Short Comments to ^{56}Fe of FENDL/MG-2.0

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Dr. Kodeli pointed out a large discrepancy between neutron spectra below 1.5 keV calculated by MCNP and ANISN with the FENDL-2 library for an iron sphere benchmark, which consisted of an iron sphere of 10 cm in radius with 14 MeV neutron source in the center. Reasons of the discrepancy were investigated in detail. The benchmark calculations with FENDL-1, FENDL-2 and EFF-3.1 by ANISN and MCNP suggested that FENDL/MG-2.0 ^{56}Fe data have some problems. It was identified that reasons of the discrepancy are the LIST data of the first neutron energy of the FILE6 in FENDL/E-2.0 ^{56}Fe, through the detail check of the original libraries of ^{56}Fe of FENDL-1, FENDL-2 and EFF-3.1. The FENDL/MG-2.0 ^{27}Al data also have the same problem, though the influence is small.

1. Introduction

At the EFF meeting in April and November, 1999, Dr. Kodeli pointed out that there was a large discrepancy between neutron spectra below 1.5 keV calculated by MCNP and ANISN with the FENDL-2 [1] library for an iron sphere benchmark, which consisted of an iron sphere of 10 cm in radius with 14 MeV neutron source in the center. [2,3] We investigated reasons of that discrepancy in detail.

2. Iron Sphere Benchmark Calculation

At first we carried out an iron benchmark calculation similar with one which Dr. Kodeli did in order to confirm the large discrepancy between neutron spectra below 1.5 keV calculated by MCNP and ANISN. The iron assembly was a natural iron sphere of 10 cm in radius (atomic density : 0.083 /barn/cm) and a point neutron source with uniform distribution in energy interval 13.84 – 14.19 MeV covering group 8 of the VIATMIN-J [4] group structure was set in the center of the iron sphere as shown in Fig. 1. A neutron spectra at the distance of 15 cm from the center of the iron sphere was compared.

We used the MCNP-4A [5] and ANISN (included in the DOORS 3.2 package [6]) codes. The iron sphere was modeled in 1D spherical geometry. The nuclear data library for MCNP was

FENDL/MC-2.0 [7], while the P_5 multigroup library for ANISN with self-shielding correction was generated from FENDL/MG-2.0 [7] by the TRANSX2.15 [8] code. Calculations with the FENDL-1 [9] nuclear data library were also performed for comparison. The inputs were the same as those for FENDL-2 except for the nuclear data library part.

The calculated neutron spectra are shown in Figs. 2 and 3. As Dr. Kodeli pointed out, there is a large discrepancy between neutron spectra below 1.5 keV calculated by MCNP and ANISN in the case of FENDL-2, while there is no large discrepancy in the case of FENDL-1. Since the neutron spectra have no rapid change around 1.5 keV in the MCNP and ANISN calculations of FENDL-1 and the MCNP calculation of FENDL-2, it is considered that the iron data of FENDL/MG-2.0 have some problems. The ^{56}Fe data of FENDL-2 is that of EFF-3.0, while the data of other iron isotopes are those of FENDL-1. It is concluded that the ^{56}Fe data of FENDL/MG-2.0 cause the discrepancy. The ^{56}Fe data of FENDL/MG-2.0 was generated with NJOY94.105, which is an older version of the NJOY code [10]. We reprocessed FENDL/E-2.0 ^{56}Fe with the newer version NJOY97.95 and recalculated a neutron spectrum by ANISN with this newly processed library. The result was, however, the same as the previous calculation.

Recently a new evaluation EFF-3.1 ^{56}Fe [11], which was re-evaluated based on EFF-3.0 ^{56}Fe, was released only for EFF members. In order to examine whether the same phenomena as EFF-3.0 ^{56}Fe appears in EFF-3.1 ^{56}Fe, we performed the benchmark calculation by ANISN and MCNP with EFF-3.1 ^{56}Fe and other iron isotopes of FENDL-2. We used the official ace file of EFF-3.1 ^{56}Fe in EFF members for MCNP, which Dr. Trkov processed [12] with NJOY. A matxs file of EFF-3.1 ^{56}Fe was newly generated with NJOY97.95 for the multigroup library for ANISN. The rapid change of neutron spectrum around 1.5 keV does not appear in this ANISN calculation.

