Generation of Fast Reactor Multigroup Cross Sections employing the NJOY System and Extended Transport Approximation

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1. Introduction

Generation of multigroup (MG) cross section (XS) data starting from the evaluated nuclear data files (ENDF) [1] is one of the most important processes in reactor analyses since it is not possible to achieve sufficient accuracy in the reactor calculation without using proper MG XSs. Numerous researches have been conducted for the generation of MG XS libraries for PWRs. Only a little attention, however, has been given to the fast reactor cross sections in Korea. Unfortunately the existing MG XS generation systems for PWRs are not appropriate for fast reactor analyses because of the significant differences in the reactor physics characteristics between the two reactor types. Thus the MG XS generation system for fast reactors should be established properly considering the special physical characteristics of fast reactors such as the inelastic and anisotropic scattering and also the strong resonance interferences due to the structural and coolant materials. This work is to develop a fast reactor XS generation system by using the NJOY raw cross section data processing system [2] and the extended transport approximation which makes it possible to consider higher order flux moments in the 0-dimensional multigroup spectrum calculation as employed in the MC^2-3 code.[3]

2. Multigroup XS Generation Code, EXUS-F

A fast MG XS generation code, EXUS-F (**E**ffective **X**Ss generation codes based on **U**ltrafine transport **S**olution for **F**ast reactor analysis), was developed at Seoul National University (SNU) in order to generate directly the MG XSs from the ENDF files. Unlike the MC^2-3 code, it does not require any pre-generation of cross section data. Its calculation procedure consists of five steps as shown in Fig. 1: the Doppler broadening processing by the NJOY routines, the consideration of the self-shielding effect, the calculation of the fission and the scattering transfer matrices, and the multigroup spectrum calculation. In the following, each step is described briefly.

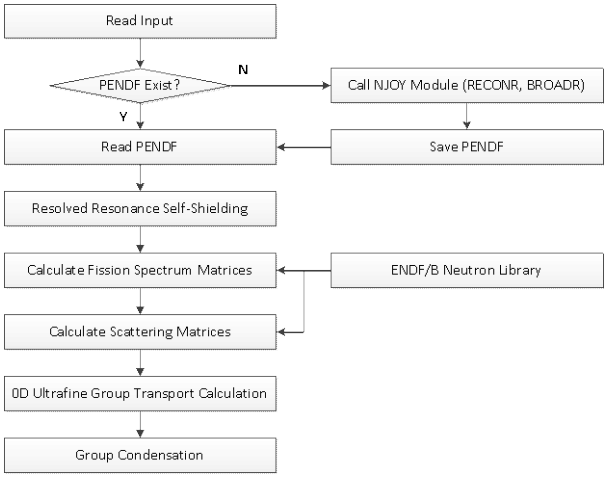

Fig. 1. Computational flow of EXUS-F

2.1. Energy Group Structure

EXUS-F uses the ultrafine energy group structure for the transport calculation. The energy group structure should be sufficiently fine to resolve the self-shielding and the resonance interference effects properly. The ultrafine energy group structure in EXUS-F is consists of 2123 energy groups. The upper and lower energy bounds of the structure are 20 MeV and 0.413 eV, respectively. All the energy groups have the same lethargy width as 1/120.

2.2. NJOY based Doppler Broadening

In the ENDF system, resonance XSs are represented in the form of the resonance parameters instead of the pointwise XSs. Therefore the reconstruction process based on the resonance parameters should be performed. The Doppler broadening effect should also be considered for a given temperature and it can be performed with the reconstruction work. It is not simple to realize the reconstruction and Doppler broadening feasibilities in EXUS-F and thus the NJOY routines which are widely used for the ENDF processing, was integrated in EXUS-F. If there is no pre-saved PENDF file for a nuclide, EXUS-F calls RECONR of the NJOY system for reconstruction using the resonance

parameters. The BROADR module is then called for processing the Doppler broadening effect at the given temperature. As a result of calling the two modules of NJOY, a PENDF file is obtained which contains the pointwise XS in the ENDF/B format. The PENDF file can be stored for a later use since the run time of an NJOY routine requires a considerable computing time. Fig. 2 represents the process to obtain the Doppler broadened pointwise XS using NJOY.

