ASTRA DPC Calculation with MCNP-GenP Library Generation Code System

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1. Introduction

KARMA-ASTRA code system is currently used in core analysis in KNF (KEPCO Nuclear Fuel Company). The accuracy of the code system highly depends on the multi-group and subgroup library of KARMA. To improve KARMA library, the subgroup data was re-generated with EXUS-GenP library generation code system developed by SNU. Additionally, MCNP-GenP library generation code system was suggested to provide more accurate resonance effective self-shielded cross-section. The reason of introducing MCNP to replace EXUS is not limited in level of cross-section accuracy. It is about considering up-scattering and enhanced Doppler broadening in the stage of cross-section library generation. In core analysis, Doppler power coefficient was less negative in ASTRA calculation and the low absorption cross-section of U238 was considered to be the reason. As a result of this work, resonance absorption cross-section of U238 has been increased in KARMA library and Doppler power coefficient in ASTRA core calculation to be more negative.

2. Background Theory

KARMA-ASTRA code system is 2-step code system for core analysis. KARMA is a 2-dimensional multi-group transport code to generate the few-group constants in forms of homogeneous group constants (HGC) files. ASTRA performs a core analysis with cross-section data from KARMA calculation.
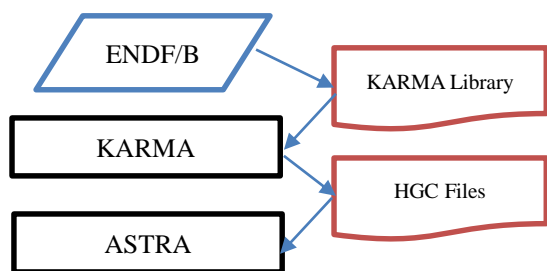

Figure 1. Cross-section data flow in KARMA-ASTRA code system

2.1 Overview of KARMA Library Generation System

KARMA library is generated by a set of code system using evaluated nuclear data file (ENDF) [1]. ENDF is processed by NJOY code [2] for single isotope. The NJOY output files are *mxs* files (gendf format) from GroupR calculations and *pxs* files (pendf format) from BroadR calculations.

The mxs files are transformed to multi-group library files (grxs) by cross-section editing code NOEX. The pxs files are used in slowingdown calculation in EXUS code. The output shielded resonance cross-sections are used to generate subgroup parameters (sgp) in GenP code. The subgroup data is used to reconstruct effective cross-section for resonance energy groups in KARMA and multi-group library is used elsewhere. In this study, MCNP code [3] was suggested to generate shielded resonance cross-section instead of EXUS code.

2.2 Effective Self-Shielded Cross-Section by EXUS Code

EXUS code was developed by SNU to provide accurate effective self-shielded cross-section in resonance energy range by performing ultrafine slowdown calculation. The slowing down calculation [4] is solved by the Boltzmann equation given as follow:

$$\vec{\Omega}\cdot\nabla\psi + \Sigma_t(\vec{r},E)\psi(\vec{r},E,\vec{\Omega}) =$$
$$\int_{4\pi} d\vec{\Omega}' \int_0^\infty dE' \Sigma_s(\vec{r},E'\rightarrow E,\vec{\Omega}'\cdot\vec{\Omega})\psi(\vec{r},E,\vec{\Omega}) + q(\vec{r},E,\vec{\Omega}) \quad (1)$$

where

$\vec{\Omega}$ = neutron direction

$\vec{r}$ = space coordinate

E = neutron energy

ψ = angular flux

Σ_t = macroscopic total cross-section

Σ_s = double differential scattering cross-section

q = external source

To simplify the equation, only isotropic scattering of elastic scattering reaction is considered. Therefore, fission source and up-scattering reaction are ignored for resolved resonance energy level. The energy group is rewritten in lethargy form.

Also, for resolved resonance range, resonant nuclides have a resonance scattering cross-section and a resonance absorption cross-section (and resonance fission cross-section when available) where non-resonant nuclides have only a constant potential cross-sections since the absorption cross section is negligible compared to it.