3. Double Differential Cross section Data Reconstructed from Multigroup Libraries

In order to specify problems included in FENDL/MG-2.0 ^{56}Fe, we reconstructed double differential cross section (DDX) data from 175 group multigroup libraries generated from the ^{56}Fe matxs files of FENDL-1, -2 and EFF-3.1 and compared each other. As the result, we found out that the only DDX data of FENDL-2 ^{56}Fe have huge sharp peaks around 1.5, 2.5 and 3.5 keV in the incident neutron energies of groups 28-33 (4.4933 - 6.0653 MeV), 11-12 (12.214 - 12.84 MeV) and 13-14 (11.052 - 12.214 MeV), respectively, as shown in Fig. 4. Particularly the peak around 1.5 keV in the incident neutron energy of group 32 is very large. This peak energy, 1.5 keV, is the same as the energy, below which the neutron spectra calculated by MCNP and ANISN with FENDL-2 were different. The reason of the discrepancy is considered to be this huge peak in the DDX.

4. Comparison of ^{56}Fe among FENDL/E-1.1, FENDL/E-2.0 and EFF-3.1

Next we checked the original libraries of ^{56}Fe in FENDL/E-1.1, FENDL/E-2.0 and EFF-3.1 in detail. The FILE2, FILE3 and FILE4 data seemed to have no problem. But we detected two different points for the FILE6. One point is the reference system of secondary energy and angle; the laboratory (LAB) coordinates are used in FENDL/E-1.1, while the center-of mass (CM) coordinates are used in FENDL/E-2.0 and EFF-3.1, though all the libraries use Legendre coefficients for the angular presentation of the FILE6. The other point is the LIST data of the first incident neutron energy. Figure 5 shows the LIST data of the first incident neutron energy in FILE6, MT91. The highest secondary energy is 1 x 10^{-5} eV in FENDL-1 and EFF-3.1, while it is 1 eV in FENDL-2 (the difference of the b_0 data is due to normalization and interpolation scheme). From these two points, we suspected that the GROUPR module of NJOY could not deal with the LIST data of the first incident neutron energy of the FILE6 in FENDL-2 ^{56}Fe correctly since the CM to LAB conversion in the GROUPR module of NJOY seemed to have no problem in EFF-3.1 ^{56}Fe. Then we modified the highest energy and b_0 data of the LIST data of the first incident neutron energy of all the MTs (MT16, MT22, MT28 and MT91) in FENDL/E-2.0 ^{56}Fe to those in EFF-3.1 ^{56}Fe, made a new matxs file of FENDL-2 ^{56}Fe with NJOY97.95 and executed the ANISN calculation with the multigroup library generated from the new matxs file. The calculated neutron spectrum is shown in Fig. 6 with the previous MCNP result. The discrepancy between the ANISN and MCNP calculations disappears. Figure 7 plots the DDX data reconstructed from 175 group multigroup libraries generated from the original and modified ^{56}Fe matxs files of FENDL-2. The huge peak around 1.5 keV disappears in the modified FENDL-2 ^{56}Fe. It is concluded that the GROUPR module of NJOY can not deal with the LIST data of the first incident neutron energy of the FILE6 in FENDL/E-2.0 ^{56}Fe correctly. On the contrary, the ACER module of NJOY can process the LIST data of the first incident neutron energy of the FILE6 in FENDL/E-2.0 ^{56}Fe without problem, since the MCNP calculation shows no strange results.

5. FENDL/MG-2.0 ^{27}Al

The ^{27}Al data of FENDL/E-2.0 are also from EFF3.0. Since the highest energy and b_0 data in the LIST data for the first incident neutron energy of the FILE6 of FENDL/E-2.0 ^{27}Al have the same as those of FENDL/E-2.0 ^{56}Fe, the same trouble may appear in calculations with FENDL/MG-2.0 ^{27}Al. Figure 8 shows calculated leakage neutron spectra (at the distance of 15 cm from the center of an aluminum sphere) for an aluminum sphere of 10 cm in radius with 14 MeV neutron source in the center by ANISN and MCNP with FENDL-2. The large discrepancy between ANISN and MCNP calculations does not appear in ^{27}Al seemingly. The FENDL/MG-2.0 ^{27}Al data, however, have the same huge sharp peak as FENDL/MG-2.0 ^{56}Fe as shown in Fig. 9. Probably the reason why the discrepancy does not appear is because the sharp peak in FENDL/MG-2.0 ^{27}Al is smaller by one order than that in FENDL/MG-2.0 ^{56}Fe.

