

Benchmarking FENDL-2.1 with Impact of ENDF/B-VII.0 Release

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FENDL-2.1 Background

- FENDL development initiated in 1987
- Latest version FENDL-2.1 released December 2004, INDC(NDS)-467
- Library is comprehensive collection of highquality nuclear data selected from existing national libraries
- During FENDL evolution, a set of calculational and integral experimental benchmarks were utilized for validation
- FENDL-2.1 has been extensively validated and is the reference data library for nuclear analysis of ITER and other fusion systems



Data Source for FENDL-2.1

No.	Library	NMAT	Materials
1	ENDF/B-VI.8	40	² H, ³ H, ⁴ He, ⁶ Li, ⁷ Li, ⁹ Be, ¹⁰ B, ¹¹ B, ¹⁶ O, ¹⁹ F, ²⁸⁻³⁰ Si, ³¹ P, S,
	(E6)		^{35,37} Cl, K, ^{50,52-54} Cr, ^{54,57,58} Fe, ⁵⁹ Co, ^{61,62,64} Ni, ^{63,65} Cu, ¹⁹⁷ Au, ²⁰⁶⁻²⁰⁸ Pb, ²⁰⁹ Bi, ^{182-184,186} W
2	JENDL-3.3 (J33)	18	1 H, 3 He, 23 Na, $^{46-50}$ Ti, , 55 Mn, $^{92,94-98,100}$ Mo, 181 Ta,V
3	JENDL-3.2 (J32)	3	Mg, Ca, Ga
4	JENDL-FF (JFF)	4	¹² C, ¹⁴ N, Zr, ⁹³ Nb
5	JEFF-3 (EFF) JEFF3	4	²⁷ Al, ⁵⁶ Fe, ⁵⁸ Ni, ⁶⁰ Ni
6	BROND-2.1 (BR2)	2	¹⁵ N, Sn

> Data for 40 isotopes/elements were taken from ENDF/B-VI.8

- ENDF/B-VII.O library was officially released on December 15, 2006 [M.B. CHADWICK, et al., "ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology," Nuclear Data Sheets, 107, 2931 (2006)]
- We examined changes in data for these 40 isotopes/elements and assessed possible impact on nuclear analysis of ITER and other fusion system



Isotopes for which data did not change (7 isotopes)

H-2, He-4, Li-7, B-11, Fe-58, Co-**59**, Bi-209

"ENDF/B-VII CONVERTED FROM ENDF/B-VI BY NNDC OCT 2004"

For the following isotopes only change is in the product energyangle distributions (MF=6) using corrected gnash code to fix an earlier bug (19 isotopes)

Si-28, Si-29, Si-30, P-31, Cr-50, Cr-52, Cr53, Cr-54, Fe-54, Fe-57,Ni-61, Ni-62, Ni-64, Cu-63, Cu-65, W-182, W-183, W-184, W-186

"Possible impact on secondary particle production"

For following isotopes ENDF/B-VII.0 data were taken from JEFF-3.1 (2 isotopes)

Pb-206, Pb-207



Only minor change in cross sections above ~5 MeV



Only isotopic data are provided in ENDF/B-VII.0 for S and K Data for S isotopes (*S*-*32*, *S*-*33*, *S*-*34*, *S*-*36*) and K isotopes (*K*-*39*, *K*-*40*, *K*-*41*) were taken from JENDL-3.3



No isotopic data for K in ENDF/B-VI.8 (except for K-41(n,p)) Large changes in cross sections



H-3

Changes in (n,total), (n,elastic) and (n,2n) cross sections



Large changes in (n,2n) and elastic scattering cross sections

Only possible impact on ICF target neutronics

Does not impact ITER



Li-6

Changes in (n,total), (n,elastic) and (n,t) cross sections, angular distribution



Minor increase in (n,t) at very low and high energies that could lead to impact on predicting tritium production in breeding blankets





Minor impact on ITER expected



F-19

Changes in (n,total), (n,elastic), (n,inelastic) and (n,γ) cross sections



Some large change in (n,γ) and inelastic scattering Expected impact on analysis of breeding blankets with Flibe

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12



Changes in (n,total), (n,elastic), (n,p) and (n, γ) cross sections



Some large changes in (n,γ) , (n,p) and elastic scattering Minor impact on ITER expected since CI is not used