The final form of slowing down equation is given in terms of region k and nuclide i in function of lethargy:

$$\vec{\Omega} \cdot \nabla \psi_k + \sum_i \Sigma_{i,t}(u)\psi_k(u,\vec{\Omega}) =$$

$$\sum_i \int_{u-\Delta_i}^{u} \Sigma_{i,s}^{k}(u')\phi_k(u')\frac{\exp(u'-u)}{1-\alpha_i}\,du' \qquad (2)$$

where

$$u = \ln(E_0/E) \text{, lethargy}$$

$$\Sigma_{i,x} = N_i \sigma_{i,x},$$

$$\Sigma_{i,s}^{k}(u) = \Sigma_{i,p}^{k} + \Sigma_{i,rs}^{k}(u),$$

$$\Sigma_{i,t}^{k}(u) = \Sigma_{i,s}^{k}(u) + \Sigma_{i,ra}^{k}(u)$$

$$\alpha_i = (A_i - 1)^2 / (A_i + 1)^2,$$

$$\Delta_i = -\ln(\alpha_i)$$

In the equation (2), $\Sigma(u)$ and N are a macroscopic cross-section and an atomic number density. In subscription, p and t means potential and total cross-section as well as rs and ra means resonance scattering and resonance absorption, respectively. Also, A_i, Δ_i and $1-\alpha_i$ is an atomic mass, the maximum lethargy gain per collision with isotope i and the maximum fractional energy loss per collision with isotope i, respectively. The scalar flux over the ultrafine energy group can be obtained by solving equation (2). The group-wise cross-section is obtained using with the integrated over energy group with the cross-section and scalar flux.

$$\sigma_{x,g} = \frac{\int_{\Delta u_g} \sigma_x(u)\phi(u)du}{\int_{\Delta u_g} \phi(u)du} \qquad (3)$$

The self-shielded cross-section is provided with various dilutions cases, providing different background cross-section sets along with temperature sets.

2.3 Effective Self-Shielded Cross-Section by MCNP Code

The implementation of Monte Carlo code to generate self-shielded resonance cross-section had been tried to consider resonance up-scattering effect at the library generation stage which previously EXUS ignored. Doppler broadening rejection correction (DBRC) method was suggested by Becker [5]. As a result of adopting DBRC method in MCNP code, resonance up-scattering effect is considered correctly.

Neglecting the resonance up-scattering effect is thought to be main reason for underestimating a Doppler power defect in core analysis. Modifying the Sampling the Velocity of the Target Nucleus (SVT), MCNP can take account of the temperature dependency of target nucleus by correcting scattering kernel. The modified subroutine was taken from Becker's work.

2.4 Resonance Treatment in KARMA

The subgroup level and weight are defined by effective cross-section in GenP code. GenP calculates subgroup weights (w_n) with corresponding subgroup level (σ_n) to preserve the given effective cross-section minimizing the RMS error. Effective cross-section is defined by either of two transport codes described previously.

KARMA uses subgroup method for the effective resonance cross-section treatment. The subgroup method is based on subgroup fixed source problem of broad group calculation as following equation:

$$\vec{\Omega} \cdot \nabla \psi + \sum_i (\Sigma_{i,a} + \lambda_i \Sigma_{i,p})\psi(\vec{\Omega}) = \sum_i \lambda_i \Sigma_{i,p} \qquad (4)$$

where

Σ_a = macro absorption cross-section of target nuclide

Σ_p = macro potential cross-section of target nuclide

λ = hydrogen equivalent factor

The macroscopic cross-sections can be written in terms of number density N and microscopic cross-section σ. The solution, therefore, is given in terms of cross-section of target resonance nuclide R and background cross-section of the corresponding heterogeneous system [6]. The background cross-section which is not a physical quantity but an artificial one is defined to simplify the solution. The solution of the equation (4) can be simplified in terms of background cross-section and target resonance absorption cross-section.

$$\phi(u) = \frac{\sigma_b}{\sigma_a^{R}(u) + \sigma_b} \qquad (5)$$

where

$$\sigma_a^{R}(u) = \Sigma_a(u) / N^R$$

$$\sigma_b = \lambda \Sigma_p / N^R$$

When subgroup flux is given, the effective cross-section is reconstructed for each resonance energy group by following equation.

