

Integral Data Test of FENDL-2 Fusion Nuclear Data Library with Neutronic Integral Experiments

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FENDL-2, the latest version of Fusion Evaluated Nuclear Data Library, had been developed based on selection of evaluated data from ENDF/B-VI, JENDL-3, JENDL-FF, BROND-2 and EFF-3 and distributed for benchmark analysis recently. Integral data test of FENDL-2 has been performed to qualify and validate the working library with a variety of neutronic integral experiments. Calculations and analyses of neutron leakage spectra and reaction rates have been performed with the three dimensional Monte Carlo transport code MCNP and FENDL-2 data library. The results have been compared with the measured results as well as the results obtained previously with FENDL-1, EFF, JENDL-FF

KEYWORDS: *Fusion, nuclear data library, benchmark, calculation, neutronic experiment, integral data test, neutron spectrum, reaction rate, data evaluation, spherical shell, combined assembly, 14 MeV neutron*

I. Introduction

The Fusion Evaluation Nuclear Data Library (FENDL) is a compilation of fusion-oriented data evaluations selected from the national nuclear data files ENDF/B (USA), BROND (Russian Federation), JENDL (Japan) and EFF (Europe) in an international effort initiated and coordinated by the IAEA Nuclear Data Section.

The first version of the file, FENDL/E-1, has been compiled and released ⁽¹⁾. And the file has served as the reference library for design calculations in the Engineering Design Activity (EDA) phase of the International Thermonuclear Experimental Reactor (ITER) project.

The second version of the file, FENDL/E-2 ⁽²⁾, contains evaluated neutron, photon-atom and photon production cross sections, in ENDF format, with resonance parameters where appropriate, for 57 nuclides of importance for coupled neutron-photon transport calculations for fusion reactor design selected from the evaluated data files BROND-2, ENDF/B-VI, JENDL-3.1, JENDL-FF and EFF-3. In the development of the improved library FENDL/E-2.0, the previous version of the basic evaluated library, FENDL/E-1.0, was used as a starter file. Ten evaluations of this library were replaced and evaluations for seven additional nuclides were included ⁽²⁾. A preliminary working library (Version 1 of March 1997) is available from the IAEA Nuclear Data Section for the purpose of benchmark analysis, which contains the processed cross sections in pointwise ACE format, for use with the Monte Carlo transport code MCNP4A ⁽³⁾, and in the multigroup GENDF and MATXS formats, for use in coupled neutron-photon transport

calculations with discrete-ordinates codes such as ANISN ⁽⁴⁾, ONEDANT ⁽⁵⁾, etc.

Prior to FENDL-2 evaluation selection, a great amount of benchmark work, including integral fusion neutronic experiments and data testing, has been performed in the world for FENDL validation ^(6,7). In particular, in the Ref. (7), a large variety of existing integral 14MeV benchmark experiments had been analyzed for that purpose by means of coupled neutron-photon transport calculations with the Monte Carlo code MCNP4A, the discrete ordinates code ONEDANT and the nodal transport code NGSN/1D ⁽⁸⁾. The analyzed experiments covered a wide range of fusion-relevant materials. In particular, 14 MeV neutron transmission experiments on rectangular iron (Fe) and beryllium (Be) slabs, and on spherical iron, beryllium, aluminum (Al), silicon (Si), molybdenum (Mo), cobalt (Co), chromium (Cr), copper (Cu), titanium (Ti), manganese (Mn), zirconium (Zr), niobium (Nb), tungsten (W) and vanadium (V) shells with measurements of neutron leakage spectra were analyzed. The benchmark analysis comprise MCNP-calculations using detailed three-dimensional models of the experimental configurations and taking into account the proper energy-angle distribution of the (D,T) source neutrons, comparisons to one-dimensional calculations and comparisons to multi-group (VITAMIN-J) based deterministic transport calculations. In addition, comparisons are included of processed and measured cross-section data where appropriate and needed.

