

Benchmark test for next FENDL

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Outline



• We would like to present the following issues as the outstanding actions from the last FENDL meeting in 2018.

1. INDEN Fe56 benchmark test with QST/TIARA iron shielding experiments for FENDL-3.2

2. Benchmark test with QST/TIARA concrete shielding experiments for new O16 data

 We would like to introduce some problems of deuteron-induced files in TENDL-2017 that we newly found out.

3. Problems on neutron production data of deuteron-induced files in TENDL-2017

• Finally, let me talk about...

4. New Fe56 benchmark test with QST/TIARA iron shielding experiments for next TENDL, TENDL-2019



INDEN Fe56 benchmark test with QST/TIARA iron shielding experiments for FENDL-3.2

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Introduction



- At the last Consultants' Meeting on the FENDL Library for fusion neutronics calculations (14-18 Oct. 2018), Dr. Trkov proposed that INDEN Fe56 would be a candidate of FENDL-3.2 Fe56.
- However, it was not clear whether INDEN Fe-56 was better than FENDL-3.1d Fe56.
- Thus, we carried out **benchmark tests of INDEN Fe56** based on the action of the last FENDL meeting.
- Here the results with the QST/TIARA iron shielding experiments are presented.
- Those with the JAEA/FNS iron experiments are presented by Dr. Konno.

Experiment & Analysis



Experimental configuration





- The generated neutrons, 40 and 65MeV, were collimated and entered on the iron test shield.
- The neutron spectrum above 5MeV was measured by scintillators.

See the following report for more details about the experiments and analyses:

H. Nakashima et al., JAERI-Data/Code 96-005, 1996



Code: MCNP6.1.1

Libraries:

FENDL-3.1d (Official ACE file) TENDL-2017 (Official ACE file) JENDL-4.0/HE (Processed with NJOY2016) INDEN: Fe56 file (^{54,57,58}Fe: FENDL-3.1d)

The measured neutron spectrum was used as the neutron source in MCNP.

Result: 40MeV



Result: 65MeV



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About the FENDL-3.1d (rev.) REVIEW

• We examined the iron isotopes data in FENDL-3.1d.

<u>*mt=5:</u> Sum of all reactions not given explicitly in another mt #

• ⁵⁶Fe data of FENDL-3.1d was taken from TENDL-2011, in range of 20-150MeV.



→ The secondary neutron spectrum data of mt=5* in FENDL-3.1d are incorrect at 20MeV.

→ We replaced the incorrect data at 20MeV in FENDL-3.1d with the "normal" secondary neutron spectrum data in ENDF/B-VII.1, as it is called "FENDL-3.1d (rev.)" in the analysis results.

Result: 40MeV with FENDL-3.1d (rev.)



Result: 65MeV with FENDL-3.1d (rev.)





- In the analyses of QST/TIARA iron shielding experiments, it can not be affirmed that INDEN Fe56 is better than FENDL-3.1d Fe56.
- We propose that FENDL-3.2 adopts FENDL-3.1d Fe56, where only the secondary neutron spectrum data at 20MeV in mt=5 are revised.



Benchmark test with QST/TIARA concrete shielding experiments for new O16 data

Saerom Kwon¹

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¹National Institutes for Quantum and Radiological Science and Technology (QST) ²Japan Atomic Energy Agency (JAEA)

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Introduction



- As one of the actions at the last Consultants' Meeting on the FENDL Library for fusion neutronics calculations (14-18 Oct. 2018), Dr. Kunieda prepared new O16 data for the next FENDL library.
- The O16 data of FENDL-3.1d was taken from ENDF/B-VII.
- Dr. Kunieda replaced the O16 data of FENDL-3.1d with those of JENDL-4.0/HE over 30MeV, where the upper energy limit was changed from 200 to 150 MeV.
- As a benchmark test of the new O16 data, we analyzed the QST/TIARA concrete shielding experiments.
- Here, our results are presented.

