A Method for Generating Subgroup Parameters from Resonance Tables and the SPART Code

K. Devan and P. Mohanakrishnan
Reactor Physics Division, Indira Gandhi Centre for Atomic Research, Kalapkkam- 603 102

It is known that in certain neutron energy groups where the cross section varies significantly and in cases of interacting resonances due to the presence of many heavy isotopes, there is a loss of accuracy in the usual multigroup method. A finer group structure improves the accuracy but usually demands a large computer time. In such a situation, it is claimed, that the subgroup or multiband method [1-3] greatly improves the accuracy and is relatively economic. In this method, each group is divided into a number of total cross section ranges or bands and an average band cross section is defined in each band. Hence, the neutrons are allowed to interact not with only one cross section, as in the multigroup method, but rather with any one of the different band cross sections which are defined along with their associated statistical probabilities. Many people had used the subgroup method for fast reactors in the treatment of cell heterogeneity. Similar calculations were also done by R. J. Roth [2] for thermal reactors. At present, the subgroup method is found to be more flexible and easier to use when the spatial heterogeneity is considered.

As a first step in our attempts to implement the subgroup method for our fast reactor applications, D. E. Cullen's GROUPIE [3] code was tried to generate subgroup parameters. It was soon found that the code, as distributed by IAEA, does not include subroutines (due to restrictions) required for more than two bands. Hence we developed a method [4], which resembles Roth's method [2], to generate the subgroup parameters for any number of bands from the usual resonance tables containing multigroup unshielded cross sections and self shielding factors for a set of dilution cross sections and temperatures. A code SPART [4,5] was written which calculates the desired band parameters using the resonance tables available in Cadarache Version 2 format in binary mode.

The subgroup parameters are obtained from the resonance table by solving the following system of non-linear equations:

$$\sum_{k=1}^{N} \frac{\alpha_k}{\sigma_{tk} + \sigma_{0l}} = \frac{1}{\langle \sigma_t \rangle f_t(\sigma_{0l}) + \sigma_{0l}} \qquad \ldots\ldots (1)$$

$$\sum_{k=1}^{N} \frac{\alpha_k \sigma_{xk}}{\sigma_{tk} + \sigma_{0l}} = \frac{\langle \sigma_x \rangle f_x(\sigma_{0l})}{\langle \sigma_t \rangle f_t(\sigma_{0l}) + \sigma_{0l}} \qquad \ldots\ldots (2)$$

where α_k , σ_{tk} and σ_{xk} are subgroup parameters and k is the subgroup index. α_k is the band weight for k-th band and $f_t(\sigma_{ol})$ is the self-shielding factor for the total cross section for the dilution σ_{ol} .The index l gives the particular value of the dilution considered. Similarly, $f_x(\sigma_{ol})$ is the self-shielding factor for the reaction x (x = capture, elastic or fission) for the dilution σ_{ol} . $<\sigma_t>$ and $<\sigma_x>$ represent the unshielded cross sections for total and the reaction x and N is the total number of bands. The above set of equations satisfy the following constraints:

$$\sum_{k=1}^{N} \alpha_k = 1 \qquad \text{..... (3)}$$

$$\sum_{k=1}^{N} \alpha_k \sigma_{tk} = <\sigma_t> \qquad \text{..... (4)}$$

$$\sum_{k=1}^{N} \alpha_k \sigma_{xk} = <\sigma_x> \qquad \text{..... (5)}$$

$$\sum_{x} \sum_{k=1}^{N} \alpha_k \sigma_{xk} = <\sigma_t> \qquad \text{..... (6)}$$

The following steps were taken to solve the above set of non-linear equations with non-linear constraints:

(1) Convert eq. 1 into a polynomial equation and find its roots. The negative of these roots are the subgroup parameters for total cross section (σ_{tk}).

(2) Use σ_{tk}'s in eq. 1 and perform a least-squares fit with the constraints given by eq. 3 and 4 to find the band weights α_k 's.

(3) Use α_k and σ_{tk} in eq. 2 and perform a least-squares fit with the contraints given by eq. 5 and 6 to obtain σ_{xk}.

It should be noted that if N is the number of subgroups, the number of dilutions required to solve the above set of equations is 2N - 1. More details of the code SPART are given in ref.5.

Table 1 gives the subgroup parameters for Th-232 from JENDL-2 based multigroup binary cross section library [6] in two bands obtained using SPART. The subgroup parameters generated using GROUPIE from the JENDL-2 basic library is also given in Table 1. It should be kept in mind that SPART and GROUPIE differ in the method of generating subgroup parameters. Table. 2 gives the subgroup parameters for Pu-239 which was generated from the Cadarache Ver.2 cross section library in four bands.

1. L. B. Levitt, Nucl. Sci. Engg., 49, 450 (1972).

2. M. J. Roth, Report AEEW-R 921 (1974).

3. D. E. Cullen, Report UCRL-50400, Vol. 17, Part D (1980).

4. K. Devan and P. Mohanakrishnan, A Method of Generating Subgroup Parameters from Resonance Tables, in Proc. Tenth National Symposium on Radiation Physics (NSRP-10), Kalpakkam & Madras, Aug 17-20, 1993, p20.

5. K. Devan and P. Mohanakrishnan, SPART: A Code for Generating Subgroup Parameters from Resonance Tables, Internal Note RPD/NDS/51 (1993).

6. V. Gopalakrishnan et al., Internal Note, RPD/NDS/42 (1991)

Table 1. Subgroup parameters of Th-232 from JENDL-2 library for the broad group(276eV-101eV)

Code	Temp.	Band	Weights	Total	Capture	Elastic
SPART	300K	1	0.98281	17.810	3.703	14.10
		2	0.01719	1319.215	526.470	793.060
GROUPIE	0K	1	0.94661	10.067	0.500	9.568
		2	0.05339	593.000	245.070	347.93

Table 2. Subgroup parameters of Pu-239 from Cad. Ver.2 set at 300K for the group (22.6eV-3.06eV) using SPART code

Band	Weights	Total	Capture	Elastic	Fission
1	0.42213	15.884	1.819	9.693	4.123
2	0.32346	39.877	9.607	10.178	21.459
3	0.15690	190.880	53.301	14.307	117.010
4	0.09750	1051.300	436.210	65.548	556.190