This work has been performed to validate and qualify the second version of FENDL based on benchmark calculations with the code MCNP4A and the preliminary release of the processed FENDL-data and also comparisons to the previous calculation results in Ref. (7). In this paper, we do not intend to present the detailed analysis of any evaluation status. However, brief benchmark calculation results and major findings are presented for 14 MeV neutron transmission experiments on spherical Fe, Be, Al, Si, Mo, Co, Cr, Cu, Ti, Mn, Zr, Nb, W and V shells with measurements of neutron leakage spectra, which

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Table 1 C/E data for integrated neutron leakage spectra in the IPPE iron shell experiment

Shell Thickness (cm)	Energy Range (MeV)	Experimental Leakage (1/sn)	C/E of Integral Leakage			
			FENDL-2	FENDL-1	JENDL-FF	EFF-3
2.5 (0.5 MFP)*	0.05~1.0	.099 (5)**	0.95	0.93	1.09	0.96
	1.0~5.0	.140 (4)	1.00	0.99	1.01	1.05
	5.0~10.0	.032 (5)	0.72	0.98	0.84	0.76
	10.0~20.0	.740 (7)	1.04	1.05	1.05	1.05
	>0.05	1.01 (5)	1.02	1.03	1.04	1.03
28.0 (6.1 MFP)*	0.05~1.0	.786 (5)	1.08	1.08	1.09	1.09
	1.0~5.0	.115 (4)	1.06	1.04	0.99	1.06
	5.0~10.0	.0063 (6)	0.98	1.27	1.09	0.98
	10.0~20.0	.034 (7)	1.08	0.94	0.93	0.98
	>0.05	.94 (5)	1.08	1.07	1.07	1.08

*MFP represents Mean Free Path of neutron in the materials; ** percentage experimental errors in parentheses

Table 2 C/E data for integrated neutron flux spectra in the OKTAVIAN Be shell experiment

Energy Range (MeV)	Experimental Leakage (1/sn)	C/E of Integral Leakage		
		FENDL-2	FENDL-1	JENDL-FF
0.003~1.0	.469 (5.7)*	0.99	.98	.98
1.0~5.0	.315 (1.0)	0.84	.83	.85
5.0~10.0	.143 (1.7)	0.90	.88	.90
10.0~20.0	.324 (1.1)	1.20	1.18	1.21
>0.003	1.26 (2.9)	0.99	.98	1.00

* percentage experimental errors in parentheses

had been performed previously at Institute of Physics & Power Eng. (IPPE, Russian Federation), University of Osaka (OKTAVIAN facility, Japan) and for shielding experiments on multi-layer alternating iron-water spherical and cylindrical shells-combined assembly and multi-layer iron-polyethylene-lead slabs-combined with measurements of activation reaction rates, which have been performed recently at Southwest Institute of Nuclear Physics and Chemistry (SWINPC), China^(9,10,11).

II. Benchmark Calculation and Analysis

1. Iron Spherical Shell Experiment (IPPE)

Iron spherical shells with various thicknesses of 2.5, 7.5, 12, 18.1 and 28 cm were irradiated by 14 MeV D-T neutrons at Institute of Physics & Power Eng., Russian Federation. The neutron leakage spectra from the outer surface of five shells were measured by the Time-of-Flight (TOF) method⁽¹²⁾. Calculations have been performed for the three-dimensional (3D) spherical geometrical model with MCNP4A and FENDL-2. The measured leakage with specified uncertainty and C(calculational)/E (Experimental) ratios of integral neutron spectra for the shells with thicknesses of 2.5 and 28.1 cm are listed in **Table 1** where the previous results with EFF-3 from Ref.(7) are also included for comparison purpose.

The results show that FENDL-2 Fe data underestimated the measured leakage spectrum in the thin shell experiment by above 20%. However, a clear improvement can be observed for the thick shell experiment.

In addition, we note that the results for FENDL-2 are different from those with the previous EFF-3 data file, where FENDL-2 Fe data originated.

2. Beryllium Spherical Shell Experiment (OKTAVIAN)

A beryllium spherical shell experiment with various thicknesses was conducted at the intense 14 MeV neutron source facility OKTAVIAN at Osaka University, Japan. Neutron leakage spectra were measured applying the TOF technique⁽¹³⁾.

