

## ARTICLE

**Insufficient Self-Shielding Correction in VITAMIN-B6**

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We carried out a simple benchmark calculation test with a multigroup cross-section library VITAMIN-B6 generated from ENDF/B-VI. The model of this test consisted of an iron sphere of 1 m in radius with an isotropic 20 MeV neutron source in the center. Neutron spectra in the sphere were calculated with an Sn code ANISN and VITAMIN-B6 or FENDL/MG-1.1. A calculation with MCNP and ENDF/B-VI was carried out as a reference. The neutron spectra with ANISN and FENDL/MG-1.1 agreed with those with MCNP, while those with ANISN and VITAMIN-B6 were at most 50 % different from those with MCNP. We uncovered that the discrepancy came from insufficient self-shielding correction due to the followings; 1) The smallest background cross section of  $^{56}\text{Fe}$  in VITAMIN-B6 is 1. 2) The weighting flux used in generating VITAMIN-B6 is not adequate. VITAMIN-B6 should be revised for adequate self-shielding correction.

**KEYWORDS:** VITAMIN-B6, ANISN, self-shielding correction, background cross section, weighting flux

**I. Introduction**

An AMPX master library VITAMIN-B6<sup>1)</sup> was released from ORNL in 1996. ENDF/B-VI release 3<sup>2)</sup> data of 120 materials were processed to GENDF files (neutron 199 groups and gamma 42 groups) with the NJOY code<sup>3)</sup>. The GENDF files were converted to VITAMIN-B6 with the SMILER code<sup>4)</sup>. A multigroup library is produced with the SCAMPI code<sup>5)</sup>, where the self-shielding correction is carried out with the BONAMI code<sup>4)</sup>.

VITAMIN-B6 was verified through computational analyses of more than 30 benchmark experiments<sup>6)</sup> and has been used widely in the world. However we encountered a strange result in a simple benchmark calculation test with VITAMIN-B6. Here we investigate reasons for the strange result in detail.

**II. Simple Benchmark Calculation Test**

The model of the simple benchmark calculation test consisted of a natural iron sphere of 1 m in radius with an isotropic neutron source of 17.732-19.96 MeV, which is the first group in VITAMIN-B6, in the center. Neutron spectra in the sphere were calculated with an Sn code ANISN<sup>7)</sup> and VITAMIN-B6. For comparison we also carried out an ANISN calculation with a multigroup library produced from FENDL/MG-1.1<sup>8)</sup>, which is a MATXS file<sup>9)</sup> for fusion reactors and iron data of which were taken from ENDF/B-VI, by using the TRANXS<sup>9)</sup> code. Moreover a calculation with MCNP4C<sup>10)</sup> and ENDF/B-VI was carried out as a reference.

**Figure 1** shows the calculated neutron spectra at the distance of 40 cm from the center of the iron sphere. The neutron spectrum with ANISN and FENDL/MG-1.1 agrees with that with MCNP, while the neutron spectrum below 100 keV with ANISN and VITAMIN-B6 is at most 50 % larger than that with MCNP.

**Figure 2** shows the calculated neutron spectra at the distance of 80 cm from the center of the iron sphere. The tendency is similar with that in Fig. 1, but the neutron spectrum with ANISN and VITAMIN-B6 is at most 30 % larger below 100 keV and by a half smaller from 100 keV to 1 MeV than that with MCNP.

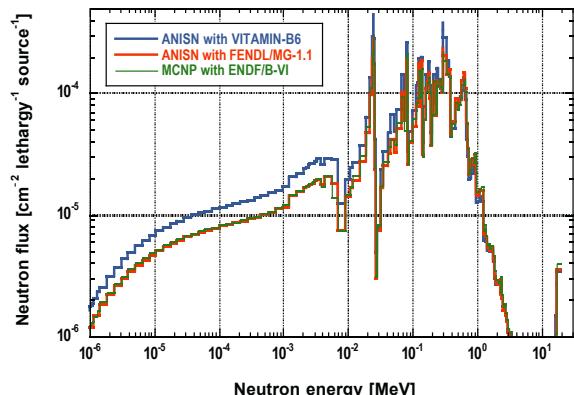


Fig. 1 Neutron spectra at 40 cm from center of iron sphere

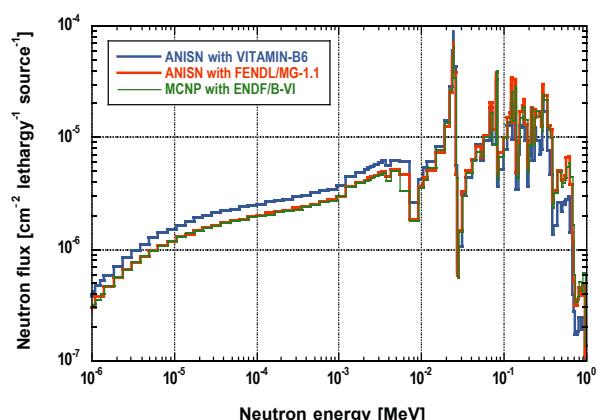


Fig. 2 Neutron spectra at 80 cm from center of iron sphere

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### III. Problems in VITAMIN-B6

In order to investigate reasons for the above discrepancy in the neutron flux below 1 MeV, we compared VITAMIN-B6 with FENDL/MG-1.1 in detail.

