Comment to VITAMIN-B6

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HILO2K is a new multigroup cross-section library for neutron and gamma energies to 2 GeV and 20 MeV, respectively. We performed a simple benchmark test in order to validate HILO2K. This benchmark test suggested that HILO2K has some problem. We investigated the problem and pointed out that the problem comes from insufficient self-shielding correction and inadequate scattering matrices in VITAMIN-B6, which provided much of the low energy data in HILO2K.

1. Introduction

Recently Oak Ridge National Laboratory prepared a new multigroup cross-section library, HILO2K [1], for neutron energy to 2 GeV and adopted it for neutronics calculations of the SNS project [2]. In this paper a simple benchmark test with HILO2K will be performed in order to validate HILO2K. Through this benchmark test, it is pointed out that the self-shielding correction in VITAMIN-B6 [3], which provided many of the low energy data in HILO2K, is insufficient and the scattering matrices in VITAMIN-B6 is inadequate.

2. Overview of HILO2K

HILO2K is an ANISN formatted multigroup cross-section library for neutron and gamma energies to 2 GeV (83 groups) and 20 MeV (22 groups), respectively. The nuclides included in HILO2K are ^{1}H, ^{2}H, He, Be, ^{10}B, ^{11}B, C, N, O, Na, Mg, Al, Si, S, K, Ca, Cr, Mn, Fe, Ni, Cu, Zr, Nb, Cd, Ba, Gd, Ta, W, Hg, Pb, ^{235}U and ^{238}U. The neutron (> 20 MeV) cross sections [42 groups] are based on data calculated with MCNPX [4]. The nonelastic scattering cross sections of ^{2}H, C, N, O, Al, Si, Ca, Cr, Fe, Ni, Cu, Nb, W, and Pb are normalized to those in LA150 [5]. On the contrary, the neutron (< 20 MeV) [41 groups] and gamma cross sections are obtained by collapsing VITAMIN-B6 (neutron 199 groups, gamma 42 groups, generated from ENDF/B-VI [6]), which has self-shielding correction with the Bondarenko method [7].

HILO2K has two versions with P_9 Legendre expansion; one is a standard version where all reaction data are taken into account, while the other is a modified version where a neutron collision with scattering angle cosines greater than 0.99 and with more than 95 % of the incident neutron energy was ignored in order to represent strongly forward peaked angular distributions in high energy region. Here we used the modified version.

3. Simple Benchmark Test

We performed a simple benchmark test to validate HILO2K. This benchmark test consisted of a concrete sphere or an iron sphere of 5 m in radius with an isotropic 2 GeV neutron source in the center. Neutron dose rates and neutron spectra in the sphere were calculated with the Sn code ANISN [8] and HILO2K. Calculations with MCNPX (neutron only mode. ENDF/B-VI was adopted for neutron cross section library below 20 MeV.), which is used to obtain neutron (> 20 MeV) cross sections of HILO2K, were carried out as a reference. It was judged through comparison between the ANISN and MCNPX calculations whether HILO2K has any problems.

The calculated neutron dose rates and neutron spectra in the spheres are shown in Figs. 1 - 5. In the concrete sphere the neutron dose rates are almost the same between the ANISN and MCNPX calculations and the discrepancy between the neutron spectra of the ANISN and MCNPX calculations was at most within 50 %, even on the sphere surface, 5 m from the center. This was not the case in the iron sphere, particularly at positions far from the center. The dose rate with ANISN was around 3 orders of magnitude smaller than that obtained with MCNPX at 4 m from the center. The calculated neutron spectra suggest that the large discrepancy in the dose rate mainly comes from the differences in the neutron flux below 1 MeV.

4. Problem in VITAMIN-B6 (1)

In order to investigate causes for the discrepancy in the neutron flux below 1 MeV, we examined VITAMIN-B6, which provided many of the low energy data in HILO2K. At first we found out the following problem; the smallest background cross section of ^{56}Fe in VITAMIN-B6 is 1, but natural iron requires a smaller background cross section of ^{56}Fe, around 0.2. It is considered that this problem leads to insufficient self-shielding correction and wrong neutron flux.

Then we performed a new ANISN calculation for the iron benchmark with two revised HILO2K libraries, HILO2K-r1 and HILO2K-r2, where neutron cross sections below 20 MeV were replaced with those of the smallest background cross section of ^{56}Fe is 10^{-5} and 1 b, respectively, processed by using NJOY99.67 [9] and TRANSX2.15 [10] from ENDF/B-VI. Figures 6 and 7 show the result. The ANISN calculation with HILO2K-r2 agrees with the MCNPX calculation best, but there is still difference. It is considered that this difference is due to the coarse group structure of HILO2K and limitation of the simple self-shielding correction.