$$\overline{\sigma}_a^{R} = \frac{\sum_n w_n \phi_n \sigma_n}{\sum_n w_n \phi_n} \qquad (6)$$

where

$\overline{\sigma}_a^{R}$ = effective resonance cross-section
w_n = subgroup weight
σ_n = subgroup level

3. Results

EXUS-GenP subgroup library generation system was tested in SNU. KNF also generated KARMA library with ENDF/VII.1 using the same code system. In the code system, MCNP was tested to generate effective resonance self-shielded cross-section which is called MCNP-GenP code system. Both libraries are verified by KARMA-ASTRA two-step core analysis. ASTRA performs many core analysis features but Doppler power coefficient calculation is considered only in this study.

3.1 Implementation of DBRC Scheme in MCNP Code

MCNP code was modified to adopt DBRC scheme in order to consider exact model for resonance up-scattering. It is known to increase resonance absorption cross-section and as a result, it is known to increase fuel temperature coefficient (FTC) by 10%.

Table 1. FTC Calculation by MCNP

FTC (pcm/K)	w/ DBRC	w/o DBRC	Diff
HFP	-2.06	-1.84	12.11%
HZP	-2.38	-2.14	10.77%

The Table 1 shows the results of FTC calculations of single pin problem. In the table, HFP and HZP means fuel temperature of 900K and 600K, respectively. FTC was calculated by reactivity difference at ±50K around target fuel temperature. MCNP calculations with DBRC show more negative FTC value. The differences are consistent with McCARD results by SNU [7].

3.2 Generation of Effective Self-Shielded Cross-Section

The resonance self-shielded cross-section was obtained with EXUS and MCNP code, respectively. The incorporated nuclides are only U235 and U238 in this study. EXUS MOC calculation is performed with 16-azimuthal and 4-polar angles as well as 0.01 cm ray width. The number of ultrafine groups is set to be 100,000 in the calculations. MCNP calculation was done for one million particles. The geometry and material information is identical in both calculations and designed for typical PLUS7 fuel with composition of 4.5 w/o enriched uranium. The number of dilution cases is 11 including infinite dilution case for 5 temperature sets. By changing fuel and/or moderator density and moderator volume, the set of dilution cases have various background cross-sections.

Subgroup data for each effective cross-section were also generated with GenP code. Subgroup data consists of subgroup levels and weights. In this case, subgroup weights are generated with fixed subgroup levels. Each library is produced with new subgroup data and KARMA transport calculation was performed with them.
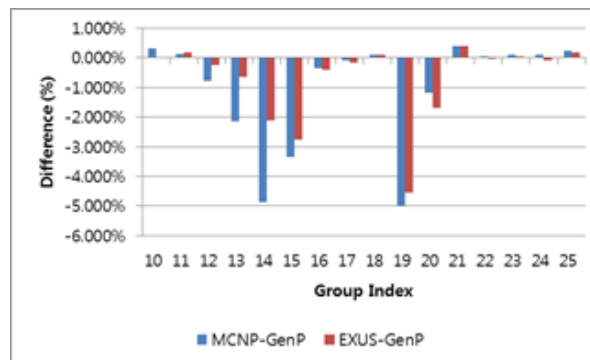

Figure 2. Differences in resonance absorption cross-section of U238 from reference MCNP results

The homogenized group-wise cross-section in KARMA outputs were compared with the results of reference MCNP calculation as shown in Figure 2. The reference calculation is MCNP calculation with the same pin problem performed by KARMA. The result shows that the effective cross-sections by MCNP are larger than those by EXUS calculation. Resonance self-shielded cross section and the subgroup library of U235 was also generated in the same way but the effect is much smaller compare to U238. The energy boundary for group index is attached in Appendix A. The multiplication factors of KARMA calculations are also compared in Table 2.