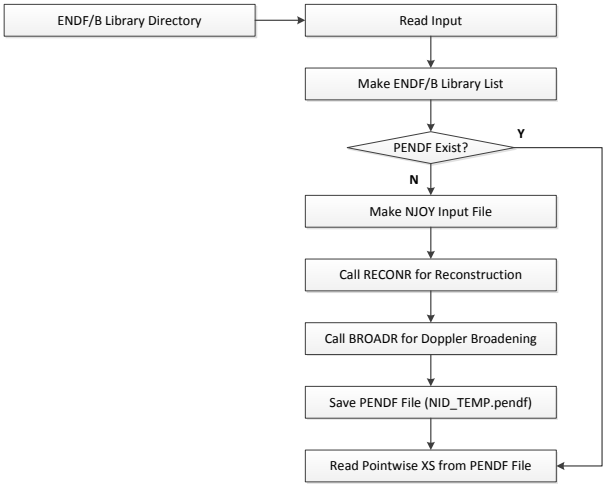

Fig. 2. Flow chart to reconstruction and Doppler broadening of resonances by calling the NJOY system

2.3. Resolved Resonance Self-shielding

The width of the ultrafine group structure is considerably large compared with the pointwise XS and thus it is demanding to use the pointwise XS directly. It means that the self-shielded XSs need to be obtained for the ultrafine group structure. The self-shielded XS can be calculated as:

$$\bar{\sigma}_{i,x,g} = \int_{\Delta u_g} \sigma_{i,x}(u)\phi(u)du \Big/ \int_{\Delta u_g} \phi(u)du \qquad (1)$$

where i, x and g are the indices for isotope, reaction type and energy group, respectively.

Eq. (1) requires a neutron flux spectrum and it brings an extra calculation. Instead of using an exact neutron flux spectrum, the narrow resonance (NR) approximation is assumed for simplifying Eq. (1) which expresses the neutron spectrum flux as:

$$\phi(u) = \Sigma_p / \Sigma_t(u)\,. \qquad (2)$$

The NR approximation is valid as far as the resonance width is much smaller than the energy loss per scattering. Therefore in the most energy range except below 100 eV, the NR approximation is valid.

The self-shielded XS with the NR approximation is written as:

$$\bar{\sigma}_{i,x,g} = \int_{\Delta u_g} \frac{\sigma_{i,x}(u)}{\Sigma_t(u)}du \Big/ \int_{\Delta u_g} \frac{1}{\Sigma_t(u)}du\,. \qquad (3)$$

The integrations in Eq. (3) are performed by using Trapezoidal rule with interpolated pointwise XSs at 200 points within a group.

Likewise, the high order moments of neutron spectrum can be approximated briefly. The l-th order moment of neutron spectrum is approximated as [4]:

$$\phi_l(u) \approx \frac{1}{[\Sigma_t(u)]^{l+1}}\,. \qquad (4)$$

2.4. Fission Spectrum Matrix

EXUS-F uses the fission spectrum matrix instead of the fission spectrum vector which is independent of the incident neutron energy. The ultrafine group fission spectrum matrix is calculated directly from the ENDF/B file. The integrations in Eq. (5) can be performed numerically or analytically based on a given data format.

$$\chi_i^g(\mathrm{E}') = \frac{\int_{E_g}^{E_{g-1}} dE\,\chi_i(\mathrm{E}', E)}{\int_{E_{\min}}^{E_{\max}} dE\,\chi_i(\mathrm{E}', E)}\,. \qquad (5)$$

Fig. 3 shows the fission spectra of ^{235}U for five different incident neutron energies. The fission spectra under 1 MeV energy are very similar, but considerable changes are observed at high energy over 1 MeV.

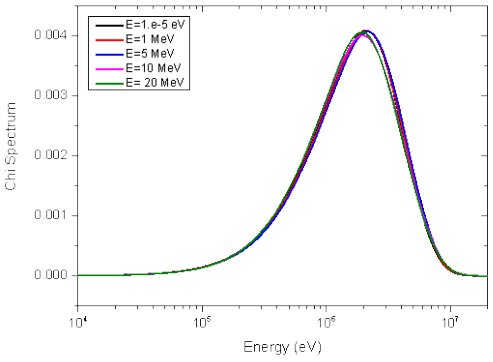

Fig. 3. Fission spectra of U235 for different incident energies

2.5. Scattering Transfer Matrix

The concept of the 'Feed function' is used in EXUS-F and it is from the NJOY system [2]. The element of the scattering transfer matrix is defined in terms of the feed function as:

$$\sigma_{l,g'\to g} = \frac{\int_g F_{l,g'}(E)\sigma_s(E)\phi(E)dE}{\int_g \phi(E)dE} \quad (6)$$

where E is the incident neutron energy and the feed function is defined as:

$$F_{lg'}(E) = \int_{g'}\int_{-1}^{+1} f(E\to E',\mu_s)P_l(\mu_s)d\mu_s dE' \quad (7)$$

with $f(E\to E',\mu_s)$ being the scattering transfer probability from incident energy E to secondary energy E' and the cosine of scattering angle μ_s in the lab system. $P_l(x)$ is the l-th order legendre polynomial. The feed function for the scattering transfer matrix has a meaning of the probability after scattering with incident energy E to reach the secondary energy group g'.