6. Conclusion

We investigated reasons of a large discrepancy between neutron spectra below 1.5 keV calculated by MCNP and ANISN with the FENDL-2 library for an iron sphere benchmark, which consisted of an iron sphere of 10 cm in radius with 14 MeV neutron source in the center. The benchmark calculations with FENDL-1, FENDL-2 and EFF-3.1 by ANISN and MCNP suggested that FENDL/MG-2.0 ^{56}Fe causes the discrepancy. Through the detail check of the original and multigroup libraries of ^{56}Fe of FENDL-1, FENDL-2 and EFF-3.1, it is identified that reasons of the discrepancy are the LIST data of the first incident neutron energy of the FILE6 in FENDL/E-2.0 ^{56}Fe. We recommend revising the FENDL/MG-2.0 ^{56}Fe data. The FENDL/

MG-2.0 ^{27}Al data have the same problem, though the influence is small. We also recommend revising FENDL/MG-2.0 ^{27}Al.

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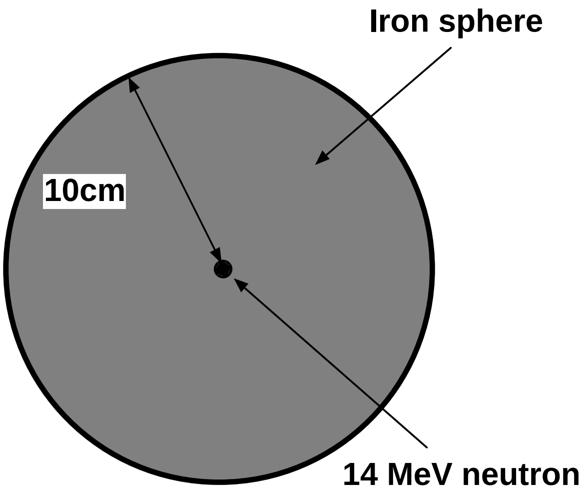

Fig.1 Calculation model.

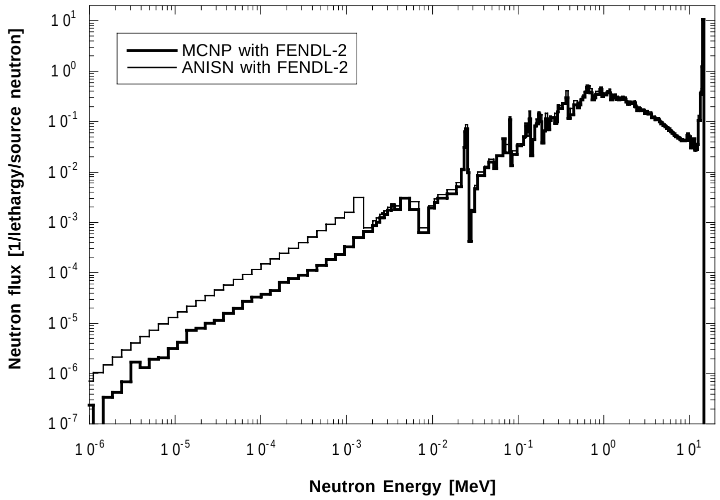

Fig. 2 Calculated neutron spectra at the distance of 15 cm from the center of the iron sphere (FENDL-2).