In this work, the sphere shell with inner radius of 5.7 cm and outer radius of 17.35 cm has been calculated using MCNP4A and FENDL-2 with isotropic 14.1 MeV point neutron source and the measured neutron energy spectrum. Results are shown in **Table 2** in comparison with the results obtained previously with FENDL-1 and JENDL-FF.

The calculation shows that the results obtained with FENDL-2 fairly well represents the measured neutron spectra although there is an overestimation of 20% around the source energy peak. In addition, the results with the current FENDL-2 beryllium data, which originated from JENDL-FF beryllium data file, well agree with those with JENFL-FF. The very slight differences probably come from the statistic errors in the calculations.

3. Vanadium Spherical Shell Experiment (IPPE)

Neutron leakage spectra were measured at the IPPE neutron source facility for two vanadium spherical shells. The inner/outer radii of the two shells amounted to 1.5cm/5cm and 1.5cm/12cm, respectively. The total uncertainty of the measured fluences is estimated at about 7%⁽¹⁴⁾.

An isotropic neutron source was adopted in the calculation with MCNP4A and FENDL-2 V data. A uniform source energy spectrum distribution between 13.36 and 14.89 MeV and the simplified 1-D geometry model was used in the calculation. The comparison of calculated and measured integral spectra is

Table 3 C/E data for integrated neutron leakage spectra in the IPPE V shell experiment

Shell Thickness (cm)	Energy Range (MeV)	Experimental Leakage (1/sn)	C/E of Integral Leakage			
			FENDL-2	FENDL-1	JENDL-FF	EFF-3
3.5 (0.6MFP)	0.1~1	.123	1.31	1.11	1.25	1.00
	1~5	.170	1.07	1.02	1.05	1.14
	5~10	.0308	1.14	1.06	1.12	.87
	10~20	.737	0.99	.996	.99	1.00
	>0.1	1.06	1.05	1.02	1.03	1.02
10.5 (1.8MFP)	0.1~1	.391	1.23	1.06	1.22	1.01
	1~5	.301	1.03	1.04	1.02	1.14
	5~10	.0377	1.27	1.13	1.25	.96
	10~20	.0381	0.97	1.00	.98	1.00
	>0.1	1.11	1.09	1.04	1.08	1.04

Table 4 Characteristic parameters of the sample sphere piles

Pile (element)	Outer diameter (cm)	Apparent density (g/cm ³)	Thickness of pile	
			(cm)	(MFPs)
Al	40	1.22	9.8	0.5
Si	60	1.29	20.0	1.1
Mo	61	2.15	27.5	1.5
Co	40	1.94	9.8	0.5
Cr	40	3.72	9.8	0.7
Cu	61	6.23	27.5	4.7
Ti	40	1.54	9.8	0.5
Mn	61	4.37	27.5	3.4
Zr	61	2.84	27.5	2.0
Nb	28	4.39	11.2	1.1
W	40	4.43	9.8	0.8

given in **Table 3**. The results obtained previously with FENDL-1, JENDL-FF and EFF-3 are also listed in Table 3.

The calculations have shown that FENDL-2 vanadium data agrees with JENDL-FF V evaluation and has the best agreement with the measured leakage spectra among the three evaluated data files. A slight difference between FENDL-2 results and previous ones with JENDL-FF in the low energy range for thin shell experiment was caused by the fact that we had included the measured source energy spectrum distribution in the previous calculation with JENDL-FF.

4. Various spherical pile experiment (OKTAVIAN)

Sphere pile experiments were performed at the intense 14 MeV neutron source facility OKTAVIAN at Osaka University, Japan, for various materials using the TOF technique. The neutron leakage spectra and the source neutron spectrum were measured. The sample piles were made by filling spherical vessels with sample powder or flakes. The characteristic parameters of the sample piles are listed in **Table 4** ⁽¹³⁾.

