Analysis of cross sections on iron and oxygen using Cf-252 neutron source

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Abstract. The leakage neutron spectra measurements have been done on benchmark spherical assemblies with Cf-252 source in center of 1) heavy water sphere with diameter of 30 cm (with Cd cover) and of 2) iron spheres with diameter of 100 cm and 50 cm. It has been stated for years that transport calculations by iron overestimate measured spectra in energy region around 300 keV by about 20-40 % (calculation to measurement ratio C/E = 1.2-1.4). The influence of an artificial changes in cross-section XS-Fe-56 (n,elastic)designed by IAEA, Nuclear Data Section, has been studied on the iron spheres. Influence of those XS-corrections to calculated neutron spectrum is presented.

1 Introduction
Validation of 56Fe and 16O cross section has been performed in Research Centre Rez (RC) in accordance with CIELO [1] project requirements. It has been stated for years that calculations for iron overestimate measured spectra in energy region around 300 keV by about 20-40 %, i.e., determination of calculation to experiment ratio C/E = 1.2-1.4 and also around 600 keV by about 12-15 %. The C/E around 300 keV grows with iron thickness, B. Jansky [2], [3]. R. Capote, A. Trkov and S. Simakov from IAEA-NDS changed cross-section of 56Fe producing new ND library IND-R22 and IND-R34 (IND - INDEN conference 2018, [4]) to test influence of such change.

2 Experimental and calculation methods

2.1 Experimental setup
Determination of C/E ratio of leakage neutron spectra from iron and heavy water spheres with Cf-252 neutron source in center was done for 4 libraries IND-R22, IND-R34, CIELO and JEFF-3.2T2 for 56Fe and CIELO for 16O. The following assemblies were used for measurement and calculation: 1) heavy water sphere with diameter of 30 cm (with Cd cover) and 2) iron spheres with diameter of 100 cm and 50 cm. Each assembly had certain acronym, e.g., FE100R150 is Fe assembly with the diameter of 100 cm and the distance of 150 cm between sphere and detector (center to center). At first, the leakage neutron (and gamma) spectrum from spherical assemblies with Cf-252 in center was measured together with background. Then, the background itself was measured with shielding cone placed between the sphere and detector. To get “pure” leakage spectrum, the measured background was subtracted from the first measurement.

2.2 Calculation
The calculations were performed using Monte-Carlo code MCNP with nuclear data library CIELO (i.e., ENDF/B-VIII.0) and JEFF-3.2T2. As for calculation geometry description, a simplified model was used, which substitutes assembly elements with concentric spherical shells around the source. Also, the MCNP model of detector is represented by a 1 cm thick spherical shell with radius equal to the real distance R of detector and source. For each calculation 10⁸ -10⁹ particle histories were computed.

Figure 1. Hydrogen proportional detector of NOK-445 type.

2.3 Spectrometry
Two hydrogen proportional spherical detectors (HPD) K4 and K8 with diameter of 40 mm were used in neutron spectrometer [5]. The detector K4 with pressure 400 kPa was used for measurement in the energy range Eₘ = 0.01-0.7 MeV, the detector K8 with pressure 1000 kPa was used for measurement in the energy range Eₘ = 0.2 -1.3 MeV, see
Figure 1. Stilbene spectrometer was used for measurement in the range $E_n = 1-10$ MeV. The HPD measured and calculated spectra were evaluated in two group structures: 40 gpd, it corresponds to the lethargy step about 6 % and in structure 200 gpd, i.e., with lethargy step 1 %. The common energy structure for stilbene had step of 100 keV.

2.4 Uncertainties

Uncertainty of single measurement is composed of uncertainty of the “A-type” that includes statistical uncertainty in measurement (in channel) and consequent calculation of each energy group and uncertainty of “B-type” that includes influence of apparatus instability, of benchmark geometry and detector position, neutron source position, detector discharges, energy calibration, during time remote repeated measurements. Uncertainties of A–type of the integral values presented in tables 1-3 are in interval from 0.3 to 5 %. Uncertainty of “B-type” we estimate 2-4 %. Uncertainties of MCNP calculations are better than 1 % in energy interval 0.1-1.3 MeV and better than 5 % in energy interval 1-5MeV, [6].