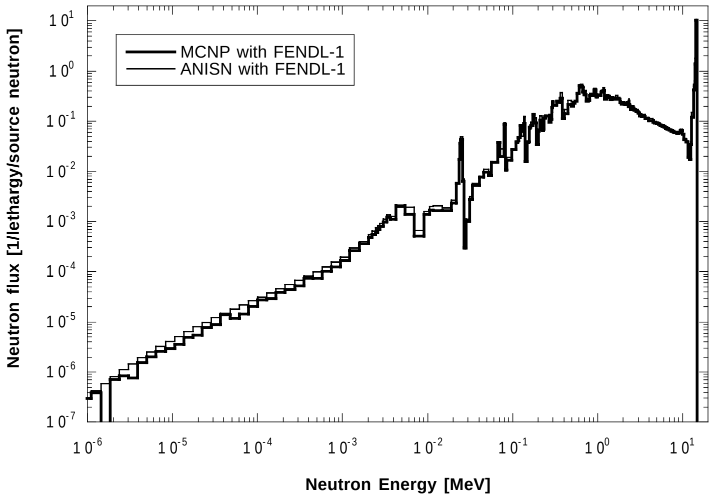

Fig. 3 Calculated neutron spectra at the distance of 15 cm from the center of the iron sphere (FENDL-2).

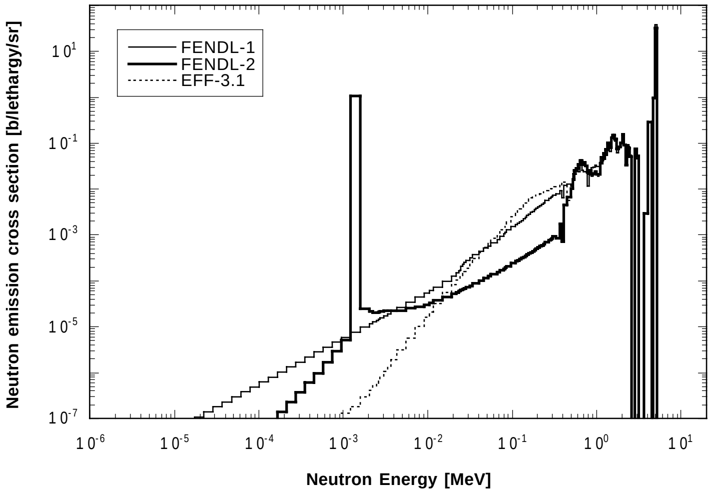

Fig. 4 ^{56}Fe DDX reconstructed from 175 group multigroup libraries in the incident neutron energy of group 31 (4.9659 – 5.2205 MeV) and the emission angle of 0 degree.

```
0.000000+0  4.620600+6           0           0          4      22631 6 91 8331
0.000000+0  1.000000+5  1.000000-5  0.000000+0                  2631 6 91 8332
```

(a) FENDL-1 (interpolation scheme is histogram)

```
  .00000+ 0   4.61780+ 6           0           0          4     22631 6 9111120
  .00000+ 0   2.00000+ 0  1.00000+ 0    .00000+ 0                 2631 6 9111121
```

(b) FENDL-2 (interpolation scheme is linear-linear)

```
0.000000+0  4.617800+6           0           0          4      22631 6 91      7
0.000000+0  2.000000+5  1.000000-5  0.000000+0                  2631 6 91      8
```

(c) EFF-3.1 (interpolation scheme is linear-linear)

Fig. 5 LIST data of FILE6, MT91 in ^{56}Fe of FENDL-1, FENDL-2 and EFF-3.1.

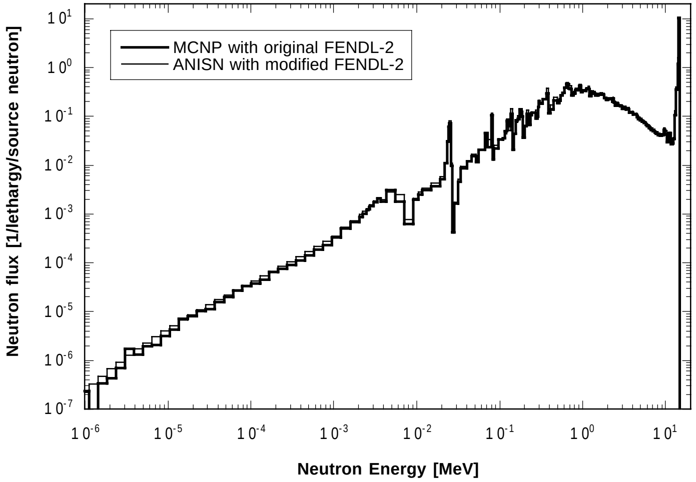

Fig. 6 Calculated neutron spectra at the distance of 15 cm from the center of the iron sphere (MCNP with original FENDL-2, ANISN with modified FENDL-2).