To calculate the feed function and the scattering transfer matrix, the scattering transfer probability $f(E\to E',\mu_s)$ should be known. It can be obtained directly from File 4 through File 6 of ENDF [5] which provide information about the energy and angle distributions of the scattered or emitted neutron.

For a two-body scattering such as elastic and discrete inelastic scattering, the secondary energy can be determined from the scattering angle. Therefore the transfer probability in Eq. (7) can be written as:

$$f(E\to E',\mu_s) = f(E,\mu_s)\delta\left(E'-E'(E,\mu_s)\right). \quad (8)$$

The feed function for two-body scattering is reformulated as:

$$\begin{aligned} F_{lg'}(E) &= \int_{g'}\int_{-1}^{+1} f(E\to E',\mu_c)P_l(\mu_s[\mu_c])d\mu_c dE' \\ &= \int_{\mu_{s,\min}}^{\mu_{s,\max}} f(E,\mu_{s,})d\mu_s \end{aligned} \quad (9)$$

where $\mu_{s,\min}$ and $\mu_{s,\max}$ are the cosine related to lower and upper energy boundaries of the secondary energy group g'. The angular distribution $f(E,\mu_s)$ can be found in File 4 of ENDF.

If the secondary particle information is given in the center of mass (CM) system, Eq. (9) is changed to:

$$F_{lg'}(E) = \int_{\mu_{c,\min}}^{\mu_{c,\max}} f(E,\mu_c)d\mu_c. \quad (10)$$

In the case of continuum inelastic scattering or *(n,Xn)* reaction, the secondary energy and scattering angle are independent. The angle and energy distribution are provided in File 4 and File 5 separately, or energy-angle coupled information is given in File 6. If the information is given in File 4 and File 5, the transfer probability can be separated to the angle and energy terms as:

$$f(E\to E',\mu_s) = f(E,\mu_s)g(E\to E'). \quad (11)$$

The double integration in the feed function can also be separated as:

$$F_{lg'}(E) = \int_{-1}^{+1} f(E,\mu_s)d\mu_s\int_{g'} g(E\to E')dE'. \quad (12)$$

The energy distribution $g(E\to E')$ can be found in File 5 of the ENDF/B files.

File 6 of ENDF provides the transfer probability as tabulated values or parameters which can construct it. The transfer probability $f(E\to E',\mu_s)$ can be obtained directly by using both of data in File 6. The feed function, consequently, can be calculated by using Eq. (7). But the Jacobian matrix should be used for the integration if the energy-angular information is given in the center-of-mass (CM) system which is defined as:

$$J(E',\mu_s) = \sqrt{E'/E'_{cms}}. \quad (13)$$

On the other hand, the feed function for energy-angular distribution in File 6 can be calculated by:

$$\begin{aligned} F_{lg'}(E) &= \int_{g'}\int_{-1}^{+1} f\left(E\to E',\mu_s\right)P_l\left(\mu_s\right)d\mu_s dE' \\ &= \int_{g'}\int_{\mu_{c,\min}}^{+1} d\mu_s f_l(E\to E'_{cms},\mu_c)\sqrt{\frac{E'}{E'_{cms}}}P_l\left(\mu_s\right)dE' \end{aligned}. \quad (14)$$

2.6. Extended Transport Approximation

In order to consider the anisotropic scattering effect, high order moments of the MG scattering transfer matrix should be required. They are calculated based on high order moments of neutron spectrum. For this reason, the extended transport approximation is introduced for 0-dimensional problem.

The MG Pn equations for a 0-dimensional problem are given as:

$$\begin{aligned} &\frac{n+1}{2n+1}iB\phi_{n+1,g} + \frac{n}{2n+1}iB\phi_{n-1,g} + \Sigma_{t,g}\phi_{n,g} \\ &= \sum_{g'}\Sigma_{sn,g'\to g}\phi_{n,g'} + S_{f,g}\delta_n^0, n = 0,1,\cdots,\mathrm{N}-1 \end{aligned}, \quad (15)$$

$$\frac{N}{2N+1}iB\phi_{N-1,g} + \Sigma_{t,g}\phi_{N,g} = \sum_{g'}\Sigma_{sN,g'\to g}\phi_{N,g'}. \quad (16)$$