Cl-37 Changes in (n,total), (n,elastic), and (n, γ) cross sections







Some large changes in (n,γ) and elastic scattering Minor impact on ITER expected since CI is not used



Changes in (n,total), (n,elastic), and (n, γ) cross sections



Moderate changes in (n,γ) and elastic scattering in resonance region Only possible impact on ICF target neutronics



Pb-208



Large changes in several cross sections with possible impact on analysis for breeding blankets with LiPb (e.g., ITER-TBM)



Findings of Data Comparison

- ➢Minor impact on ITER nuclear analysis is expected except for ITER-TBM nuclear analysis due to changes in data for Li-6, Pb-208, and F-19
- Effects of changes could be large in other fusion systems
 - Power plants with breeding blankets
 - Inertial fusion systems (e.g., H-3 and Au-197 data are important for ICF target neutronics)



ITER Calculational Benchmark

- To quantify these observations, we performed calculations for a 1-D cylindrical geometry calculational benchmark representative of an early ITER design that was utilized during FENDL development process
 - M. Sawan, "FENDL Neutronics Benchmark: Specifications for the Calculational Neutronics and Shielding Benchmark," IAEA Nuclear Data Section Report INDC(NDS)-316 (December 1994).





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Analysis for ITER Calculational WISCONSIN Benchmark

- This benchmark problem has been mainly used in discrete ordinate calculations using FENDL multigroup data
- FZK prepared MCNP geometry input and compared nuclear responses using FENDL-1.0, 2.0 and 2.1 [IRS-01/06-Fusion 271, July 2006]
- We used this MCNP model to carry out calculations using the FENDL-2.1 library with data for the 40 isotopes/elements replaced by the recent data from ENDF/B-VII.0 processed by NJOY-99.161
- [R. ARCILLA, "ENDF/B-VII.0 in ACE Format-Beta Version," Library ID D00226MNYCP00, distributed by RSICC (2007)]
- Results for flux, heating, dpa, and gas production were compared to those obtained using the FENDL-2.1 library



Peak Neutron and Gamma Flux Results

	FENDL-2.1		FENDL-2.1 +ENDF/B-VII.0			FENDL-2.1		FENDL-2.1 +ENDF/B-VII.0		0/
	Neutron	%	Neutron	%	%	Gamma	%	Gamma	%	Change
	Flux	Error	Flux	Error	Change	Flux	Error	Flux	Error	Change
IB										
FW										
Be	3.52E+14	0.05%	3.52E+14	0.05%	0.05%	3.18E+14	0.05%	3.18E+14	0.05%	0.12%
Cu	3.09E+14	0.05%	3.09E+14	0.05%	0.08%	3.08E+14	0.05%	3.08E+14	0.05%	0.10%
SS	2.96E+14	0.06%	2.96E+14	0.06%	0.10%	3.07E+14	0.06%	3.07E+14	0.06%	0.09%
VV	8.43E+11	0.19%	8.46E+11	0.19%	0.29%	4.84E+11	0.17%	4.85E+11	0.17%	0.26%
Mag										
net	3.42E+09	0.45%	3.45E+09	0.45%	1.04%	9.34E+08	0.42%	9.41E+08	0.42%	0.71%
OB										
FW										
Be	4.37E+14	0.03%	4.37E+14	0.03%	0.12%	3.61E+14	0.04%	3.62E+14	0.04%	0.15%
Cu	3.95E+14	0.03%	3.95E+14	0.03%	0.13%	3.60E+14	0.04%	3.61E+14	0.04%	0.14%
SS	3.80E+14	0.03%	3.80E+14	0.03%	0.14%	3.66E+14	0.04%	3.66E+14	0.04%	0.13%
VV	1.17E+12	0.09%	1.17E+12	0.09%	0.34%	6.60E+11	0.08%	6.62E+11	0.08%	0.27%
Mag net	4.93E+08	0.41%	4.97E+08	0.41%	0.79%	1.38E+08	0.40%	1.39E+08	0.40%	0.49%

Using ENDF/B-VII.0 data results in slightly higher flux values. However, the change is <1% with much smaller differences at the front FW zones facing the plasma



