Benchmarking FENDL-2.1 with Impact of ENDF/B-VII.0 Release on Nuclear Heating and Damage

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***Abstract*— MCNP calculations for a calculational benchmark representative of an early ITER design were carried out to investigate the impact of ENDF/B-VII.0 release on FENDL-2.1. The results presented in this work clearly show that the previously observed differences in nuclear heating and radiation damage are removed when the correctly processed ENDF/B-VII.0 data are used. Differences in all nuclear parameters are very small (<1%) implying that minimal impact is expected on ITER analysis and updating the FENDL-2.1 library is not urgently needed for ITER analysis. Calculations for an inertial fusion power plant showed larger changes in nuclear heating, and radiation damage due to the large changes in the H-3 and Au-197 data that affect the energy spectrum of neutrons emitted from the ICF target. The results confirm the need for updating FENDL-2.1 for use in analysis of fusion systems beyond ITER.**

Keywords-nuclear data; nuclear heating; radiation damage; ITER

I. INTRODUCTION

The International Atomic Energy Agency (IAEA) in cooperation with several national nuclear data centers and research groups started an effort in 1987 to develop the Fusion Evaluated Nuclear Data Library (FENDL) [1]. During the FENDL evolution, a set of calculational and integral experimental benchmarks were utilized for validation and selection of the appropriate evaluations for the different isotopes in the library [2,3]. The most recent version, FENDL-2.1, includes 71 elements or isotopes taken from different evaluations that include ENDF/B-VI.8, JENDL-3.3, JENDL-3.2, JENDL-FF, JEFF-3, and BROND-2.1 as illustrated in Table I [4]. This library has been extensively validated [3] and is the reference library for nuclear analysis of ITER and other fusion systems. Data for most of the elements/isotopes (40) were taken from ENDF/B-VI.8. A new cross section evaluation, ENDF/B-VII.0, was released in December 2006 and was recommended to replace ENDF/B-VI.8 based on extensive validation [5].

A preliminary assessment for changes made in data of the 40 isotopes/elements used in FENDL-2.1 implied that only minor impact is expected on nuclear analysis of ITER [6]. However, the effect of data changes could be large when used in analysis of other fusion systems with breeding blankets (Demo and power plants). In addition, for inertial fusion systems, large effects are expected due to changes in data for H-3 and Au-197 that are important for ICF target neutronics.

To quantify these observations, we performed MCNP calculations for an ITER 1-D calculational benchmark that was utilized during the FENDL development process [2]. In a previous work [6], calculations were carried out using FENDL-2.1 with the data for the 40 elements/isotopes replaced by the recent data from ENDF/B-VII.0. Results for both neutron and gamma fluxes were found in a previous work to agree within less than 1% for all regions. However, results for nuclear heating and atomic displacement damage were found to differ by up to 50%. This unexpected finding was attributed to a bug in the version of the NJOY code used to process the data. This was fixed in a recent version and was used to provide an updated version of the ACE formatted ENDF/B-VII.0 library [7]. In this paper, results of calculations for the ITER benchmark problem are presented and compared to the FENDL-2.1 results. Emphasis is on comparing nuclear heating and radiation damage to investigate whether the previously observed discrepancy is removed. In addition, results of calculations for a conceptual inertial fusion power plant are presented and discussed.

TABLE I. SOURCE OF DATA IN FENDL-2.1

No.	Library	NMAT	Materials
1	ENDF/B-VI.8 (E6)	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, ^{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

II. RESULTS FOR ITER CALCULATIONAL BENCHMARK

We performed calculations for the ITER 1-D cylindrical geometry calculational benchmark illustrated schematically in Fig. 1 [2]. The inboard (IB) and outboard (OB) components are modeled as cylindrical rings with the plasma in between. The source in the plasma zone is normalized to 6.1×10^{17} n/cm^{2}s yielding IB and OB neutron wall loadings of 1 and 1.5 MW/m^2, respectively. The calculations were performed with the MCNP code [8]. The 14 MeV source neutrons are sampled from a uniform isotropic distribution in the plasma. Cell importances were adjusted to reduce statistical uncertainties in calculated parameters. In these MCNP calculations, nuclear responses (flux, heating, radiation damage, and gas production) were

compared using FENDL-2.1 and the FENDL-2.1 library with the data for the 40 isotopes/elements replaced by the recent data from ENDF/B-VII.0 processed by NJOY-99.259 [7].

The calculated total neutron and gamma flux values obtained with FENDL-2.1 were compared to those obtained with data for the 40 isotopes/elements taken from ENDF/B-VII.8 replaced by data from ENDF/B-VII.0. The results are identical to those reported previously [6]. 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. The detailed neutron energy spectra with 175 energy bins also agreed very well with differences <2% as shown in Figs. 2 and 3 for the front of the OB vacuum vessel (VV).