In this work, the sphere pile experiments for Al, Si, Mo, Co, Cr, Cu, Ti, Mn, Zr, Nb, W have been calculated using MCNP4A with continuous energy cross-section data FENDL-2. The isotropic angular distribution of source neutrons along with the measured energy spectra and the simplified 1-D geometry model has been adopted in all the calculations. The C/E values of integrated neutron leakage are listed in **Table 5**. The

experimental uncertainty listed in Table 5 includes only counting statistic error. From Table 5, the following facts can be observed:

For both Al and Si, a clear improvement in the estimation of neutron spectra can be found with FENDL-2 in comparison to other data files although there is still a slight underestimation in the energy range below source peak energy with all the data files.

For Mo, the measured neutron leakage spectrum can be well reproduced by all the data evaluations except for an underestimation in the energy range 3-10 MeV. However, FENDL-2 Mo data, originating from JENDL-FF Mo data, show a much better agreement with the measured spectrum in that energy range due to an improved neutron emission spectrum. The measured total neutron leakage (>0.1 MeV) is underestimated by some 10% in total.

For Co, a serious underestimation by about 17% of the leakage spectrum as measured in the experiment is found for all of the applied data evaluations. Note the shape of leakage spectrum is nevertheless well reproduced by all the calculations. Thus there may be a normalization problem in this experiment.

For Cr, FENDL-2 Cr data, originating from ENDF/B-VI (FENDL-1) data, has a good agreement with experiment except for an overestimation of some 10% in the energy range 0.1-10 MeV.

For Cu, FENDL-2, FENDL-1 and EFF-2, which all make

Table 5 C/E of integral leakage spectra for various materials sphere pile experiments

Element	Energy Range (MeV)	Measured Leakage (1/sn)	C/E of Integral leakage			
			FENDL-2	FENDL-1	EFF-2	JENDL-FF
Al	0.1~1.0	.069 (1.9)	0.90	0.89	0.81	0.88
	1.0~5.0	.148 (3.1)	0.85	0.92	0.89	0.79
	5.0~10.	.050 (1.4)	0.74	0.60	0.79	0.81
	10.0~20	.675 (3.7)	1.10	1.10	1.10	1.11
	>0.1	.942 (3.3)	1.03	1.03	1.03	1.02
Si	0.1~1.0	.093 (3.7)	0.89	1.63	0.67	0.89
	1.0~5.0	.171 (5.0)	0.93	0.69	0.79	0.89
	5.0~10.	.047 (2.1)	0.94	0.71	0.79	0.83
	10.0~20	.482 (4.6)	1.11	0.97	1.17	0.93
	>0.1	.793 (4.4)	1.03	0.97	1.00	0.90
Mo	0.1~1.0	.516 (8.5)	0.90	0.90	0.81	0.89
	1.0~5.0	.287 (6.9)	0.89	0.96	1.03	0.89
	5.0~10.	.043 (2.1)	0.82	0.60	0.63	0.83
	10.0~20	.524 (4.7)	0.93	0.97	0.97	0.93
	>0.1	1.37 (6.5)	0.91	0.93	0.91	0.90
Co	0.1~1.0	.242 (4.3)	0.63	0.63	0.63	0.62
	1.0~5.0	.295 (6.2)	0.61	0.61	0.61	0.64
	5.0~10.	.055 (2.1)	0.49	0.49	0.49	0.65
	10.0~20	.729 (5.2)	1.02	1.02	1.02	1.00
	>0.1	1.32 (5.1)	0.83	0.83	0.83	0.83
Cr	0.1~1.0	.211 (4.9)	1.07	1.07	1.07	1.15
	1.0~5.0	.221 (3.2)	1.13	1.13	1.25	1.11
	5.0~10.	.041 (1.2)	1.14	1.14	0.98	0.96
	10.0~20	.549 (2.8)	0.97	0.97	0.96	0.96
	>0.1	1.02 (3.3)	1.04	1.03	1.05	1.03
Cu	0.1~1.0	.660 (10)	1.09	1.08	1.09	1.04
	1.0~5.0	.145 (4.8)	1.05	1.06	1.06	0.97
	5.0~10.	.013 (1.2)	1.28	1.27	1.27	0.99
	10.0~20	.079 (2.0)	0.99	0.99	0.99	1.04
	>0.1	.898 (8.4)	1.07	1.07	1.07	1.03
Ti	0.1~1.0	.086 (2.2)	1.31	1.31	1.31	1.38
	1.0~5.0	.152(3.8)	1.33	1.34	1.34	1.06
	5.0~10.	.038 (1.5)	0.98	0.98	0.98	1.00
	10.0~20	.598 (4.4)	1.19	1.19	1.19	1.23
	>0.1	.874 (4.0)	1.22	1.21	1.21	1.20
Mn	0.1~1.0	.661 (9.4)	1.08	1.08	1.08	1.08
	1.0~5.0	.271 (6.5)	1.14	1.14	1.14	1.13
	5.0~10.	.028 (1.7)	1.00	1.00	1.00	1.15
	10.0~20	.154 (2.7)	0.95	0.94	0.94	1.00
	>0.1	1.14 (7.5)	1.05	1.07	1.07	1.08
Zr	0.1~1.0	.442 (7.7)	1.21	1.07	0.95	1.21
	1.0~5.0	.307 (8.2)	1.07	1.24	1.58	1.07
	5.0~10.	.033 (2.2)	0.99	1.20	1.74	0.98
	10.0~20	.317 (4.9)	1.21	1.26	1.19	1.21
	>0.1	1.10 (6.9)	1.16	1.18	1.22	1.16
Nb	0.1~1.0	.335 (6.1)	1.37	1.27	1.12	1.37
	1.0~5.0	.219 (3.2)	1.04	1.26	1.47	1.04
	5.0~10.	.036 (1.1)	0.93	1.09	1.17	0.94
	10.0~20	.510 (2.7)	1.04	1.04	1.05	1.04
	>0.1	1.10 (3.8)	1.14	1.15	1.16	1.14
W	0.1~1.0	.360 (7.2)	0.93	0.84	0.87	0.94
	1.0~5.0	.241 (7.0)	0.79	0.86	0.84	0.79
	5.0~10.	.040 (2.1)	0.69	0.67	0.61	0.68
	10.0~20	.710 (6.3)	0.94	0.94	0.95	0.94
	>0.1	1.35 (6.6)	0.90	0.90	0.89	0.90