Experiment & Analysis



Experimental configuration



(Units in cm)

- 43 and 68MeV of protons were bombarded on the Li-7 target.
- The generated neutrons, 40 and 65MeV, were collimated and entered on the concrete test shield.
- The neutron spectrum above 5MeV was measured by scintillators.

See the following report for more details about the experiments and analyses:

N. Nakao et al., JAERI-Data/Code 97-020, 1997



- Code: MCNP6.1.1
- Libraries:

FENDL-3.1d (Official ACE file) JENDL-4.0/HE (Processed with NJOY2016) FENDL-3 new1:

O16 new 1 (Processed with NJOY2016) others FENDL-3.1d (Official ACE file)

The measured neutron spectrum was used as the neutron source in MCNP.

•

Result: 40MeV (FENDL-3 new1 from Dr. Kunieda)

Neutron spectra in 40MeV experiment





- <u>Continuous region:</u> Although the calculated neutron flux still overestimates the experimental one with FENDL-3 new1, it is improved a little bit.
- <u>Peak region</u>: The calculated neutron flux agrees well the experimental one with FENDL-3 new1 (improved!).

Result: 65MeV (FENDL-3 new1 from Dr. Kunieda)

Neutron spectra in 65MeV experiment





- <u>Continuous region</u>: The calculated neutron flux agrees well the experimental one with FENDL-3 new1.
- <u>Peak region</u>: The calculated neutron flux still overestimates the experimental one with FENDL-3 new1 (improved a little bit).

Impact of data above 20MeV

- GQST
- Dr. Kunieda replaced O16 data of FENDL-3.1d with those of JENDL-4.0/HE over 30MeV (FENDL-3 new1).
- The effects of the above modification are slightly different those by Dr. Konno (Fusion Eng. Des. 98-99 (2015) 2178).
- The difference between the data modified by Kunieda and Konno is the energy region (Kunieda: over 30MeV, Konno: over 20MeV)
- In order to clarify an impact of data between 20 and 30MeV, we modified the Kunieda's O16 data (O16 new2); the data above 20 MeV were replaced with those in JENDL-4.0/HE.
 - Library:

FENDL-3 new2:

O16 new 2 (Processed with NJOY2016) others FENDL-3.1d (Official ACE file)

Result: 40MeV (FENDL-3 new2)



Neutron spectra in 40MeV experiment





- <u>Continuous region</u>: Although the calculated neutron flux still overestimates the experimental one with FENDL-3 new2, it is improved.
- <u>Peak region</u>: The calculated neutron flux agrees well the experimental one with FENDL-3 new2 (improved!).

Result: 65MeV (FENDL-3 new2)



Neutron spectra in 65MeV experiment





- <u>Continuous region</u>: The calculated neutron flux agrees well the experimental one with FENDL-3 new2.
- Peak region: The calculated neutron flux still overestimates the experimental one with FENDL-3 new2 (improved a little bit).

Impact of data between 20 and 30MeV





- <u>Continuous region</u>: The calculated neutron flux using FENDL-3 new2 is better than that of FENDL new1.
- <u>Peak region</u>: The calculated neutron fluxes using FENDL-3 new1 and 2 are almost the same.

→ The data between 20 and 30MeV in FENDL-3.1d should be replaced with JENDL-4.0/HE.



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- The analyses of QST/TIARA concrete shielding experiments affirm that the new O16 data from Dr. kunieda is better than FENDL-3.1d O16 (the same as those of ENDF/B-VII).
- We affirm that our new O16 data is also better than FENDL-3.1d O16.

- The O16 data over 20MeV in FENDL-3.1d should be replaced with those in JENDL-4.0/HE.
- The two new O16 data will be candidates for those in the FENDL-4.