#### 1. Background Cross Section Data

The self-shielding correction in VITAMIN-B6 and FENDL/MG-1.1 is performed with the BONAMI code and the TRANSX code, respectively, by using the Bondarenko method<sup>11)</sup>. In the Bondarenko method, the following weighting flux is used for averaging cross section data in a group,

$$W_\ell(E) = \frac{C(E)}{[\sigma_0 + \sigma_t(E)]^{\ell+1}}, \quad (1)$$

where  $C(E)$  is a smooth part of the shape of the flux,  $\sigma_0$  is called a background cross section,  $\sigma_t(E)$  is a total cross section and  $\ell$  is a Legendre order.

We found out that the prepared background cross section data for  $^{56}\text{Fe}$  were different between VITAMIN-B6 and FENDL/MG-1.1; Bondarenko factors for self-shielding correction for the background cross sections of  $10^{10}, 10^5, 10^3, 10^2, 50, 10$  and 1 barn are included in  $^{56}\text{Fe}$  of VITAMIN-B6, while those of  $10^{10}, 1000, 100, 10, 3, 1, 0.3$  and 0.1 barn are included in  $^{56}\text{Fe}$  of FENDL/MG-1.1. Natural iron requires Bondarenko factors for the background cross section of approximately 0.2 for  $^{56}\text{Fe}$ , but Bondarenko factors for the background cross section of 1 are used for self-shielding correction in VITAMIN-B6, which leads insufficient self-shielding correction, because the smallest background cross section is 1. On the contrary, the self-shielding correction for natural iron is adequate in FENDL/MG-1.1 because the smallest background cross section is 0.1. The multigroup macroscopic total cross sections of natural iron are plotted in Fig. 3. The total cross section of VITAMIN-B6 is different from that of FENDL/MG-1.1. VITAMIN-B6 should include Bondarenko factors for the background cross section of 0.1. Note that BUGLE96<sup>12)</sup> (a

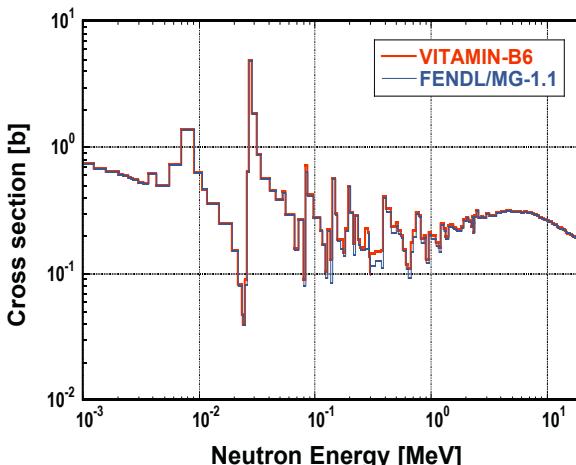


Fig. 3 Total cross section of natural iron

broad group version of VITAMIN-B6) and HILO2K<sup>13)</sup> (data below 20 MeV : VITAMIN-B6) also have the same problem. The same problem occurred in the FENDL/MG-1.0<sup>14)</sup> and it was revised in FENDL/MG-1.1 based on our comment<sup>15)</sup>. Other material data in VITAMIN-B6 should be also checked whether the prepared background cross sections are enough or not.

#### 2. Weighting Flux

The weighting flux in Eq. 1 should be used for adequately averaging cross section data in a group. However the weighting fluxes for  $\ell \geq 1$  used in VITAMIN-B6 and FENDL/MG-1.1 are the followings and are different from Eq. 1,

$$W_{\ell \geq 1}(E) = W_0(E) : \text{VITAMIN-B6}, \quad (2)$$

$$W_{\ell \geq 1}(E) = W_1(E) : \text{FENDL/MG-1.1}. \quad (3)$$

Next influences of the difference between the weighting fluxes in Eqs. 2 and 3 were examined.