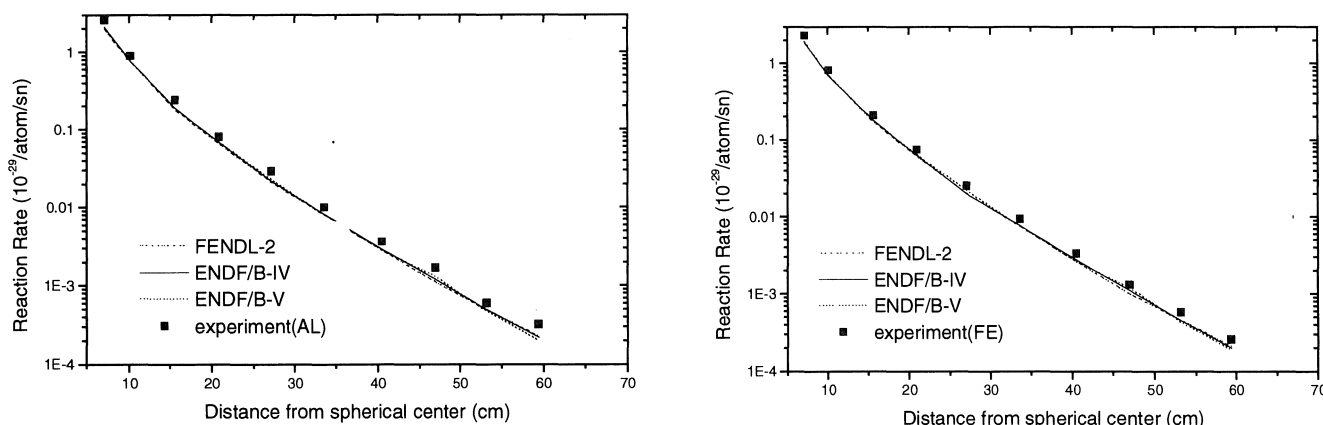


Fig. 1 Measured and calculated reaction rates for iron-water combination experiment