Table 2. KARMA Multiplication Factor

k-eff	EXUS-GenP/ KARMA	MCNP-GenP/ KARMA	Diff (pcm)
HFP	1.33604	1.33464	140
HZP	1.34776	1.34709	67

As the table shows, the multiplication factors are lower in results of MCNP-generated library. The reactivity difference mostly comes from the cross-section differences. Also, the difference depends on the temperatures as well since DBRC method in MCNP considers Doppler broadening effect.

3.3 Verification with ASTRA Core Calculation

ASTRA core calculation was performed with KARMA cross-section. For core analysis, FTC cannot be obtained directly because the fuel temperature for each assembly is provided with fuel temperature profile, rather than a single value. Therefore, the Doppler Power Coefficient (DPC) is calculated by reactivity difference as the power changes. ASTRA will increase power by 5% and calculate the reactivity.

ASTRA DPC calculation showed less negative value compared to measured value in general. Various methods were taken including introduction of Correction Factor to ASTRA [8]. The correction factor modifies fast group capture cross-section of U238 used in ASTRA core analysis. By increasing the resonance capture cross-section of U238 in epithermal energy region, ASTRA

DPC calculation can show more negative value.

In Figure 2, the effective absorption cross-section is generally larger when MCNP code was used due to considering up-scattering effect and improving Doppler broadening effect. As a result, the difference should be reflected in ASTRA DPC calculation.

Both KARMA library by EXUS and MCNP are used to KARMA calculation to generate the few-group constants for ASTRA. ASTRA uses the cross-section data and performs various core analysis – in this case, DPC calculation. The results of ASTRA DPC calculation are listed in Table 3 as well as measured data. The unit for DPC is given as [pcm/%P]. In ASTRA code, the correction factor was removed.

Table 3. ASTRA DPC Calculation

Power	Measured	Predicted (EXUS)	Predicted (MCNP)
20%	-13.76	-11.10	-11.86
50%	-11.69	-9.84	-10.40
80%	-9.73	-8.71	-9.25
95%	-9.47	-8.07	-8.61

The results show that using MCNP code to generate the resonance effective cross-section make the DPC in ASTRA be about 6% more negative which is an improvement. The effect became smaller in low power because the fuel temperature is generally lower and the Doppler broadening effect is also smaller. Also, the uncertainty is generally larger at low power.

In the previous MCNP calculation, the effect of FTC change is almost 10%. DPC does not necessarily coincides the change rate of FTC. In core analysis, the effect becomes smaller since reactor core consists of a many fuel pins at different temperatures and various temperature profiles. Also, during DPC calculation, the core power increases and increasing power changes power distribution. The distribution effect is considered to be main reason for smaller change.

Therefore, at this stage, the correction factor in ASTRA should stay until the remaining cause is identified. The value of correction factor, however, should be adjusted since some of the effect are represented in KARMA library.

4. Conclusion

The resonance self-shielded cross-section plays an important role in the accuracy of transport code that uses subgroup method for resonance treatment. Both EXUS which uses ultrafine slowing down MOC calculation and MCNP which was modified to use DBRC method are considered in this study. Using resonance effective cross-section by MCNP showed better DPC calculation results in core analysis. Therefore, it is suggested to use MCNP code for generating resonance effective cross-section or equivalent treatment should be considered when generating KARMA library.

Appendix A. Group Structure of KARMA Library

For resonance group

Group	Upper Boundary	Lower Boundary
10	9.1188E+03	2.0347E+03
11	2.0347E+03	1.3007E+02
12	1.3007E+02	7.8893E+01
13	7.8893E+01	4.7851E+01
14	4.7851E+01	2.9023E+01
15	2.9023E+01	1.3710E+01
16	1.3710E+01	1.2099E+01
17	1.2099E+01	8.3153E+00
18	8.3153E+00	7.3382E+00
19	7.3382E+00	6.4760E+00
20	6.4760E+00	5.7150E+00
21	5.7150E+00	5.0435E+00
22	5.0435E+00	4.4509E+00
23	4.4509E+00	3.9279E+00
24	3.9279E+00	2.3824E+00
25	2.3824E+00	1.8554E+00

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