Problems on neutron production data of deuteron-induced files in TENDL-2017

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- A-FNS is a fusion neutron source for irradiation tests of fusion materials, and it is similar to IFMIF/DONES in Europe.
- A-FNS produces fusion-like neutrons by the Li(d,xn) reaction (E_d=40MeV).
- Design activity of A-FNS in Japan is ongoing.
- Neutronics analyses of A-FNS have been carried out with Monte Carlo code and FENDL-3.1d (neutron-induced).
- In the near future, we will use deuteron-induced nuclear data for the analyses.
- Candidates of the deuteron-induced nuclear data are FENDL-3.1d, new JENDL file (release soon) and TENDL-2017.

Purpose



- Charged particles-induced files (p, d, t, He3, α up to 200MeV) in TENDL-2017 was released on Dec. 30, 2017.
- ONE nuclide has 3 kinds of ENDF files as the following description:

Evaluated formatted data (i.e. ENDF)

- 1. The TENDF file (Evaluated Nuclear Data File, explicit channels up to 30 MeV, then MF6/MT5 up to 200 MeV)
- 2. <u>Special ENDF file</u> (all explicit channels up to 200 MeV)
- 3. Another special ENDF file (all channels in MF6/MT5 from 0 to 200 MeV)
- There is only official ACE file from "the TENDF file" in TENDL-2017.
- Up to TENDL-2015, the TENDL libraries have only the file corresponding to "Another special ENDF file" of TENDL-2017.
- Recently, K.L.Paaren et al. reported that "The TENDF file" of ⁹Be in the αinduced files of TENDL-2017 produced strange neutron spectra, while "Another special ENDF file" produced reasonable neutron spectra^[1].
- The THREE files must be consistent.

...But they are NOT!

> We investigate whether the deuteron-induced files in TENDL-2017 have the similar problem with the α -induced files or not.

Method 1



- In order to investigate the three ENDF files of ⁹Be in TENDL-2017, they are downloaded from the official TENDL-2017 web page.
- Make ACE files of "The TENDF file", "Special ENDF file" and "Another special ENDF file" of ⁹Be using NJOY2016.49.mod.
- Extract and compare neutron production cross sections and secondary neutron energy distributions from NJOY outputs of the three ENDF files (no ACE format information for neutron production)

WHY is ⁹Be first?

→ The TENDF files from H to Li are not calculated with TALYS but taken from ENDF/B-VII.1.

Due to bug of NJOY:

→ MCNP calculations do not finish or produce neutrons when the official ACE file (processed from "The TENDF file") are used.

Modify NJOY2016.49: → See the next slide

Strange NJOY output of the TENDF file

- We found out strange data in the NJOY output of the TENDF file.
- No such data in the NJOY outputs of the Special ENDF file and Another special ENDF file.

