

1

The Impact of Neutron and Photon Cross Section Libraries on ITER Neutronics Calculations

Tim Bohm Mohamed Sawan* (* retired) University of Wisconsin-Madison CSEWG 2016, Brookhaven National Lab, NY November 14-16, 2016



Bohm



Outline

- 1) Introduction
- 2) Nuclear data libraries examined
- 3) Benchmark calculations considered
- 4) Results
- 5) Conclusion/Future Work



Introduction

- - In the design of fusion reactors, radiation transport calculations are very important
 - Both deterministic (Discrete Ordinates) and stochastic (Monte Carlo) methods are used
 - These transport codes need to have accurate cross section libraries







ITER



Fusion Neutronics Calculations

- Neutron flux/fluence (neutron)
 - magnet
- Radiation damage/dpa (neutron)
 - structural material degradation
- He production (neutron)
 - reweldability
- T production (neutron)
 - breeding, environmental
- Radiation dose (neutron+photon)
 - insulator
- Total nuclear heating (neutron+photon)
 - coolant system design, thermal stress, magnets

Need accurate neutron and photon libraries



Shield Block





FENDL

The Fusion Evaluated Nuclear Data Library (FENDL) is an international effort coordinated by the IAEA Nuclear Data Section
Assembles a collection of the best nuclear data from national cross section data libraries for fusion applications

- ENDF/B (US), JENDL (Japan), JEFF (Europe), BROND (Russia)
- Process uses fusion specific experimental and calculational benchmarks to evaluate the data

Bohm

Hot Topics = ENDF/8-VII	1 • TENDL-2012 • JENDL-4 • IBAND	L News » 50 year anniversary of ND	S, June 2014		
Request CD/DVD with documentation, data, codes, etc.	NEW IF	EFF-3.2 - Joint Evaluated Fission and Fit RDFF - International Reactor Dosimetry D/DVD-ROMs available for on-line down ortable Empire-3.2.2 for Windows - nuc	usion File, coord. by NEA Data Bar and Fusion File v1.03 [page] [archi nloading [page] clear reaction model code system fr	k, 2014 [page] [archive] [retrieve] ve] [retrieve] or data evaluation [page] [download]	
Culck Links ADS-Lb Alomic Mass Data Centre CINDA	Main All Reaction Da	tal Structure & Decay by A	pplications Doc & Codes uclides	Index Events Links News CINDA Nuclear reaction biolography	
Charged particle reference cross section DROSG-2000 EMPIRE-3.2	ENDF Evaluated nuclear realibraries	action ENSDF evaluated nuclear stru	cture and decay data (+XUNDL) **	NSR Nuclear Science References *	
ENDF-Archive ENDF Retrieval ENDF-6 Codes	NuDat 2.6 selected evaluated nuclear structure data **	RIPL reference parameters for nuclear model calculations	IBANDL Ion Beam Analysis Nuclear Data Library	Charged particle reference cross section Beam monitor reactions	
ENDVER	PGAA Prompt gamma rays from neutron capture	FENDL 3.0 Fusion Evaluated Nuclear Data Library, Version 3.0	Photonuclear cross sections and spectra up to 140MeV	IRDFF International Reactor Dosimetry and Fusion File	
ENSDF ASCII Files ENSDF programs EXEOR	NAA Neutron Activation Analysis Portal	Safeguards Data recommendations, August 2008	Standards - Neutron cross-sections, 2006 - Decay data, 2005		
Electron and Photon Interaction Data FENDL 3.0	*Database at the IAEA, Venna IAEA Nuclear Data Secti	**Database at the US NNDC			
Fission Yields	IAEA-NDS Mission, Staff and more Molecular	Newsletters Newsletters	Nuclear Structure & Decay Data Network	ents	



THE UNIVERSITY

ISCONSIN

5



FENDL continued

- FENDL-2.1 (71 isotopes, 2003) is reference library for ITER
 FENDL-3.1b has recently been released with 180 isotopes and energies up to 150 MeV for neutrons, protons, and deuterons
- Libraries available on-line:
 - <u>https://www-nds.iaea.org/fendl21/</u>
 - <u>https://www-nds.iaea.org/fendl3/</u>

Source of FENDL-2.1 data:

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	3	Mg, Ca, Ga
	(J32)		
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	2	¹⁵ N, Sn
	(BR2)		





- 65/180 isotopes in FENDL-3.1b come from ENDF/B-VII.1
 •See Table 1 in INDC(NDS)-0628
- Some key isotopes for this work:

Isotope	FENDL-2.1	FENDL-3.1b
H-1	JENDL-3.3	ENDF/B-VII.1
0-16	ENDF/B-VI.8	ENDF/B-VII.1
Cr-52	ENDF/B-VI.8	ENDF/B-VII.1
Fe-56	JEFF-3	JEFF-3.1.1
Ni-58	JEFF-3	ENDF/B-VII.0
Cu-63,65	ENDF/B-VI.8	ENDF/B-VII.0



Photon Data Libraries in FENDL/MCNP

- Significant efforts performed evaluating neutron data for FENDL
 - FENDL provides ACE formatted neutron data libraries for use with MCNP
- Less effort examining photon cross section data in the FENDL evaluation process
 - No MCNP (ACE formatted) photon libraries provided with FENDL
- But photon heating contributes 90% of the nuclear heating for important fusion materials (e.g. stainless steel, Cu, tungsten)

MCNP Photon Data:

•Standard library: mcplib04/84 (note: mcplib84 corrects bug in mcplib04)

•New library: eprdata12 (for MCNP6)

includes low energy < 1keV data





- Want to look at the impact of using the updated neutron and photon libraries in a realistic model of ITER
- Libraries examined:
 - <u>Neutron:</u>
 - 1. FENDL-2.1 (21c)
 - 2. FENDL-3.1b (31c)
 - 3. ENDF/B-VII.0 (70c)
 - 4. ENDF/B-VII.1 (80c)
 - <u>Photon:</u>
 - 1. mcplib84 (84p)
 - 2. eprdata12 (12p)



ITER 1-D Cylindrical Calculation Benchmark

- Based on an early ITER design
 Developed for the FENDL evaluation process
- Simple but realistic model of ITER with the Inboard and Outboard portions modeled with the plasma in between
- D-T fusion (14.1 MeV neutrons)
- Flux (neutron and photon), heating, dpa, and gas production calculated



M. Sawan, FENDL Neutronics Benchmark: Specifications for the calculational and shielding benchmark, INDC(NDS)-316, December 1994

ITER 1-D Cylindrical Benchmark continued



U.S.



THE UNIVERSITY

Plasma

Plasma



Results: Neutron Flux



• With updated FENDL-3.1b neutron library (31c) see neutron fluxes up to 8% higher than FENDL-2.1 (21c) at deep depths in TF coil

- With ENDF/B-VII.1 (80c) see neutron fluxes up to 3% lower
- In FENDL-3.1b, Fe-56 and Cu data come from JEFF-3.1.1 and ENDF/B-VII.0



Results: Neutron Spectrum at OB TF coil



U.S.

With ENDF/B-VII.0-1 (70c, 80c) see lower flux at TF coil
With updated FENDL-3.1b neutron library (31c) see a harder spectrum than FENDL-2.1 (21c) at TF coil
With ENDF/B-VII.0-1 (70c, 80c) also see a harder spectrum at TF coil





Results: Photon Flux



• Photon fluxes roughly follow neutron fluxes (see structure at VV shell)

• With updated FENDL-3.1b neutron library (31c) see photon fluxes up to 9% higher than FENDL-2.1 (21c) at deep depths in TF coil

• With ENDF/B-VII.1 (80c) see neutron fluxes up to 6% lower





Results: Total nuclear heating



With updated FENDL-3.1b neutron library (31c) see total heating up to 6% higher than FENDL-2.1 (21c) at deep depths in TF coil
With ENDF/B-VII.1 (80c) see total heating up to 3% lower





Results: neutron heating



• With updated FENDL-3.1b neutron library (31c) see neutron heating up to 15% higher than FENDL-2.1 (21c) at deep depths in TF coil

• With ENDF/B-VII.1 (80c) see neutron heating up to 70% higher





Results: photon heating



 With updated FENDL-3.1b neutron library (31c) see photon heating up to 5% higher than FENDL-2.1 (21c) at deep depths in TF coil

• With ENDF/B-VII.1 (80c) see photon heating up to 4% lower





Results: Impact of Photon Library



• With the updated photon library (12p), we see good agreement with the standard photon library (84p)