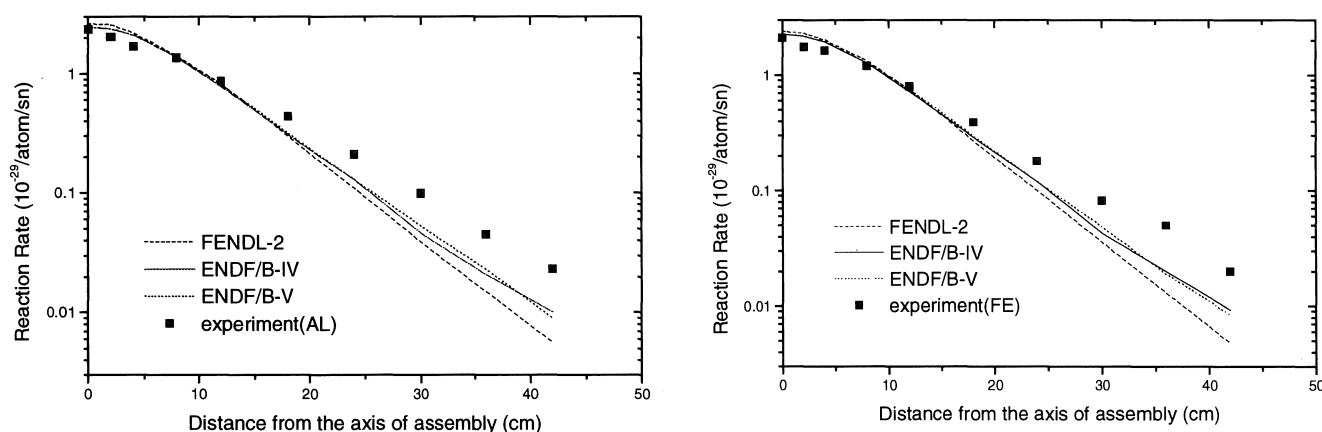


Fig.2 Measured and calculated reaction rates inside lead plate for Fe-Pb-PE combination experiment

use of the Cu ENDF/B-VI evaluation, give a strong overestimation of measured integral leakage spectra by 28% in the energy range 5-10 MeV.

For Ti, all the data totally overestimate the measured leakage spectra by about 20% whereas JENDL-FF shows much better agreement in the energy range of above 1 MeV. FENDL-2 shows the same results as FENDL-1 and EFF-2 due to application of the same Ti ENDF/B-VI evaluation.

For Mn, FENDL-2, FENDL-1 and EFF-2 data rather well reproduce the experimental spectrum except for a slight overestimation of about 10% in the energy range below 5 MeV.

For Zr, FENDL-2, which makes use of JENDL-FF Zr evaluation, shows the best agreement with the experimental spectrum among the evaluations. However, an overall overestimation of 16% can still be observed with FENDL-2 and other data although FENDL-2 shows an improvement.

For Nb, FENDL-2 Nb data shows an improvement in reproduction of the experimental leakage spectrum above 1 MeV although the measured leakage spectrum is overestimated by about 15% in total with all the evaluations.

For W, the measured leakage spectrum is underestimated by some 10% in total with all the evaluations. In particular, there is a strong underestimation for FENDL-2, originating from

JENDL-FF, around 1 MeV and for EFF-2 in the energy range 2-6 MeV.

In addition, it is noted that all the calculated results with FENDL-2 for the OKTAVIAN spherical shell experiments are nearly the same as those with the other corresponding data files, from which FENDL-2 originated.

5. Iron-Water Combination Experiment

The experimental assembly was constructed from a combination of alternating iron-water multi-layers of spherical and cylindrical shells. The spherical shell was made of three layers of iron and two layers of water. The inner and outer radii were as follows:

R (inner/outer, cm) =

7.1/13.1(Fe)/18.1(H₂O)/23.8(Fe)/30.5(H₂O)/35(Fe)

The D-T target was surrounded by foam polystyrene of 0.04 g/cm³ in density inside the spherical shell and placed at the center of spherical shell.