reaction descriptors

	reaction	mt	tyr	lsig	land	ldlw	emin	emax	q
	elastic	2			1		1.00000F-11	2.000000F+02	
1	(d.x)	5	-101	1	_1	49	2,999999E+01	2.000000E+02	0,000000F+00
2	(d,n*)d	32	-1	35	-1	10994	2.036442E+00	2.000000E+02	-1.664540F+00
3	inelastic	104	-1	132	-1 .	15115	2.060250E+00	2.000000E+02	-1.684000E+00
4	(d,pd)	115	-1	226	mt=	=113 810 -2	2nd 65920E+01	2.000000E+02	-1.688630E+01
_5	(d.da)	117	-1	272	-1	18825	2.823290E+00	2.000000E+02	-2.307690E+00
6	(d,n)	4	0	359	-1	20548	1,0000000-11	2 AAAAAAF+A2	1 362160F+00
7	(d,2n)	16	0	1011			4.		-
8	(d,3n)	17	0	1091		Т	2. Althoud	ah there	is no cross
9	(d,n*)a	22	0	1128			2.		
10	(d,2n)a	24	0	1268		1	7. section	data of n	nt-11 (d 2nd)
11	(d,n*)p	28	0	1342					n=11 (a,211a),
12	(d,n*)t	33	0	1430			1. accord	any days	aran data of
13	(d,n*)he3	34	0	1483				ary deut	eron data or
14	(d,2np)	41	0	1539			4.		
15	(d,gma)	102	0	1620	I		1. mt=11 e	exists.	
16	(d,p)	103	0	2272		_	1.		
17	(d,t)	105	0	2924	<u></u>	9	1.		
18	(d,he3)	106	0	3576	<u> </u>	<u> </u>	1.		
19	(d,a)	107	0	3641		-			NIOVO04C 40
20	(d,2a)	108	0	4293	/		6. VVE INV	estigated	NJU12010.49
21	(d,2p)	111	0	4370	/		1.		
22	(d,pa)	112	0	4420	/		³ in detai		
23	(d,pt)	116	0	4504			1.		
24	(d,xp)	203	0	4563			1.0000000-11	2.000000E+02	0.00000E+00
25	(d,xd)	204	0	5215			2.036442E+00	2.000000E+02	0.00000E+00
26	(d,xt)	205	0	5312			1.000000E-11	2.000000E+02	0.00000E+00
27	(d,xhe3)	206	0	5964			1.393830E+01	2.000000E+02	0.00000E+00
28	(d,xa)	207	0	6029			1.000000E-11	2.000000E+02	0.000000E+00
29	~@~@~@^@^@^	0~0~0~0	0	0	0		1.04	+3467 - 320 2.8	00000E+01 0.000000E+00

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Modify NJOY2016.49



- We found out that the mt=11 data was not processed adequately in acefc.f90 of NJOY2016.49.
- We added "mt.eq.11" to line 5297 in acefc.f90.

```
from

if(mt.eq.2.or.mt.eq.32.or.mt.eq.35.or.&

to

if(mt.eq.2.or.mt.eq.11.or.mt.eq.32.or.mt.eq.35.or.&
```

- We compiled the modified acefc.f90, "NJOY2016.49.mod".
- We produced a new ACE file of the TENDF file with NJOY2016.49.mod.



The NJOY output of the TENDF file seems normal using the modified NJOY.

reaction descriptors

reaction	mt	tyr	lsig	land	ldlw	emin	emax	q
elastic	2					1.000000F-11	2.000000F+02	
(d,x)	5	-101			• •	.999999E+01	2.000000E+02	0.000000E+00
(d,2nd)	11	-1 m	mt-	t—11	DYICTC	.515756E+01	2.000000E+02	-2.056320E+01
(d,n*)d	32		1110-		CABL	.036442E+00	2.000000E+02	-1.664540E+00
inelastic	104	-1	1/3	-1	10040	∠.060250E+00	2.000000E+02	-1.684000E+00
(d,pd)	115	-1	267	-1	18397	2.065920E+01	2.000000E+02	-1.688630E+01
(d,da)	117	-1	313	-1	19356	2.823290E+00	2.000000E+02	-2.307690E+00
(d,n)	4	0	400			1.000000E-11	2.000000E+02	4.362160E+00
(d,2n)	16	0	1052			4.985412E+00	2.000000E+02	-4.074960E+00
(d,3n)	17	0	1132			2.771231E+01	2.000000E+02	-2.265140E+01
(d,n∗)a	22	0	1169			2.275022E-01	2.000000E+02	-1.859550E-01
(d 2n)a	24	A	1200	omitte	ed below	7 040710F+00	2 AAAAAAF+A2	<u>-</u> 5 769970F+00

- MCNP calculations finished and produced neutrons without any troubles using the newly processed ACE file.
- The official deuteron-induced ACE files of TENDL-2017 with mt=11 should be replaced with those using the "bugfixed NJOY", NJOY2016.49.mod.

Neutron production xs of ⁹Be



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 Neutron production cross section of Special ENDF file differs markedly from those of The TENDF file and Another special ENDF file.