Results: dpa

	21c+84p	31c+84p	% diff.	80c+84p	% diff.
IB					
FW Cu	9.16416E+00	9.13434E+00	-0.33	9.18390E+00	0.22
FW SS (Fe)	7.78771E+00	7.78131E+00	-0.08	8.22207E+00	5.58
VV Inconel (Ni)	1.01076E-02	1.04166E-02	3.06	1.01171E-02	0.09
VV SS (Fe)	3.35716E-03	3.45015E-03	2.77	3.46625E-03	3.25
Magnet Cu	3.88072E-05	4.06994E-05	4.88	3.84160E-05	-1.01
ОВ					
FW Cu	1.37635E+01	1.37245E+01	-0.28	1.37831E+01	0.14
FW SS (Fe)	1.18140E+01	1.18099E+01	-0.03	1.24828E+01	5.66
VV Inconel (Ni)	1.38127E-02	1.42400E-02	3.09	1.38188E-02	0.04
VV SS (Fe)	5.02005E-03	5.16308E-03	2.85	5.18489E-03	3.28
Magnet Cu	5.61928E-06	5.95996E-06	6.06	5.55328E-06	-1.17

Max. relative error <0.15%

• different neutron flux and spectrum at FWSS, VV, magnet





Results: He production

	21c+84p	31c+84p	% diff.	80c+84p	% diff.
IB				-	
FW Be	4.09900E+03	4.10018E+03	0.03	4.12365E+03	0.60
FW CuBeNi	2.10289E+02	2.11113E+02	0.39	2.12205E+02	0.91
FW SS316	1.77311E+02	1.84877E+02	4.27	1.88600E+02	6.37
VV Inconel	6.76921E-02	7.98705E-02	17.99	7.68869E-02	13.58
VV SS316	7.62989E-02	8.24488E-02	8.06	7.97493E-02	4.52
Magnet Cu	3.80472E-04	4.01679E-04	5.57	3.79698E-04	-0.20
OB					
FW Be	5.98127E+03	5.98538E+03	0.07	6.01139E+03	0.50
FW CuBeNi	3.23240E+02	3.24749E+02	0.47	3.26056E+02	0.87
FW SS316	2.45343E+02	2.56222E+02	4.43	2.62737E+02	7.09
VV Inconel	9.04495E-02	1.06787E-01	18.06	1.02669E-01	13.51
VV SS316	1.07582E-01	1.16363E-01	8.16	1.12537E-01	4.61
Magnet Cu	5.56782E-05	5.93275E-05	6.55	5.53346E-05	-0.62

Max. relative error <0.19%

• different neutron flux and spectrum at FWSS, VV, magnet





Results: Tritium production

	21c+84p	31c+84p	% diff.	80c+84p	% diff.
IB	-				
FW Be	6.10392E+01	6.10362E+01	0.00	6.11245E+01	0.14
FW CuBeNi	1.56402E+00	1.56365E+00	-0.02	1.56666E+00	0.17
FW SS316	1.19527E-01	1.19116E-01	-0.34	2.22290E-01	85.97
VV Inconel	2.92231E-06	6.92198E-06	136.87	6.86316E-06	134.85
VV SS316	2.47763E-05	2.53464E-05	2.30	4.19001E-05	69.11
Magnet (Cu)	1.34326E-06	1.42722E-06	6.25	1.30178E-06	-3.09
OB					
FW Be	8.96548E+01	8.96782E+01	0.03	8.97799E+01	0.14
FW CuBeNi	2.44711E+00	2.44778E+00	0.03	2.45166E+00	0.19
FW SS316	1.86724E-01	1.86228E-01	-0.27	3.49079E-01	86.95
VV Inconel	3.78742E-06	9.02266E-06	138.23	8.95916E-06	136.55
VV SS316	3.57871E-05	3.66218E-05	2.33	6.04256E-05	68.85
Magnet (Cu)	1.82708E-07	1.95836E-07	7.19	1.76016E-07	-3.66

Max. relative error <0.27%

- different neutron flux and spectrum at FWSS, VV, magnet
- T production substantially different in SS 316 for 31c versus 80c
- FENDL-3.1b (31c) and ENDF/B-VII.1 (80c) still missing rxn mt=205 for tungsten isotopes Bohm





- For realistic ITER calculations, use of updated photon and neutron libraries produces neutron fluxes from 3% lower to 8% higher than the reference libraries
- For realistic ITER calculations, use of updated photon and neutron libraries produces photon fluxes from 6% lower to 9% higher than the reference libraries
- For realistic ITER calculations, use of updated photon and neutron libraries produces total nuclear heating from 3% lower to 6% higher than the reference libraries





Future Work

- Repeat with FENDL-3.2 and ENDF/B-VIII when released
- Repeat comparisons with a detailed 3-D model of ITER using DAG-MCNP (CAD based version of MCNP developed at UW)







Questions?

ACKNOWLEDGMENTS

Support for this work has been provided from the United States Department of Energy, Office of Science.

The views and opinions expressed herein do not necessarily reflect those of the ITER Organization.