An extended cylinder shell with a radius of 17.5cm was arranged just outside the spherical shell. The thicknesses (cm) of multi-layers of cylindrical shell are:

1.5(Fe)/8.1(H₂O)/5(Fe)/7.6(H₂O)/5(Fe)/7.3(H₂O)/0.5(Fe).

The measurements of activation reaction rates, neutron angular

flux spectra, neutron leakage spectra were performed at the D-T neutron source facility of SWINPC⁽⁹⁾.

The calculation for 3-D geometrical model with 14.1 MeV isotropic neutron source has been performed with FENDL-2. In this work, the measured and calculated reaction rates of $^{56}\text{Fe}(n,p)^{56}\text{Mn}$ and $^{27}\text{Al}(n,\alpha)^{24}\text{Na}$ at the positions with various penetration depths are presented in Fig. 1, where the calculated results with ENDF/B-IV and ENDF/B-V data are also included for comparison purpose.

The calculation shows the all calculated results fairly represent the spatial distribution trend of the measured rates, expect for ~20% underestimation over the measured results at all positions. In addition, the underestimation with FENDL-2 appears to be ~3% stronger than those with ENDF/B-IV and ENDF/B-V at the inner surface position (7.1 cm) of iron-water spherical assembly and nearly the same at other positions.

6. Iron-Lead-Polyethylene Combination Experiment

The experiment assembly was constructed from a combination of 100x80 cm² plates of iron, lead, polyethylene (PE) and iron with thicknesses of 5.5, 10, 6, 5.5 cm. Measurements of neutron angular spectra and activation reaction rates were performed at the D-T neutron source facility of SWINPC. The 14 MeV D-T neutron source was located in the front of the plates at the axis of the slab assembly. The activation foils were placed at the middle vertical plane inside the lead plate and at the cross surface of polyethylene plate and iron plate. The reaction rates at various distances away from the axis of the experimental assembly were measured⁽¹⁰⁾.

The calculation for 3-D geometrical model with 14.1 MeV isotropic neutron source has been performed with MCNP4A and data files FENDL-2, ENDF/B-IV and ENDF/B-V. The measured and calculated reaction rates of $^{56}\text{Fe}(n,p)^{56}\text{Mn}$ and $^{27}\text{Al}(n,\alpha)^{24}\text{Na}$ are presented in Fig. 2 for the measured positions inside lead plate. An underestimation of 10%~40% is observed for all the calculations expect for an overestimation of 10%~30% at the measured positions near the axis of the experimental assembly inside lead plate with the three data files. That underestimation and overestimation with FENDL-2 are ~10% stronger than those with ENDF/B-IV and ENDF/B-V data files.

III. Summary

A variety of 14 MeV neutronic experiments have been analyzed by means of Monte Carlo transport calculations with the preliminary release of Fusion Evaluated Nuclear Data Library FENDL-2. The calculated results with FENDL-2 were compared with the measured neutron spectra and reaction rates and the calculated results obtained previously with FENDL-1, EFF-2/-3 and JENDL-FF from which FENDL-2 evaluations originated.

Transmission experiments on spherical shells made of iron, vanadium, aluminum, silicon, molybdenum, cobalt, chromium, copper, titanium, manganese, zirconium, niobium, tungsten,

respectively and on a combined spherical and cylindrical shell assembly consisting of iron-water alternating layers and on a combined slab assembly consisting of iron, lead and polyethylene plates were included in the analysis.

In general, the FENDL-2 evaluations show a high quality level and have an overall good agreement with integral experiments. However, some exceptions were found and need to be analyzed further. All the calculated results with FENDL-2 rather well reproduced those obtained previously with the corresponding data evaluations in the libraries ENDF/B-VI, EFF and JENDL-FF, from which FENDL-2 data originated.

It should be mentioned that the above found disagreements between the calculated and measured results may be caused partly by the data files and partly by the experimental data themselves. We do not intend to clarify any detailed explanation of data deficiencies in the FENDL-2, but to provide the basis for further analyses. As a next step, calculations with more integral experiments are needed for cross-checking. Furthermore, there is required a sensitivity analysis for tracing down the discrepancies to specific cross section data and further improvement of the corresponding cross section data.

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