2 Validation of $^{16}$O cross section

Validation of $^{16}$O cross section was performed on D2O30R100 assembly. Neutron spectrum was measured by 2 HPDs K4 and K8 (Research Centre Rez) and stilbene (Military Academy Brno, F. Cvachovec, [6]). The CIELO (ENDF/B-VIII.0) was used for calculation. Results of C/E are in Figures 2 (table) and 3 (graph).

4 Analysis of $^{56}$Fe(n, el) cross section

4.1 Energy region 300 keV

Results of validation of 4 different ND libraries including corrected ND IND-R22 and IND-R34 in the energy region $E_n < 1$ MeV are in Figure 4 (table) and Figure 5 (graph), [2], [3], [8].

| $E_n$ [MeV] | To | CIELO | JEFF-3.2T2 | IND-R22 | IND-R34 |
|------------|----|-------|------------|---------|---------|
| 0.013      | 1.290 | 1.0450 | 1.0520 | 1.0460 | 1.0290 |
| 0.033      | 0.060 | 0.9005 | 1.0190 | 0.9890 | 1.0940 |
| 0.060      | 0.090 | 0.9702 | 0.9894 | 1.0720 | 1.1290 |
| 0.090      | 0.150 | 0.9934 | 1.0070 | 1.1150 | 1.0130 |
| 0.150      | 0.200 | 1.0370 | 1.0070 | 1.1790 | 1.0900 |
| 0.200      | 0.250 | 1.0280 | 1.0130 | 1.1670 | 1.0390 |
| 0.250      | 0.289 | 1.0360 | 1.0050 | 0.9749 | 0.9561 |
| 0.289      | 0.333 | 1.3330 | 1.2290 | 1.0140 | 0.9150 |
| 0.333      | 0.367 | 1.3050 | 1.2680 | 1.0640 | 0.9819 |
| 0.367      | 0.410 | 1.1910 | 1.1710 | 0.8036 | 1.0450 |
| 0.410      | 0.520 | 1.0330 | 1.0810 | 0.9663 | 1.0170 |
| 0.520      | 0.780 | 1.0890 | 1.0620 | 1.0430 | 1.0440 |
| 0.780      | 1.060 | 0.7834 | 1.0490 | 0.9974 | 0.9984 |
| 1.060      | 1.290 | 0.7584 | 0.8654 | 1.0510 | 1.0530 |

Figure 4. Comparison of calculated and measured spectra - assembly FE100R53, “HPD region”, E: HPD, C: CIELO, JEFF, IND-R22 and IND-R34.

4.2 Comparison of ND libraries on two Iron Benchmarks

The measurements were performed on iron spheres with diameter of 50 cm (FE50) and of 100 cm (FE100). Two type of spectrometry results were used for cross section
validation:

1) FE100R53, $E_{th} = 0.013-1.3$ MeV, “HPD” region
2) FE50R100, $E_{th} = 0.8-17$ MeV, “stilbene region”

The spectra in the stilbene region were averaged from 4 independent measurements (L.A. Trykov [3], F. Cvachovec [6], M. Košt’ál - stilbene type and J. Adams "ROSPEC" type-HPD [9]) to minimize uncertainty of “B-type” in individual authors methodology of measurement, gamma discrimination, evaluation. Cf neutron source properties description, see [8], [9]. The cross section of $^{56}$Fe(n,el) isotope is dominant iron reaction in energy region $E_{th} < 0.7$ MeV. Moreover $^{56}$Fe has 92 % share in iron. Results of IND-R22 and IND-R34 with corrected $^{56}$Fe(n,el) cross section validation and also of CIELO and JEFF-3.2T2 are in the Figures 4 (table), Figure 5 (graph) and Figures 6 (table), Figure 7 (graph).