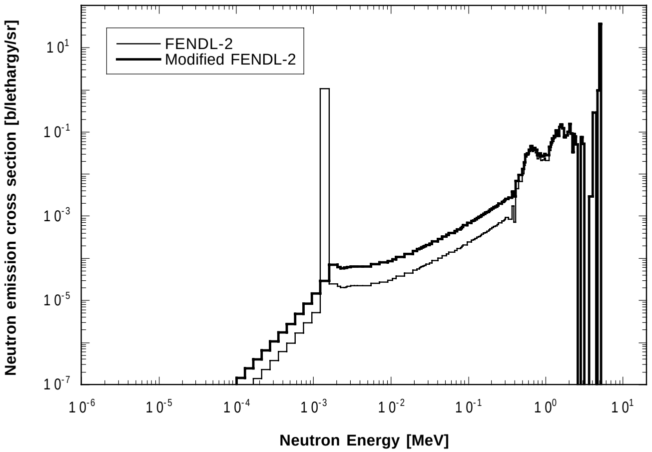

Fig. 7 ^{56}Fe DDX reconstructed from 175 group multigroup libraries of the original and modified FENDL-2 in the incident neutron energy of group 31 (4.9659 – 5.2205 MeV) and the emission angle of 0 degree.

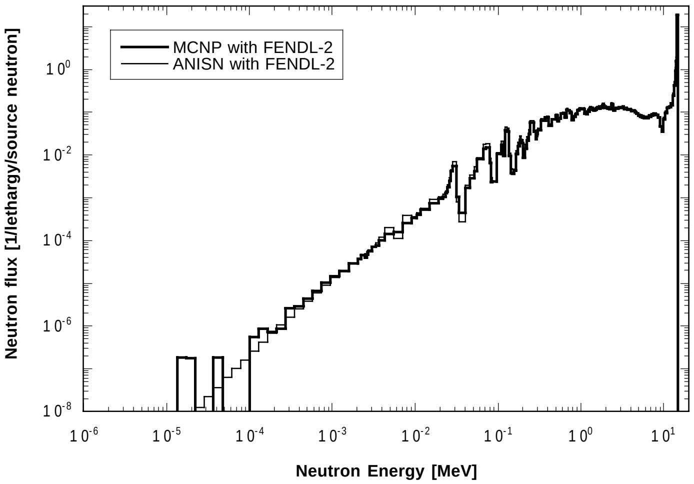

Fig. 8 Calculated neutron spectra at the distance of 15 cm from the center of the iron sphere (FENDL-2).

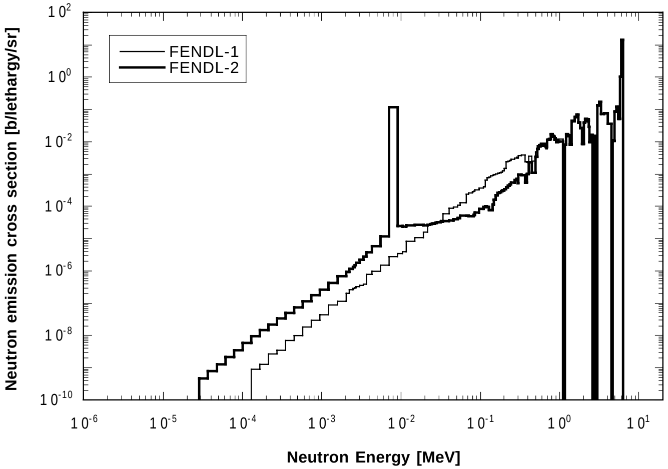

Fig. 9 ^{27}Al DDX reconstructed from 175 group multigroup libraries in the incident neutron energy of group 27 (6.0653 – 6.3763 MeV) and the emission angle of 0 degree.