The extended transport approximation assumes that the number of neutrons scattered into an energy group g is the same as the number of neutrons scattered out from the group for $n > 1$, namely,

$$\sum_{g'} \Sigma_{sN,g' \to g} \phi_{g'} = \Sigma_{sN,g} \phi_g , \; n = 2,3,\cdots N \; . \qquad (17)$$

By inserting Eq. (17) into Eqs. (15) and (16), the set of consistent P_1 order N extended transport equations is obtained as:

$$iB\phi_{1,g} + \Sigma_{t,g}\phi_{0,g} = \sum_{g'} \Sigma_{s0,g' \to g} \phi_{0,g'} + S_{f,g} , \qquad (18)$$

$$\frac{2iB}{3}\phi_{2,g} + \frac{iB}{3}\phi_{0,g} + \Sigma_{t,g}\phi_{1,g} = \sum_{g'} \Sigma_{s1,g' \to g} \phi_{1,g'} , \qquad (19)$$

$$\begin{aligned} &\frac{n+1}{2n+1} iB\phi_{n+1,g} + \frac{n}{2n+1} iB\phi_{n-1,g} \\ &+ (\Sigma_{t,g} - \Sigma_{sn,g})\phi_{n,g} = 0, \quad n = 2,3,\cdots, N-1 \end{aligned} , \qquad (20)$$

$$\frac{N}{2N+1} iB\phi_{N-1,g} + (\Sigma_{t,g} - \Sigma_{sN,g})\phi_{N,g} = 0 . \qquad (21)$$

Eqs. (20) and (21) can be solved successively from n=N to yield:

$$\phi_{N,g} = -\frac{N}{2N+1} \frac{\mathrm{iB}}{\Sigma_{t,g} - \Sigma_{sN,g}} \phi_{N-1,g} . \qquad (22)$$

Eq. (20) can be rewritten with Eq. (22) when n=N-1.

$$\begin{aligned} &\left(\frac{N}{2N-1} \frac{N}{2N+1} \frac{B^2}{\Sigma_{t,g} - \Sigma_{sN,g}} + (\Sigma_{t,g} - \Sigma_{sN-1,g}) \right) \phi_{N-1,g} \\ &= -\frac{N-1}{2(N-1)+1} iB\phi_{N-2,g} \end{aligned} \qquad (23)$$

Eq. (23) can be reformulated with the similar form of Eq. (22) as:

$$\phi_{N-1,g} = -\frac{N-1}{2(N-1)+1} \frac{iB}{A_{N-1,g}} \phi_{N-2,g} . \qquad (24)$$

where

$$A_{N-1,g} = \left[\frac{N}{2N-1} \frac{N}{2N+1} \frac{B^2}{\Sigma_{t,g} - \Sigma_{sN,g}} + (\Sigma_{t,g} - \Sigma_{sN-1,g}) \right] . \qquad (25)$$

Likewise, the relation between ϕ_{n-1} and ϕ_n is defined as:

$$\phi_{n,g} = -\frac{n}{2n+1} \frac{iB}{A_{n,g}} \phi_{n-1,g} , \; n = 2,3,\cdots \mathrm{N} \qquad (26)$$

where

$$\begin{aligned} A_{n,g} &= b_{n-1,g} + \frac{a_n}{A_{n+1,g}} \\ &= b_{n-1,g} + \cfrac{a_n}{b_{n,g} + \cfrac{a_{n+1}}{b_{n+1,g} + \cfrac{a_{n+2}}{\cdots + \cfrac{a_{N-1}}{b_{N-1,g}}}}} \end{aligned} , \qquad (27)$$

$$A_{N,g} = b_{n-1,g} , \qquad (28)$$

$$a_n = \frac{n+1}{2n+1} \frac{n+1}{2(n+1)+1} B^2 , \qquad (29)$$

and

$$b_{n,g} = \Sigma_{t,g} - \Sigma_{s,g}^{n+1} . \qquad (30)$$

For n=1, Eq. (19) can be rewritten by substituting Eq. (26) for n=2 as:

$$\frac{iB}{3}\phi_{0,g} + A_{1,g}\phi_{1,g} = \sum_{g'} \Sigma_{s1,g' \to g} \phi_{1,g'} . \qquad (31)$$

Now the P_1 order N extended transport equations can be written as:

$$iB\phi_{1,g} + \Sigma_{t,g}\phi_{0,g} = \sum_{g'} \Sigma_{s0,g' \to g} \phi_{0,g'} + S_{f,g} , \qquad (32)$$

$$\frac{iB}{3}\phi_{0,g} + A_{1,g}\phi_{1,g} = \sum_{g'} \Sigma_{s1,g' \to g} \phi_{1,g'} , \qquad (33)$$

$$\phi_{n,g} = -\frac{n}{2n+1} \frac{iB}{A_{n,g}} \phi_{n-1,g} , \; n = 2,3,\cdots N . \qquad (34)$$