4.3 Influence of spectrometer resolution on spectra assessment

Measurements and calculations use 200 gpd energy structure, i.e., lethargy step is about 1 %. Spectrometer with HPD has relatively good resolution, because in the energy interval 200-400 keV 4-6 peaks are visible: 218, 242, 272, 309, 352 and 375 keV. See Figure 5. Other spectrometers that use stilbene or TOF method resolve usually only one “thick” peak at 300 keV in the region 200-400 keV. Results are in Figure 4 and Figure 5. Correction of $^{56}$Fe(n,el) cross section is in the Figure 8, where CIELO is compared with IND-R34 data version.

| $E_{th}$(MeV) | C/E ratio |
|---------------|-----------|
| From | To | CIELO | JEFF-3.2T2 | IND-R22 | IND-R34 |
| 0.8 | 0.9 | 0.892 | 0.921 | 1.120 | 0.979 | 0.979 |
| 0.9 | 1.0 | 0.957 | 0.957 | 1.080 | 1.038 | 1.038 |
| 1.0 | 1.2 | 0.874 | 0.941 | 0.967 | 0.967 |
| 1.2 | 1.4 | 0.868 | 0.971 | 1.034 | 1.034 |
| 1.4 | 1.6 | 0.773 | 0.901 | 0.971 | 0.971 |
| 1.6 | 1.8 | 0.893 | 1.032 | 1.083 | 1.083 |
| 1.8 | 2.0 | 0.913 | 1.095 | 1.116 | 1.116 |
| 2.0 | 3.0 | 0.852 | 1.114 | 1.044 | 1.044 |
| 3.0 | 4.0 | 0.817 | 1.193 | 1.089 | 1.089 |
| 4.0 | 5.0 | 0.843 | 1.200 | 1.064 | 1.064 |
| 5.0 | 6.0 | 0.857 | 1.022 | 1.035 | 1.035 |
| 6.0 | 7.0 | 0.874 | 1.029 | 1.020 | 1.020 |
| 7.0 | 8.0 | 0.878 | 1.040 | 1.013 | 1.013 |
| 8.0 | 9.0 | 0.940 | 1.110 | 1.083 | 1.083 |
| 9.0 | 10.0 | 0.912 | 1.058 | 1.041 | 1.041 |
| 10.0 | 12.0 | 0.895 | 0.975 | 0.983 | 0.983 |
| 12.0 | 14.0 | 0.799 | 0.803 | 0.824 | 0.824 |
| 14.0 | 16.0 | 0.672 | 0.638 | 0.673 | 0.673 |

Figure 6. Comparison of calculated and measured spectra - assembly FE50R100, “stilbene region”. C: CIELO, JEFF-3.2T2, IND-R22, IND-R34.

5 Conclusion

Validation of $^{16}$O cross section - Figure 2 (table) and Figure 3 (graph), assembly D2O30R100, C/E = 1.02-1.09, C/E = 1.18 for 7-10 MeV - proves that calculation systematically slightly overestimates the measurement.

Analysis of $^{56}$Fe(n,el) cross section - Figure 4 (table) and Figure 5 (graph), IAEA corrections for $E_{th} = 0.013-0.7$ MeV, “HPD region” - shows that changes of Fe cross section in IND-R34 ND bring better agreement in C/E, but changes affect other surrounding energy regions. Undesirable changes of C/E ratio for correction performed in IND-R34 opposite to IND-R22 are in following energy intervals ($E_{th}$ is in MeV):

$E_{th}=0.033-0.060$: C/E increases from 0.989 to 1.094
$E_{th}=0.060-0.090$: C/E increases from 1.072 to 1.129
$E_{th}=0.289-0.333$: C/E decreases from 1.014 to 0.915

Analysis of $^{56}$Fe(n,el) cross section - Figure 6 (table), energy region $E_{th} = 0.8-1.6$ MeV, “stilbene region” - proves that for CIELO all values of C/E are very low, i.e., calculation underestimates measurements systematically by 5-20 %. Calculation with data versions IND-R22 and IND-R34 exhibits better values than CIELO and JEFF in mentioned region. The ratio C/E = 1.08-1.12 for both IND-R22 and IND-R34 libraries is worse in energy region $E_{th} = 1.6-2$ MeV than in the other.

It seems to be important to reassess the creation of the $^{56}$Fe(n,el) cross section, e.g. M. Diakaki, CEA Cadarache, [10].

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Figure 7. Comparison of calculated and measured spectra - FE50R100, “stilbene region”. E: red line, C: IND-R34, blue line.
Figure 8. Cross section of $^{56}\text{Fe}(n,\text{tot})$ comparison: CIELO (black), R34 (blue), R34/CIELO - norm = 1000 (red).

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