Figures 6 and 7 also indicate that the ANISN calculation with HILO2K-r1 agrees with MCNPX calculation better than that with the original HILO2K. This result appears very strange since the smallest background cross section of HILO2K-r1 is the same as that of the original HILO2K. Next we investigate this phenomenon.

5. Problem in VITAMIN-B6 (2)

We still more comb through VITAMIN-B6 and found out that the ingroup scattering matrices of Legendre order $l \geq 1$ in HILO2K-r1 is different from those in VITAMIN-B6 or the original HILO2K as shown in Fig. 8. This difference causes from whether the transport approximation (consistent-P approximation) [9] is applied. The consistent-P approximation for a group g is the following approximation;

$$\sigma_{l\ g\leftarrow g}^{SN} = \sigma_{l\ g\leftarrow g}^{PN} - (\sigma_{ltg}^{PN} - \sigma_{0tg}^{PN}), \tag{1}$$

$$\sigma_{g}^{SN} = \sigma_{0tg}^{PN}, \tag{2}$$

$$\sigma_{ltg}^{PN} = \frac{\int_g \sigma_t(E) W_l(E) dE}{\int_g W_l(E) dE}, \tag{3}$$

$$\sigma_{l\ g\leftarrow g}^{PN} = \frac{\int_g dE' \int_g dE \sigma_t(E' \rightarrow E) W_l(E')}{\int_g dE'\, W_l(E')}, \tag{4}$$

$$W_l(E) = \frac{C(E)}{[\sigma_0 + \sigma_t(E)]^{l+1}}, \tag{5}$$

where PN means PN cross sections, SN means SN cross sections, l is Legendre order, σ_t is the total cross section, $W_l(E)$ is a weight function, $C(E)$ is a smooth function of neutron energy E, and σ_0 is the background cross section. HILO2K-r1 has the consistent-P approximation. On the contrary, no transport approximation seems to be applied to VITAMIN-B6 or the original HILO2K since the term in parentheses in the right side of Eq. (1) is neglected. Therefore the ingroup scattering matrices of Legendre order $l \geq 1$ in VITAMIN-B6 or the original HILO2K is not adequate. We also confirmed that the ANISN calculation by using HILO2K-r1 without the consistent-P approximation agreed with that by using the original HILO2K. It is concluded that this is the reason of the ANISN calculation with HILO2K-r1 agrees with MCNPX calculation better than that with the original HILO2K in the iron sphere benchmark test.

The term in parentheses in the right side of Eq. (1) is very small since $W_l(E)$ is a smooth function of neutron energy E and σ_{ltg}^{PN} is almost the same as σ_{0tg}^{PN} if the self-shielding effect is small. Thus the effect of no transport approximation in VITAMIN-B6 or the original HILO2K does not appear in the concrete sphere benchmark test, where the self-shielding effect is small.

It should be noted that multigroup libraries for shielding, such as JSSTDL [11], often have no transport approximation and that they cause the same problem as VITAMIN-B6.

6. Conclusion

We investigated the validity of the multigroup library HILO2K for neutron energy to 2 GeV through the simple benchmark tests, which consisted of a concrete sphere or an iron sphere of 5 m in radius with an isotropic 2 GeV neutron source in the center, with ANISN and MCNPX. The benchmark tests indicated that ANISN with HILO2K gave similar results as MCNPX in the concrete sphere, while the ANISN calculation with HILO2K was very different from the MCNPX one in the iron sphere.

We examined VITAMIN-B6, from which the low energy data in HILO2K come, since this discrepancy appeared in neutron flux below 1 MeV. It was concluded that the discrepancy between the ANISN and MCNPX calculations for the iron sphere was due to the smallest background cross section 1 of ^{56}Fe in VITAMIN-B6 and no transport approximation (consistent-P approximation), which produced inadequate multigroup cross sections for materials with large self-shielding effect .

We generated a natural iron multigroup library below 20 MeV without the above two defects by using ENDF/B-VI, NJOY and TRANSX and replaced the natural iron multigroup library below 20 MeV in HILO2K by the new one. This new natural iron multigroup library improved the discrepancy between the ANISN and MCNPX calculations in the iron sphere. The next version of HILO2K will contain this newly generated natural iron multigroup library below 20 MeV.

