Methodology and the BFS-73-1 Fuel Unit Cell Test Results of the Fast Reactor Cross-section Generator, FXGen

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1. Introduction

Korea Atomic Energy Research Institute (KAREI) had studied pool-type sodium cooled fast reactors (SFRs), and the specific design of Proto-type Gen-IV SFR (PGSFR) had been done in 2017. In the PGSFR design, KAERI collaborated with Argonne National Laboratory (ANL). Hence, ANL deterministic code suite had been used for reactor core design to meet the time schedule of the PGSFR project.

Currently, the PGSFR project has been suspended temporarily, and KAERI focus on developing a long-term sustainable SFR concept for the emerging SMR worldwide market. In this situation, it is required to have own code system for an SFR design. As a multi-group cross-section generation code for fast reactor system, Fast reactor cross-section (XS) Generator (FXGen) has been developed. In the PGSFR design, MC^2-3 code [1] was used for multi-group cross-section generation, and the current version KAERI have is limited to the ENDF/B-VII.0 library due to lack of library preprocessing code.

In this paper, the methodology for resonance treatment and generation of few-group constants will be described. As a validation, BFS-73-1 fuel unit cell problem is analyzed.

2. Methodology

3.1. Resonance treatment

For fast reactor systems, the neutron spectrum level around keV ~ MeV is high in which complicated resonance structure of heavy nuclides exists. Therefore, accurate resonance self-shielding treatment is required. For the fast neutron energy, resonance width is small enough, so narrow resonance (NR) approximation can be applied. Under the NR approximation, neutron flux around resonance can be expressed as follow:

$$\phi(u) = \frac{\Sigma_{pot}}{\Sigma_t(u)} \tag{1}$$

where Σ_{pot} is potential scattering.

By using Eq. (1), self-shielded group constants can be expressed as:

$$\overline{\sigma}^i_{x,g} = \int_{u_g}^{u_{g-1}} \frac{\sigma^i_x(u)\Sigma_{pot}}{\Sigma_t(u)} du \Bigg/ \int_{u_g}^{u_{g-1}} \frac{\Sigma_{pot}}{\Sigma_t(u)} du \tag{2}$$

where *x* denotes the type of reaction and *i* is isotope index.

In the FXGen code, integration of Eq. (2) is calculated numerically for the resolved resonance region. The cross-section of hyper-fine group (HFG; 424,600 groups) structure can be prepared by interpolation of the PENDF file processed by NJOY [2], and numerical integration (Eq. (2)) gives self-shielded ultra-fine group (UFG; 2123 groups) cross-sections.

For the unresolved resonance region, probability table is used to incorporate the self-shielding effect. If we assume that p-table values within UFG group are constant, self-shielded cross-cross section of the unresolved resonance region can be expressed as:

$$\overline{\sigma}^i_{x,g} = \frac{\sum_k \frac{p_{g,k}\sigma^i_{x,g,k}}{\Sigma^i_{t,g,k} + \Sigma_{0,g}}}{\sum_k \frac{p_{g,k}}{\Sigma^i_{t,g,k} + \Sigma_{0,g}}} \tag{3}$$

where $p_{g,k}$ is probability of k-th probability bin and $\sigma^i_{x,g,k}$ is cross-section of k-th probability bin.

The probability table values are prepared by PURR module in NJOY code.

At the UFG group which have unresolved/resolved resonance boundary energy, self-shielded UFG cross-section is obtained by:

$$\overline{\sigma}^i_{x,g} = \frac{\int_{u_g}^{u_b} \frac{\sigma^i_x(u)}{\Sigma_t(u)} du + (u_{g-1} - u_b)\sum_k \frac{p_{g,k}\sigma^i_{x,g,k}}{\Sigma^i_{t,g,k} + \Sigma_{0,g}}}{\int_{u_g}^{u_b} \frac{1}{\Sigma_t(u)} du + (u_{g-1} - u_b)\sum_k \frac{p_{g,k}}{\Sigma^i_{t,g,k} + \Sigma_{0,g}}} \tag{4}$$

For heterogeneous geometry, escape cross-section must be considered and it can be obtained based on the Tone's method [3]. In the heterogeneous problem, Eq. (1) is modified as:

$$\phi(u) = \frac{\Sigma_{pot}}{\Sigma_t(u) + \Sigma^i_{e,g}} \tag{4}$$

where $\Sigma^i_{e,g}$ is the escape cross-section of resonant isotope *i*

In Ref. [4], it is shown that escape cross-section can be easily obtained by solving simple two fixed source

problems. In the FXGen code, the method described in Ref. [4] is used to get escape cross-section for heterogeneous geometry.