3. Verification

To verify the functionality of EXUS-F to generate MG XS, a simple problem was considered consisting of 5 nuclides, ^{23}Na, ^{56}Fe, ^{235}U, ^{238}U and ^{239}Pu. Note that ^{23}Na and ^{56}Fe are the important coolant and structural materials in fast reactors. Other nuclides are fissile nuclides. To assess the result of EXUS-F, the McCARD [6] Monte Carlo continuous energy calculation was performed and its result was used as reference in the comparison.

Fig. 4 shows the ultrafine group neutron flux spectrum of the problem. As shown in the figure, EXUS-F spectrum is in a very good agreement with that of McCARD. By using the ultrafine group flux spectrum, the group condensation was performed into a 244 energy group structure. In the case of ^{23}Na, the total XSs appear to be approximately the same as the reference as shown in Fig. 5. Errors of about 2% are, however, observed in total XS of ^{56}Fe around some resonances as shown in Fig. 6. The errors would be from the error in the ultrafine group flux spectrum or from the error of determining the ultrafine group XSs by considering the self-shielding effect with the NR approximation..

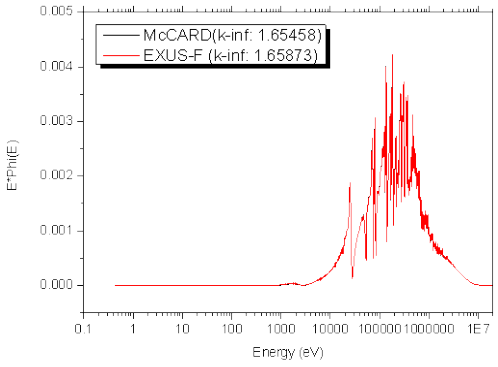

Fig. 4. Ultrafine group neutron spectrum flux obtained from McCARD and EXUS-F calculations

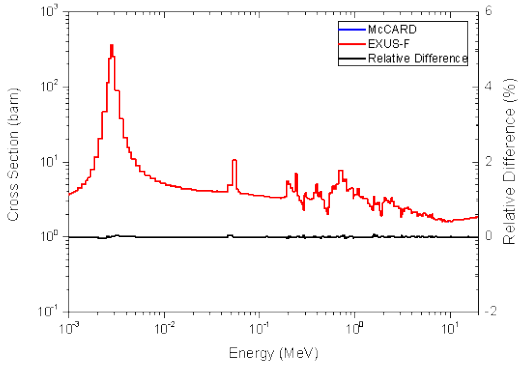

Fig. 5. Group condensed total XS of ^{23}Na obtained from McCARD and EXUS-F calculations and its relative difference

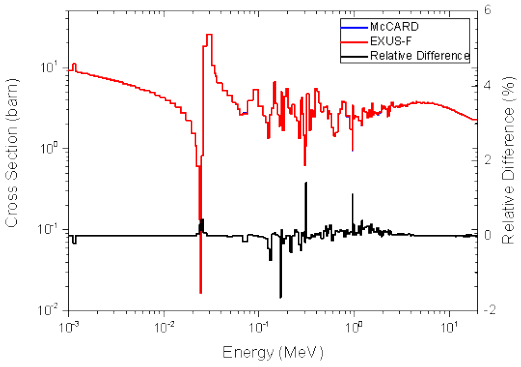

Fig. 6. Group condensed total XS of ^{56}Fe obtained from McCARD and EXUS-F calculations and its relative difference

4. Summary and Conclusions

A fast reactor multigroup cross section generation code EXUS-F was developed that is capable of directly processing the ENDF data files and solving the consistent P_1 order N extended transport equation with a ultrafine group structure. The NJOY modules were integrated to process the resonance data of the ENDF/B file directly and the functions to generate self-shielded ultrafine group XSs, fission spectrum matrices and scattering transfer matrices directly from the ENDF files were realized in EXUS-F. The extended transport approximation was used in the 0-dimensional calculation to obtain higher order moment spectra. To verify EXUS-F, the simple problem calculation for a mixture consisting of five representative fast reactor nuclides was performed. The resulting spectrum and condensed multigroup cross sections agree well with those of the McCARD results. It can thus be stated that the cross section preparation and 0-dimensial ultrafine group spectrum calculation in EXUS-F works properly. The extension of EXUS-F to one-dimensional problems using the method of characteristics transport solver with anisotropic scattering is underway.

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