar plotted for 2**σ**

4. Conclusion

Monte Carlo transport calculation is a credible method for reactor analysis. The Monte Carlo method can provide researchers with accurate and precise results based on experimentally obtained cross-sections and other nuclide-related data. However, unresolved resonance is one of the issues that nuclear data faces. Omitting the unresolved resonance affects reactor analysis accuracy due to its self-shielding effect. The probability table method is one of the methods to handle the unresolved resonance properly. This paper studied fundamental and applicational aspects of the probability table method. Also, after the implementation of the method in the iMC code, two benchmarks were considered for testing the validity of the implemented module. Both benchmarks imply that the implementation was successful. This study is expected to be a cornerstone for fast reactor analysis.

Future studies will focus on two aspects. First, further validation is required regarding other benchmark models which have significant changes due to the utilization of the unresolved resonance treatment. Also, research and implementation of the on-the-fly unresolved resonance broadening treatment are required to apply the method to the actual reactor model, in which temperature differs from the tabulated temperature in nuclear data libraries.

ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea Grant funded by the Korean government NRF-2016R1A5A1013919.

REFERENCES

[1] I.KIM, H.KIM, and Y.KIM, "Development and Validation of Depletion Module in the Monte Carlo Code iMC", Transactions of ANS (2022)
[2] J.CONLIN, "A compact ENDF(ACE) format specifications", (2020) https://doi.org/10.2172/1561065
[3] J. LEPPANEN, M. PUSA, T. VIITANEN, V. VALTAVIRTA, and T. KALTIAISENAHO, "The Serpent Monte Carlo code: Status, development and applications in 2013." Ann. Nucl. Energy, 82 (2015)
[4] K.KIM, "Specification for the VERA Depletion Benchmark Suite." (2015) https://doi.org/10.2172/1256820