Nuclear Heating, Radiation Damage Results

- With excellent agreement obtained for neutron and gamma fluxes one expects excellent agreement in response parameters as well
- However, comparison of calculated nuclear heating showed large differences with ~55%, ~10%, and ~4% reduction for the Be, CuBeNi, and SS zones of FW and smaller differences in VV and magnet
- Differences in gamma heating are negligible (<0.5%) and large differences in total heating are fully attributed to differences in neutron heating
- This explains also the larger differences for Be and CuBeNi where neutron heating is dominant



Nuclear Heating, Radiation Damage Results (cont'd)

- The large difference in neutron heating was attributed to a bug in versions of NJOY between 99.115 and 99.180 that led to erroneously low neutron heating values. This bug was fixed in subsequent versions of NJOY and new ACE formatted data was processed by LANL and will be released by RSICC
- Results show also large reductions of ~70% in Cu dpa and ~ 6% in Fe dpa that are also attributed to the bug in HEATER module of NJOY. The smaller reduction in Fe dpa is due to the fact that while all Cu isotopes in FENDL-2.1 were replaced and reprocessed, Fe-56 in FENDL-2.1 was taken from JEFF-3 and was not reprocessed



Gas Production Results

Gas production rates (helium, hydrogen, and tritium) were very close using the two libraries and reflect changes obtained in neutron flux

	FENDL-2.1		FENDL-2.1 +ENDF/B-V		
		%		%	%
	He Prod.	Error	He Prod.	Error	Change
IB					
FW					
Be	4.10E+03	0.07%	4.10E+03	0.07%	0.06%
Cu	2.10E+02	0.07%	2.10E+02	0.07%	0.04%
SS	1.77E+02	0.06%	1.77E+02	0.06%	0.05%
VV SS	7.62E-02	0.22%	7.63E-02	0.22%	0.18%
Magnet	3.30E-04	0.63%	3.36E-04	0.62%	1.72%
OB					
FW					
Be	5.98E+03	0.03%	5.98E+03	0.03%	0.06%
Cu	3.23E+02	0.03%	3.23E+02	0.03%	0.04%
SS	2.45E+02	0.03%	2.45E+02	0.03%	0.03%
VV SS	1.08E-01	0.11%	1.08E-01	0.11%	0.28%
Magnet	4.86E-05	0.59%	4.94E-05	0.58%	1.69%

Peak He appm/FPY



Peak Magnet Radiation Effects

21	FENDL-2.1		FENDL-2.7 +ENDF/B-	1 -VII.0	
	Value	% Error	Value	% Error	% Change
INBOARD					
Fast n fluence,E>0.1 MeV (n/cm2/FPY)	6.27E+16	0.46%	6.36E+16	0.46%	1.42%
Insulator dose (Gy/FPY)	5.59E+05	0.47%	5.49E+05	0.46%	-1.63%
Cu dpa/FPY	3.75E-05	0.49%	2.73E-05	0.46%	-27.09%
Winding pack nuclear heating (mW/cm3) OUTBOARD	3.66E-02	0.45%	3.59E-02	2 0.45%	-1.87%
Fast n fluence,E>0.1 MeV (n/cm2/FPY)	9.10E+15	0.42%	9.21E+15	0.42%	1.21%
Insulator dose (Gy/FPY)	8.15E+04	0.44%	8.01E+04	0.42%	-1.73%
Cu dpa/FPY	5.48E-06	0.43%	3.97E-06	0.41%	-27.54%
Winding pack nuclear heating (mW/cm3)	5.38E-03	0.43%	5.26E-03	0.43%	-2.13%

- The peak fast neutron (E>0.1 MeV) fluence increased by ~1.4%, the insulator dose was reduced by ~1.6%, and the winding pack heating decreased by ~1.9% and stabilizer damage rate decreased by 27%
- Despite the error in processing neutron heating data, heating changes are small since heating is dominated by gamma heating resulting from secondary gamma generation in thick shielding zones in front of magnets



Analysis for ICF System

≻ We performed 3-D calculations for the chamber of a power plant concept that utilizes the Z pinch driven inertial confinement technology Thick PbLi jets are utilized to breed tritium, absorb energy, and shield the chamber wall





Neutron Spectrum Emitted from Target



Changes in ENDF/B-VII.0 result in softer neutron spectrum emitted from target

Total number of neutrons emitted from target per fusion reduces from 1.047 to 1.039. This is primarily due to reduced neutron multiplication in tritium. Gamma production in target per fusion changed slightly from 4.73x10⁻³ to 4.75x10⁻³