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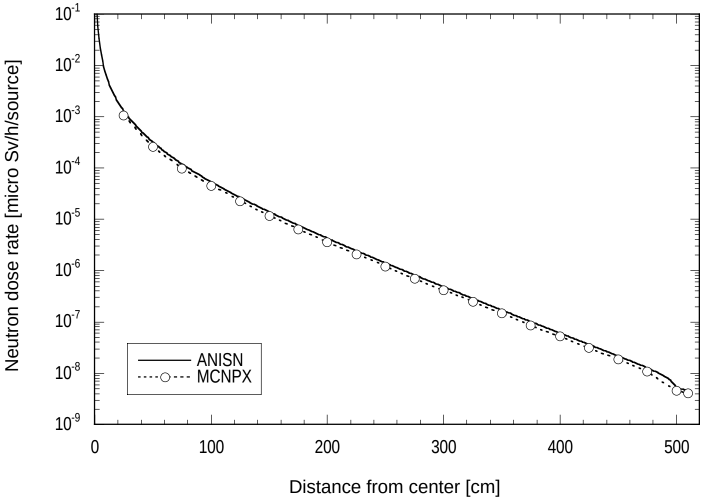

Fig. 1 Calculated neutron dose rates in the concrete sphere.

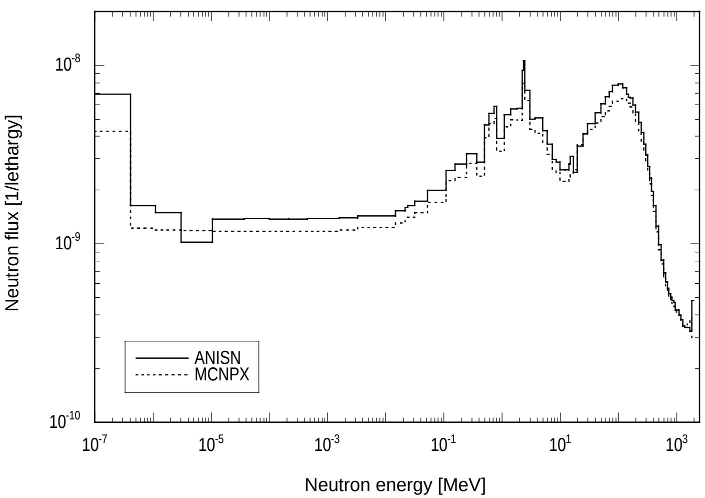

Fig. 2 Calculated neutron spectra at 4 m from the center in the concrete sphere.

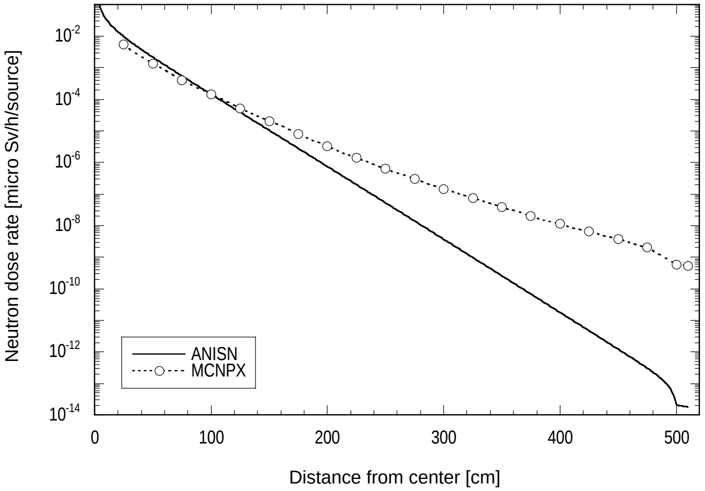

Fig. 3 Calculated neutron dose rates in the iron sphere.

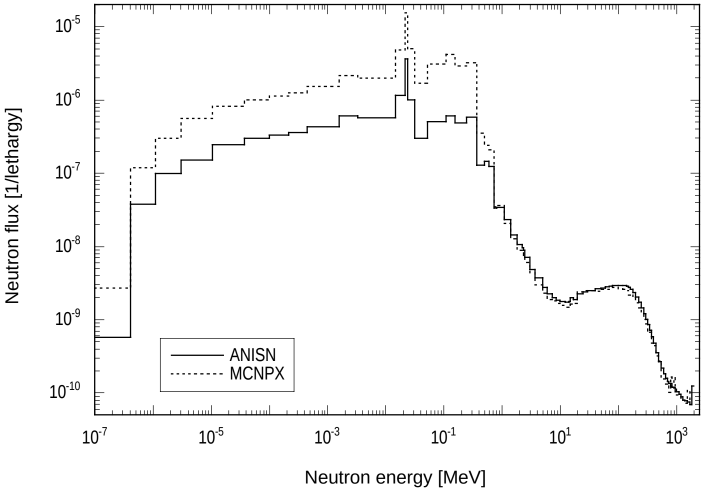

Fig. 4 Calculated neutron spectra at 2 m from the center in the iron sphere.