3.2. Fission spectrum and scattering transfer kernel

Fission spectrum matrix $\chi(E \rightarrow E')$ can be obtained in the nuclear data library such as ENDF. In the ENDF format, MF5 and MT18 stores fission spectrum matrix. It can be condensed into UFG level by following integration:

$$\chi(E \rightarrow g') = \frac{\int_{g'} \chi(E \rightarrow E')dE'}{\int_0^{E_0} \chi(E \rightarrow E')dE'} \qquad (5)$$

In the ENDF format, MF4~MF6 stores each reaction's transfer kernel. This transfer kernel can be condensed into UFG level by following integration:

$$f_{g \rightarrow g'}^{l} = \int_{g'} \int_{g} \int_{-1}^{1} f(E \rightarrow E', \mu) P_l(\mu) d\mu dE \, dE' \qquad (6)$$

The integration of Eq. (5) and (6) is evaluated by Gaussian quadrature sets. In the FXGen code, the anisotropy of (n,2n) and (n,3n) reaction is considered as a result of Eq. (6). In the MC^2-3 code, (n,2n) reaction is assumed as isotropic and (n,3n) reaction is not considered.

3.3. Neutron spectrum for few-group condensation

The UFG level cross-section and transfer kernel will be generated by Eq. (2) ~ (6). Using this UFG group constants, 0-D slowing down calculation or 1-D slab/cylinder collision probability method will be performed to get neutron spectrum. This neutron spectrum will be used to get 34-group condensed and homogenized group constants.

3. BFS-73-1 fuel unit cell analysis

To analyze the accuracy of newly developed code, FXGen, the BFS-73-1[5] fuel unit cell analysis has been conducted.

The BFS-73-1 experiments had been performed to validate KALIMER-150 core design. BFS-73-1 fuel unit cell consists of two enriched uranium pellets, one U-238 pellet, and four sodium pellets. Homogenized uranium enrichment of unit cell is matched with KALIMER-150 fuel element. Fig.1 shows general BFS-73-1 pellet geometry.

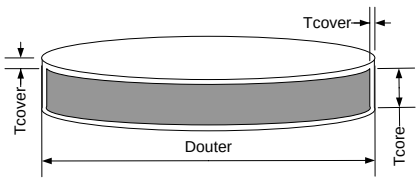

Fig. 1. BFS-73-1 pellet geometry

The volume of the cover is relatively low, core and cover of pellet are homogenized in this study. The BFS-73-1 fuel unit cell geometry is shown in Fig.2.

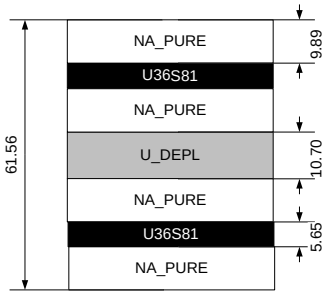

Fig. 2. BFS-73-1 fuel unit cell

As a reference, McCARD [6] Monte Carlo code is used. The number of histories per cycle is 500,000, and 50 inactive cycle and 200 active cycle are used. Fig.3 shows neutron spectrum of the BFS-73-1 fuel unit cell.

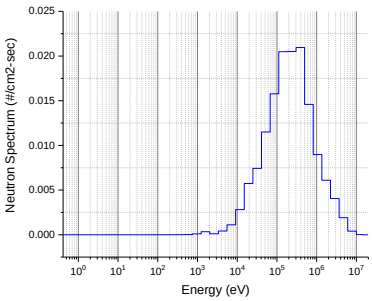

Fig. 3. Neutron spectrum of the BFS-73-1 fuel unit cell (McCARD simulation)

As shown in Fig.3, neutron spectrum is extremely low below 1.0 keV. Hence, 34-group cross-section comparison will be presented for the higher energy than 1.0 keV.

When the ENDF/B-VII.0 library is used, microscopic cross-section comparison for the FXGen and MC^2-3 are shown in Fig.4~7. The reference calculation is performed by McCARD NucGrpXS tally with same library.

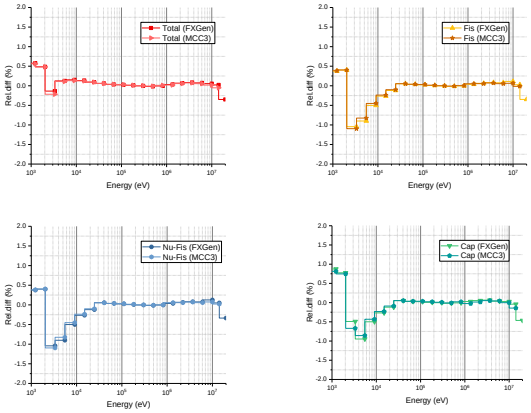

Fig. 4. 34-group homogenized cross-section comparison of U-235 isotope (ENDF/B-VII.0 results)

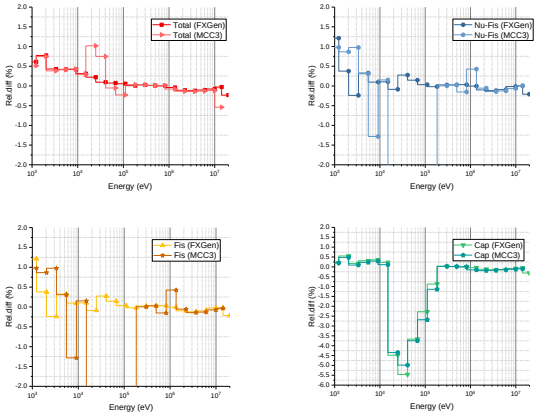

Fig. 5. 34-group homogenized cross-section comparison of U-238 isotope (ENDF/B-VII.0 results)