Tritium Breeding in ICF Chamber

	FENDL-2.1		FENDL- 2.1+ENDF/I		
	Tritons per fusion	% orror	Tritons per fusion	%	% Change
Jets	7.13E-01	0.12%	7.15E-01	0.12%	0.28%
Nozzle	5.32E-02	0.27%	5.46E-02	0.27%	2.59%
Pool	3.64E-01	0.21%	3.75E-01	0.21%	3.20%
RTL	5.44E-03	0.27%	5.42E-03	0.27%	0.52%
TBR	1.14E+00		1.15E+00		1.32%



Tritium breeding in different PbLi zones was calculated
The overall TBR increased by 1.32% (not negligible when addressing tritium self-sufficiency)



Nuclear Heating in ICF Chamber

2°,

	FENDL-2.1		FENDL-2.1+ENDF/B-VII.0					
	MeV per		MeV per					
	fusion	% Error	fusion	% Error	% Change			
Jets	9.51E+00	0.12%	5.62E+00	0.14%	-40.93%			
Pool	2.93E+00	0.30%	0 1.07E+00	0.51%	-63.47%			
Cham Wall	1.88E+00	0.15%	1.95E+00	0.15%	4.07%			
Nozzle Zone	9.34E-01	0.34%	6.85E-01	0.37%	-26.65%			
RTL sup str	4.96E-01	0.43%	4.93E-01	0.42%	-0.50%			
RTL	4.30E-02	0.53%	3.78E-02	0.52%	-12.20%			
RTL Foam	1.33E-01	0.59%	1.03E-01	0.70%	-22.97%			
Total	1.52E+01		9.96E+00)	-37.45%			



Changes in nuclear heating are much higher (up to ~70%) and are caused by the bug in the NJOY version used for processing ENDF/B-VII.0
Differences are smaller in steel chamber wall and support structure where heating is dominated by gamma heating

Peak Damage and Helium WISCONSIN Production in ICF Chamber

End-of-life cumulative peak dpa and He production after 40 FPY with 3 GJ yield at 0.1 Hz

FENDL-2.1 FENDI -2, 1+ENDE/B-VILO % Error Value Value % Error % Change 0.45% -2.30% 1.23E+03 0.49% 1.20E+03 dpa 3.85E+03 1.71% 3.85E+03 1.71% -0.08% He appm



Peak He production in chamber wall changed only by 0.08% while peak dpa decreased by 2.3% as a result of the bug in the NJOY version used

21



Started Calculations for Three Benchmark Experiments

Frascati 14-MeV Neutron Generator (FNG)



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M. Sawan



Tungsten Experiments

Tungsten block (armor material for plasma facing components)





DENSIMET-176 (93.2%w W, 2.6%w Fe, 4.2%w Ni, 17.70 g/cm³). DENSIMET-180 (95.0%w W, 1.6%w Fe, 3.4%w Ni, 18.075 g/cm³)

Measurements of neutron flux at different depths by activation foils

P. Batistoni, et al, "Compilation of the Tungsten Experiment," SINBAD 2000 Archive Data Base



- Used MCNPX-2.6f with geometrical input and source subroutine provided by Paola Batistoni (ENEA)
- Calculations were performed at the 4 locations in the W block for 9 reactions with activation foils to cover the whole energy range of the neutron flux
- Calculations performed with the recently released ENDF/B-VII.0 data for all 71 elements/isotopes and compared to results performed with FENDL-2.1
- Calculated reaction rates in both cases using the most recent dosimetry data library IRDF-2002
- Calculation results compared to experimental results



Very High Energy (E> 9 MeV) Flux for Tungsten Experiments





- ENDF/B-VIII.0 results in differences (larger than 1_o statistical error in MCNP calculations) for very high energy flux at some locations in the block
- Both libraries agree with experiments to within <10%</p>



High Energy (E>3 MeV) Flux for Tungsten Experiments



 ENDF/B-VIII.0 results in differences (larger than statistical error in MCNP calculations) for high energy flux at some locations in the block
Both libraries agree with experiments to within <10%



Intermediate Energy (E>0.1 MeV) Flux for Tungsten Experiments



- ENDF/B-VIII.0 results in differences (larger than statistical error in MCNP calculations) for intermediate energy flux at some locations in the block
- Both libraries do not agree well experiments