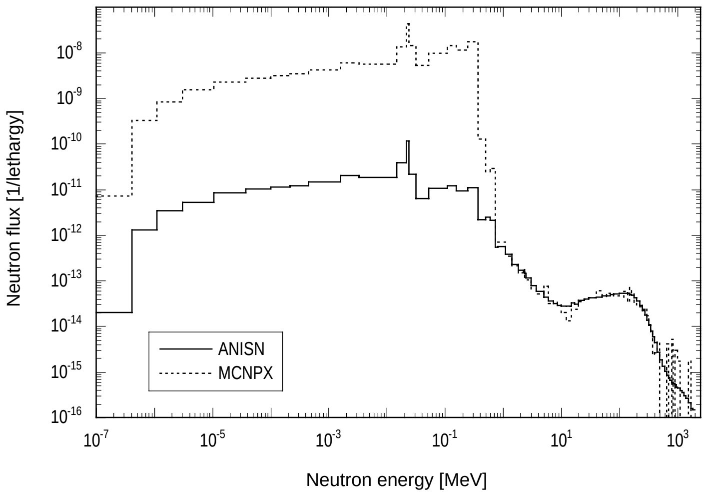

Fig. 5 Calculated neutron spectra at 4 m from the center in the iron sphere.

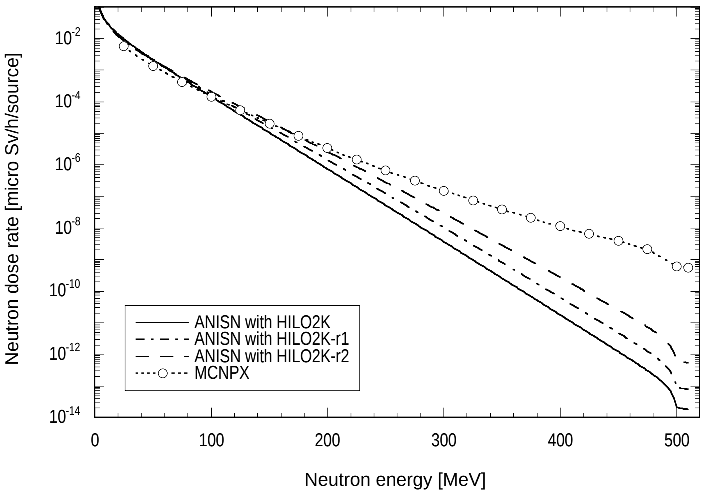

Fig. 6 Calculated neutron dose rates in the iron sphere.

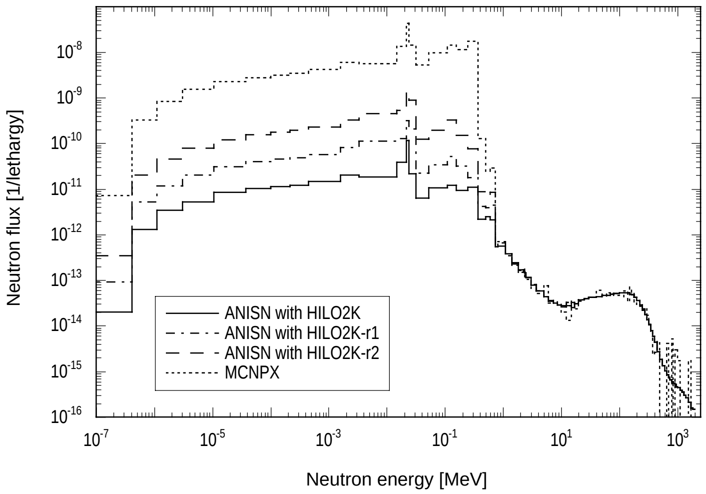

Fig. 7 Calculated neutron spectra at 4 m from the center in the iron sphere.

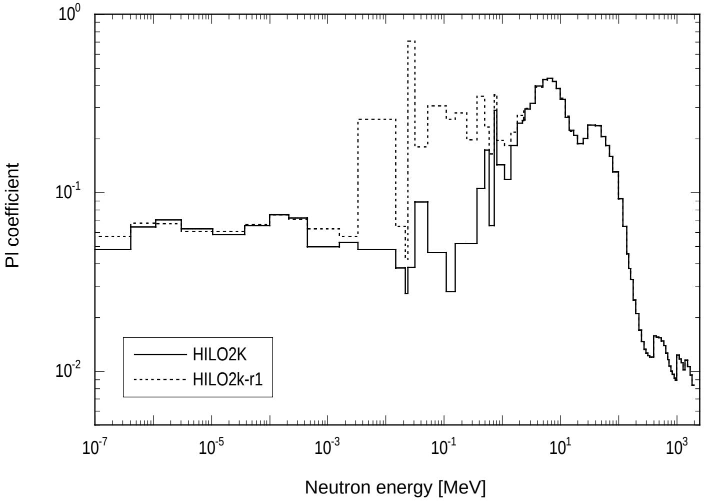

Fig. 8 Legendre coefficient of l =1 of ingroup scattering matrices for natural iron.