Secondary neutron energy distribution of ⁹Be (E_d=5MeV) ③ QST



A summation with following item of each reactions: Secondary neutron spectrum * Neutron yield * xs



Others have mt=5 data above 2MeV.

Secondary neutron energy distribution of ⁹Be (E_d=20MeV) QST



A summation with following item of each reactions: Secondary neutron spectrum * Neutron yield * xs

- ^{10⁻³} 10⁻³ 10⁻² 10⁻¹ 10⁰ 10¹ Neutron energy [MeV]
- No neutrons above 12MeV in the TENDF file.

• Others have mt=5 data above 12MeV.

Method 2



- We found out that neutron production cross section and secondary neutron energy distribution data of the TENDF file, Special ENDF file and Another special ENDF file have large differences each other.
- We calculated neutron spectra with a virtual model and MCNP6 to examine effects of the differences.

<Calculation condition>

- Beryllium sphere of radius 1cm
- Isotropic 5MeV, 20MeV, 40MeV, 50MeV deuterons in the center
- ACE files (The TENDF file, Special ENDF file and Another special ENDF file) processed by ourselves using NJOY2016.49.mod
- Calculate leakage neutron flux from Be sphere



Leakage neutron flux from Be sphere (E_d=5MeV)



- Upper energy limit of calculated neutron spectra using the TENDF file and Special ENDF file is small.
- Calculated neutron spectra using the TENDF file and Special ENDF file have an unnatural peak near 30keV.
- Calculated neutron spectrum using Special ENDF file has unphysical neutron flux over 3MeV.

Leakage neutron flux from Be sphere (E_d=20MeV)



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- Upper energy limit of calculated neutron spectrum using the TENDF file is small.
- Calculated neutron spectra using the TENDF file and Special ENDF file still have the unnatural peak near 30keV.

Leakage neutron flux from Be sphere (E_d=40MeV)



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- Calculated neutron spectra using the TENDF file and Special ENDF file still have the unnatural peak near 30keV.
- Calculated neutron spectrum using the TENDF file has a small peak near 30MeV (Never seen up to 30MeV of deuteron energy).

Leakage neutron flux from Be sphere (E_d=50MeV)



- Calculated neutron spectra using the TENDF file and Special ENDF file still have the unnatural peak near 30keV.
- Calculated neutron spectrum using Special ENDF file is smaller than those using other files. → Due to small neutron production cross section!
- Calculated neutron spectrum using the TENDF file has the small peak near 30MeV.

Reason of difference in neutron spectra (1)



- We prepared modified ACE file of Special ENDF file where mt=5 data was deleted.
- Calculated neutron spectrum using the modified ACE file has no neutron flux over 3MeV.

→ The mt=5 data in Special ENDF file caused the unphysical neutron flux over 3MeV.

Reason of difference in neutron spectra (2)



- We found out unphysically small secondary neutron energy of mt=4 data (<3MeV) in the TENDF file and Special ENDF file.
- The peak disappeared using deuteron cut off option in MCNP input (cut:d j 0.1 → cut:d j 3.0).

→ We figured out that the reason of unnatural peak near 30keV is small secondary neutron energy of mt=4 (<3MeV) in the TENDF file and Special ENDF file.

Reason of difference in neutron spectra (3) \bigcirc QST



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28 MeV 30 MeV 35 MeV

10⁰

10¹

that

suggest

10⁻²

 10^{-1}

Status of other nuclides





Concluding remarks



- We figured out that neutron production data significantly differed among <u>three ENDF files</u> of ⁹Be in TENDL-2017.
 - 1) Neutron production cross section above 30 MeV in Special ENDF file differs markedly from those in the other ENDF files.
 - → Special ENDF file produces smaller neutron fluxes for deuteron > 30 MeV.
 - 2) Wrong secondary neutron energy distribution data in the TENDF file and/or special ENDF file :
 - \rightarrow Broad peak near 30 keV in the calculated neutron spectrum
 - \rightarrow Small peak near 30 MeV in the calculated neutron spectrum
- Another special ENDF file seems to be physically correct in the three ENDF files. Hereafter, we will validate it with experimental data (EXFOR?).
- Probably the same problems occur in other nuclei of TENDL-2017.
- The official deuteron-induced ACE files in TENDL-2017 should be revised based on our study.