In ENDF/B-VII.0 calculations, data for all 71 isotopes were replaced by data from ENDF/B-VII.0



 ENDF/B-VIII.0 results are nearly identical to FENDL-2.1 results (within statistical error in MCNP calculations) for low energy flux
Both libraries give large overestimate for ⁵⁵Mn(n,γ)⁵⁶Mn



- Results of ENDF/B-VII.0 and FENDL-2.1 are almost identical at low energy but modest differences are observed at some locations at high energies
- ➤While both calculated results agree to within ~10% at high energies, larger differences between calculations and experiments are obtained at low energies



Streaming experiments



Mock-up of the ITER inboard FW/ shield/vacuum vessel/TF coil with a streaming channel (3 cm diam)

Measurements of the neutron flux as a function of depth by activation foils



Results for Streaming experiments





Nearly identical results obtained from FENDL-2.1 and ENDF/B-VII.0

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Results for Streaming experiments





Although FENDL-2.1 and ENDF/B-VII.0 produce nearly identical large differences exist between calculated and experimental results

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Conclusions

- Modifying FENDL-2.1 to include the most recent ENDF/B-VII.0 is not urgently needed for ITER analysis
- The larger changes in calculated ICF target neutronics parameters and tritium breeding confirm the need for updating FENDL-2.1 for use in analysis of fusion systems beyond ITER
- Additional calculations are in progress for integral experimental benchmarks to fully understand the impact of data changes introduced in ENDF/B-VII.0 as compared against experimental data



UW Contribution to Development of FENDL-3.0

- Fusion devices beyond ITER include IFMIF, component test facility, DEMO, and commercial reactors.
- Additional materials and/or energy ranges are required for nuclear analysis of such devices.
- Identifying these needs is essential part of the development of the new FENDL-3.0 library.
- This requires close coordination with the users.
- National cross section libraries went through several upgrades since the release of FENDL-2.1.
- This requires assessment of these changes and their possible impact on FENDL.
- Benchmark calculations for both computational and experimental benchmarks are needed for proper validation of the FENDL-3.0 library.
- These calculations should be carried out in parallel to the development of the library.
- The research carried out at the University of Wisconsin will aim at:
 - Provide input from the fusion neutronics community in the USA regarding additional materials and/or energy ranges needed to extend the usefulness of the new FENDL-3.0 library for applications beyond ITER.
 - Perform benchmark calculations using FENDL-2.1 with the most recent upgrades of the national evaluations (e.g., replacing ENDF/B-VI.8 data used for 40 materials by ENDF/B-VII.0) to provide guidance in the process of developing FENDL-3.0.
 - Carry out calculations for computational and experimental benchmarks in parallel to FENDL-3.0 development to ensure adequate validation.



Proposed Work Plan

<u>Year 1</u>:

•Perform calculations for the FENDL computational benchmark (INDC(NDS)-316) and integral experiments at Frascatti to assess the impact of replacing ENDF/B-VI.8 data used for 40 materials in FENDL-2.1 by ENDF/B-VII.0.

•Perform similar calculations to assess impact of changes in other national cross section libraries as they are made available.

•Make recommendations to the FENDL-3.0 developers regarding the need for updates in FENDL-3.0.

•Solicit input from the fusion neutronics users community in the USA regarding needs for evaluations for additional materials and/or energy ranges beyond those in FENDL-2.1 to make sure that nuclear data needs are addressed satisfactorily in FENDL-3.0.

<u>Year 2</u>:

•Develop new computational benchmarks that are representative of of DEMO or commercial reactors with more representative breeding blankets, divertors, vacuum vessel, shielding, and magnets.

•Perform calculations for the new computational benchmarks as well as available integral experiments to validate the added data in FENDL-3.0.

•The latest version of MCNP will be used in the calculations with possible use of DAG-MCNP developed at the University of Wisconsin if CAD models of the experiments are available. DAG-MCNP allows direct neutron transport in the CAD model and hence eliminates possible modeling approximations or errors.

•Continue interacting with the users to ensure enhanced usability of FENDL-3.0. Year 3:

•Continue benchmark calculations as FENDL-3.0 development approaches completion to ensure adequate validation.

•Extend the benchmark calculations to validate the activation sub-library using the ALARA code.



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- Carry out calculations for computational and experimental benchmarks in parallel to FENDL-3.0 development to ensure adequate validation.