We have to remember that the  $S_N$  multigroup cross sections for discrete ordinates codes are not the same as the  $P_N$  multigroup cross sections which are included in VITAMIN-B6 and FENDL/MG-1.1.<sup>9)</sup> The relation between the  $S_N$  and  $P_N$  multigroup cross sections are following,

$$\sigma_{\ell tg}^{PN} = \frac{\int_g \sigma_t(E) W_\ell(E) dE}{\int_g W_\ell(E) dE}, \quad (4)$$

$$\sigma_{\ell g \leftarrow g'}^{PN} = \frac{\int_g dE' \int_g \sigma_\ell(E' \rightarrow E) W_\ell(E') dE'}{\int_g W_\ell(E') dE'}, \quad (5)$$

$$\sigma_{\ell g \leftarrow g'}^{SN} = \sigma_{\ell g \leftarrow g'}^{PN} \text{ for } g \neq g', \quad (6)$$

$$\sigma_{\ell g \leftarrow g}^{SN} = \sigma_{\ell tg}^{PN} - (\sigma_{\ell tg}^{PN} - \sigma_{0 tg}^{PN}) - \Delta_g^N, \quad (7)$$

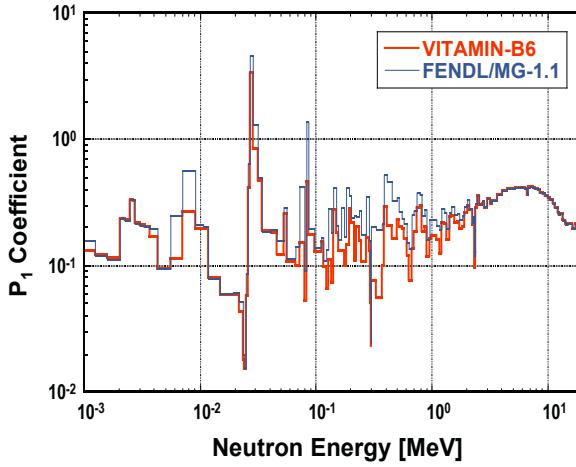
$$\sigma_g^{SN} = \sigma_{0 tg}^{PN} - \Delta_g^N, \quad (8)$$

where  $\sigma_\ell(E' \rightarrow E)$  is a scattering cross section and  $\Delta_g^N$  can be chosen to minimize the effects of truncating the Legendre expansion at  $\ell = N$ . “ $\Delta_g^N = 0$ ” is usually chosen, which is called “Consistent-P approximation”. In this case, Eqs. 7 and 8 become

$$\sigma_{\ell g \leftarrow g}^{SN} = \sigma_{\ell g \leftarrow g}^{PN} - (\sigma_{\ell tg}^{PN} - \sigma_{0 tg}^{PN}), \quad (9)$$

$$\sigma_g^{SN} = \sigma_{0 tg}^{PN}. \quad (10)$$

The difference between the  $S_N$  and  $P_N$  multigroup cross sections is only in Eq. 9. The term in parentheses of the right hand side in Eq. 9 is zero in VITAMIN-B6 because of Eq. 2, which leads  $\sigma_{\ell g \leftarrow g}^{SN} = \sigma_{\ell g \leftarrow g}^{PN}$ . However it is not always zero in FENDL/MG-1.1 because of Eq. 3, which leads  $\sigma_{\ell g \leftarrow g}^{SN} \neq \sigma_{\ell g \leftarrow g}^{PN}$ . Figure 4 shows the  $P_1$  coefficient of ingroup scattering cross section for natural iron. The  $P_1$  coefficient of the ingroup  $S_N$  scattering cross section  $\sigma_{\ell g \leftarrow g}^{SN}$  in VITAMIN-B6 is different from that in FENDL/MG-1.1 in the resonance energy region of natural iron. Note that the



**Fig. 4**  $P_1$  coefficient of ingroup  $S_N$  scattering cross section

ingroup  $S_N$  scattering cross section  $\sigma_{\ell g \leftarrow g}^{SN}$  in VITAMIN-B6 is almost the same as that in FENDL/MG-1.1 in the no-resonance region, because the weighting flux has a smooth shape in the no-resonance region.

The weighting flux for  $\ell \geq 2$  in Eq. 3 is different from that in Eq. 1, but its influence is considered to be not so large because the neutron spectra calculated with ANISN and FENDL/MG-1.1 are similar to those with MCNP as shown in Figs. 1 and 2.

### 3. Influences of Background Cross Section Data and Weighting Flux in VITAMIN-B6

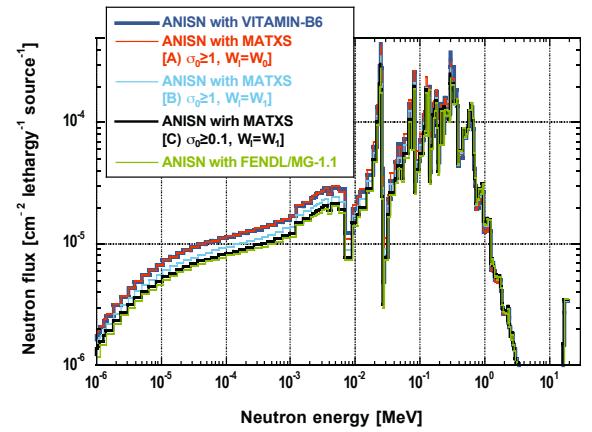
In order to examine influences due to the background cross section data and the weighting flux in VITAMIN-B6, three test MATXS files with the following conditions were produced from ENDF/B-VI by using NJOY99;