Supplementary material: Total xs of ⁹Be





Special ENDF file:

- Total cross section over 30MeV is smaller than those of others.
- Due to including only reactions for activation calculations? The TENDF file: a little bit strange?

Supplementary material: simple question



- Up to TENDL-2015, the TENDL libraries have only the file corresponding to "Another special ENDF file" of TENDL-2017.
- There is only official ACE file from "the TENDF file" in TENDL-2017.
- However, we found out some problems in data of "the TENDF file" and its ACE file.
- Our study suggests that "Another special ENDF file" is the best in the three ENDF files.

(Q) WHY is "the TENDF file" a default in TENDL-2017?

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Prompt report

New Fe56 benchmark test with QST/TIARA iron shielding experiments for next TENDL, TENDL-2019

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Introduction



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- We pointed out strange data in TENDL-2017 at the last FENDL meeting (14-18 Oct. 2018).
- 2595 nuclei in TENDL-2017 had incorrect secondary neutron spectrum data at 30MeV (among 2807 data).
- Dr. Koning prepared new Fe56 data for TENDL-2019 where a format error at 30MeV was corrected.
- Thus, we carried out a benchmark test of the new Fe56 data with the QST/TIARA iron shielding experiments.
- Here the results are presented.

The format error was fixed in Fe56





The incorrect secondary neutron energy spectrum data in Fe56 of TENDL-2017 are corrected well in the new Fe56 data.

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Experiment & Analysis



Experimental configuration





- 43 and 68MeV of protons were bombarded on the Li-7 target.
- The generated neutrons, 40 and 65MeV, were collimated and entered on the iron test shield.
- The neutron spectrum above 5MeV was measured by scintillators.

See the following report for more details about the experiments and analyses:

H. Nakashima et al., JAERI-Data/Code 96-005, 1996



Code: MCNP6.1.1

Libraries:

FENDL-3.1d (Official ACE file) TENDL-2017 (Official ACE file) JENDL-4.0/HE (Processed with NJOY2016) New Fe56 file from Dr. Koning (^{54,57,58}Fe: , FENDL-3.1d)

• The measured neutron spectrum was used as the neutron source in MCNP.

Result: 40 MeV



Neutron spectra of 40MeV neutrons





- <u>Continuous region</u>: No peak around 30 MeV. The calculated neutron fluxes still overestimate the experimental ones using new Fe56 (but improved!).
- <u>Peak region</u>: The calculated neutron fluxes agree well the experimental ones using new Fe56 (almost the same to those using TENDL-2017).

Result: 65 MeV



Neutron spectra of 65MeV neutrons





- <u>Continuous region</u>: No peak around 30 MeV. The calculated neutron fluxes agree well the experimental ones using new Fe56 (similar C/E to FENDL-3.1d).
- <u>Peak region</u>: The calculated neutron fluxes underestimate the experimental ones using new Fe56 (similar C/E to FENDL-3.1d, TENDL-2017).

Other iron isotopes in TENDL-2017





- The incorrect secondary neutron energy spectrum data in Fe54 and Fe58 of TENDL-2017 have to be corrected.
- Only Fe57 have correct secondary neutron energy spectrum data.

Result: 40 MeV (Effect of other iron nuclei)



Result: 65 MeV (Effect of other iron nuclei)





- The analyses of QST/TIARA iron shielding experiments affirmed that the new Fe56 data are better than those in TENDL-2017, although the new Fe56 data are not "perfect".
- We checked the effect of other iron nuclei data.
- Further study should be performed including to improve other iron nuclei data.
- The new Fe56 data will be a candidate for that in the next FENDL.



Thank you for your attention!

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