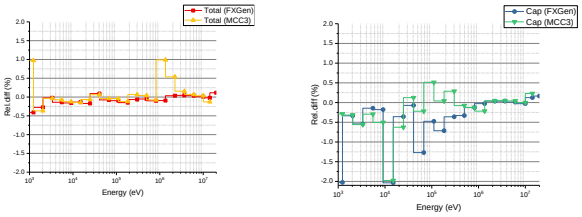

Fig. 6. 34-group homogenized cross-section comparison of Fe-56 isotope (ENDF/B- VII.0 results)

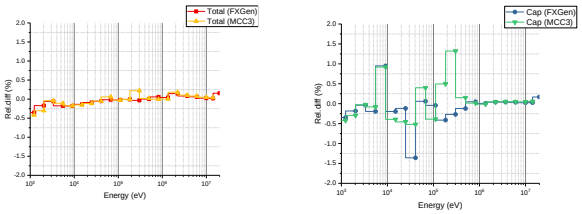

Fig. 7. 34-group homogenized cross-section comparison of Na-23 isotope (ENDF/B- VII.0 results)

As shown in Fig.4, relative errors on microscopic cross-section of U-235 shows similar trends for those FXGen and MC^2-3. For total cross-section comparison, FXGen shows better agreement with reference. For capture cross-section comparison of Fe-56 and Na-23 isotope, absolute errors are similar on two deterministic codes.

The interesting part is U-238 fission cross-section comparison. MC^2-3 code treats U-238 fission cross-section around 10 keV ~ 100 keV as zero. Hence, MC^2-3 has no relative errors around this energy range in Fig.5 fission cross-section comparison. The absolute value of U-238 fission cross-section at this energy range is very small, so this treatment is valid for reactor core calculation. For FXGen code, there is no approximation on U-238 fission cross-section.

When the ENDF/B-VII.1 library is used, microscopic cross-section comparison for the FXGen is shown in Fig.8. The reference calculation is performed by McCARD NucGrpXS tally with same library.

The trends of relative errors on microscopic cross-section for each isotope are similar with ENDF/B-VII.0 results (Fig. 4 ~ 7)

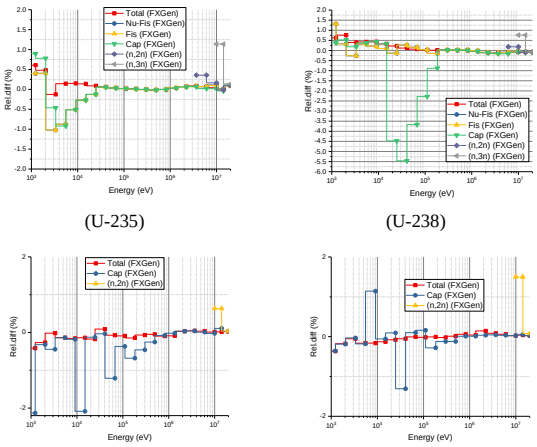

Fig. 8. 34-group homogenized cross-section comparison (ENDF/B-VII.1 results)

The keff results for FXGen, MC^2-3 and McCARD codes are shown in table I.

Table I: k_{eff} results of FXGen and MC^2-3

	McCARD	FXGen	MC^2-3
ENDF/B-VII.0	1.48761	1.48996	1.48857
ENDF/B-VII.1	1.48801	1.49037	-

The k_{eff} difference of MC^2-3 compared to McCARD is 96 pcm while the difference of FXGen is 235 pcm when ENDF/B-VII.0 library is used. When ENDF/B-VII.1 library is used, FXGen code gives 235 pcm discrepancy from the McCARD result.

In k_{eff} comparison FXGen code shows more biased result, but it gives consistent result with two ENDF library versions.

4. Conclusion

The multi-group cross section generation code FXGen has been developed. For the resonance treatment, narrow resonance approximation and probability table for unresolved resonance are utilized. At this moment, 0-D slowing down and 1-D slab and cylinder geometry can be analyzed. 2-D MOC heterogeneity calculation will be implemented as a further study.

For the validation of the FXGen code, BFS-73-1 fuel unit cell is tested and compared with McCARD and MC^2-3 code results. In multi-group cross-section comparison, FXGen and MC^2-3 code shows similar trends and FXGen has smaller relative errors for some isotope and reactions. However, in k_{eff} comparison, FXGen results shows slightly large discrepancy than MC^2-3 code. As a further study, FXGen code will be

tested for the other fast reactor experiments with various evaluated nuclear data library version and improvement on accuracy will be achieved.

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