- A)  $\sigma_0 \geq 1, W_\ell = W_0$  (the same condition as that in VITAMIN-B6)
- B)  $\sigma_0 \geq 1, W_\ell = W_1$  (revised weighting flux)
- C)  $\sigma_0 \geq 0.1, W_\ell = W_1$  (the same condition as that in FENDL/MG-1.1)

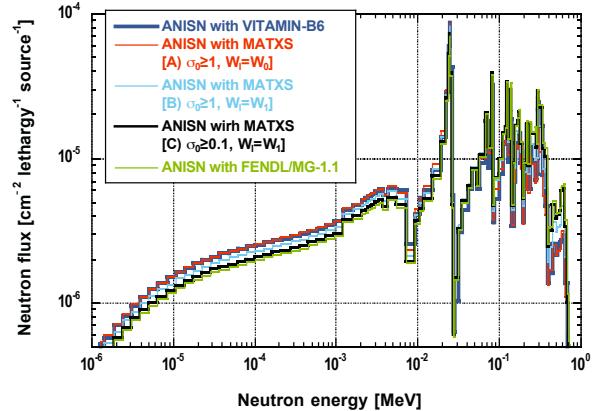
ANISN calculations with multigroup libraries produced from these MATXS files by using TRANSX were carried out. **Figures 5 and 6** show the results. The neutron spectra with the case A) MATXS file are almost the same as those with VITAMIN-B6. The neutron spectra with the case B) MATXS file are improved, but not completely. On the contrary, the neutron spectra with the case C) MATXS file are almost the same as those with FENDL/MG-1.1. It is demonstrated that the difference between the neutron spectra with VITAMIN-B6 and FENDL/MG-1.1 comes from both the inadequate background cross section data and weighting flux in VITAMIN-B6.

### 4. Processing Flow

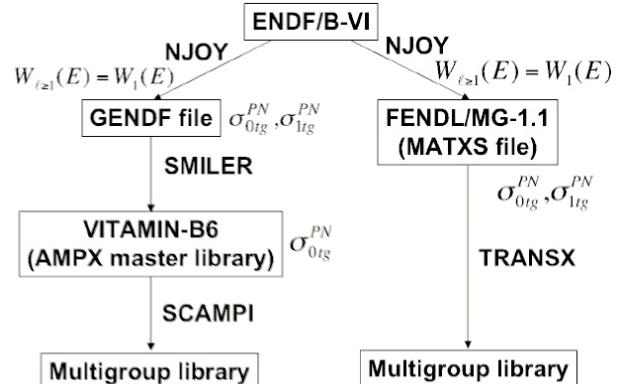
**Figure 7** shows the flow of processing nuclear data for VITAMIN-B6 and FENDL/MG-1.1. At the first step the NJOY code is used for both VITAMIN-B6 and



**Fig. 5** Neutron spectra at 40 cm from center of iron sphere



**Fig. 6** Neutron spectra at 80 cm from center of iron sphere



**Fig. 7** Processing flow in VITAMIN-B6 and FENDL/MG-1.1

FENDL/MG-1.1. However the SMILER code omits the  $\sigma_{1g}^{PN}$  in VITAMIN-B6 at the second step because the AMPX master format cannot include  $\sigma_{1g}^{PN}$ . Thus other multigroup libraries in the AMPX master format, e.g. BUGLE96 and HILO2K, also have the same problem for the weighting flux as VITAMIN-B6.

### IV. Conclusion

We carried out a simple benchmark calculation test with VITAMIN-B6 generated from ENDF/B-VI. The model of

this test consisted of an iron sphere of 1 m in radius with an isotropic 20 MeV neutron source in the center. The neutron spectra calculated with ANISN and FENDL/MG-1.1 agreed with those with MCNP, while those with ANISN and VITAMIN-B6 were at most 50 % different from those with MCNP.

We examined VITAMIN-B6 in detail in order to investigate reasons for the discrepancy. It was found out that VITAMIN-B6 had two problems :

- 1) The smallest background cross section of  $^{56}\text{Fe}$  in VITAMIN-B6 is 1, which is larger than that required for natural iron.
- 2) The weighting flux used in generating VITAMIN-B6 is not adequate.

These problems caused insufficient self-shielding correction, which leaded the discrepancy between neutron spectra with VITAMIN-B6 and FENDL/MG-1.1. VITAMIN-B6 should be revised based on this study. BUGLE96 and HILO2K also have the same problems.

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