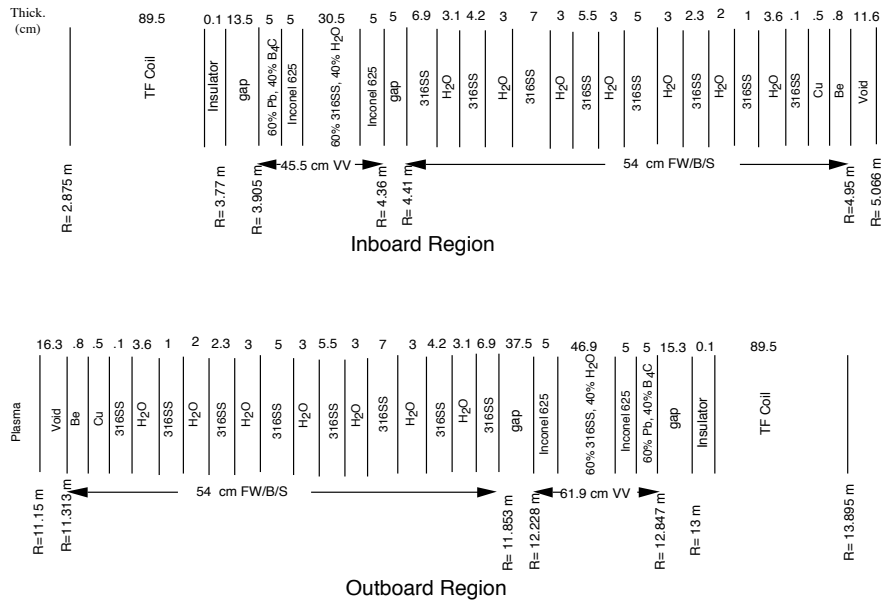

Figure 1. Radial build of ITER calculational benchmark.

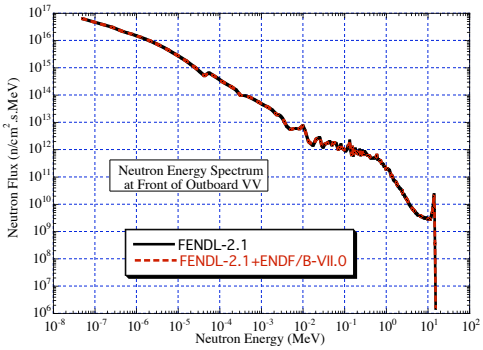

Figure 2. Neutron energry spectrum comparison at front of OB VV.

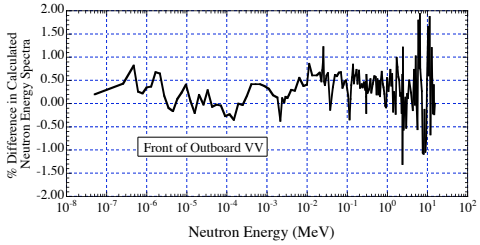

Figure 3. Differences in calculated neutron energy spectra.

The excellent agreement obtained for neutron and gamma fluxes implies excellent agreement in response parameters as well. However, in previous work [6] the comparison of calculated nuclear heating and atomic displacement damage showed large differences of up to ~55%. This large difference was attributed to a bug in versions of NJOY between 99.115 and 99.180 that led to erroneously low neutron heating values in some instances [9]. This bug was fixed in subsequent versions of NJOY and new ACE formatted data were processed. We used these data [7] to compare nuclear heating and radiation damage results.

Table II gives the calculated peak nuclear heating (in W/cm^3) in the different zones. The 1σ statistical uncertainties are also provided. Excellent agreement is obtained between the results of the two libraries with differences less than ~0.8% and much smaller differences in the front zones closer to the plasma. Investigation of the results for the separated neutron and gamma heating components revealed similar agreement.

Table III compares the peak atomic displacement damage rates (dpa/FPY) in Fe for the different zones, obtained using the two libraries. Unlike the large differences of up to ~70% observed in the previous calculations [6], the results with the corrected data show excellent agreement between the two libraries with differences less than ~0.3% and much lower differences in zones close to the plasma. Calculated gas production rates (helium, hydrogen, and tritium) were similar to those determined in the previous analysis [6] and are very close using the two libraries. These results showed nearly identical results in the FW and blanket with <1.7% change in the magnet.

TABLE II. PEAK POWER DENSITY (W/CM^3) RESULTS

	FENDL-2.1		FENDL-2.1 +ENDF/B-VII.0		
	Power Density	% Error	Power Density	% Error	% Change
IB					
FW					
Be	1.008E+01	0.05	1.008E+01	0.05	-0.02
Cu	2.017E+01	0.06	2.019E+01	0.07	0.07
SS	1.783E+01	0.08	1.786E+01	0.08	0.16
VV SS	2.619E-02	0.18	2.632E-02	0.18	0.51
Magnet	3.659E-05	0.45	3.691E-05	0.45	0.87
OB					
FW					
Be	1.391E+01	0.03	1.391E+01	0.03	-0.02
Cu	2.474E+01	0.04	2.478E+01	0.05	0.13
SS	2.230E+01	0.05	2.233E+01	0.05	0.10
VV SS	3.573E-02	0.09	3.582E-02	0.09	0.24
Magnet	5.376E-06	0.43	5.419E-06	0.43	0.79

TABLE III. PEAK FE RADIATION DAMAGE (DPA/FPY) RESULTS

	FENDL-2.1		FENDL-2.1 +ENDF/B-VII.0		
	Fe dpa/FPY	% Error	Fe dpa/FPY	% Error	% Change
IB					
FW	7.789E+00	0.07	7.795E+00	0.07	0.07
Blanket	4.430E+00	0.07	4.432E+00	0.07	0.05
VV	3.354E-03	0.24	3.365E-03	0.24	0.32
OB					
FW	1.182E+01	0.03	1.183E+01	0.03	0.13
Blanket	6.938E+00	0.03	6.945E+00	0.03	0.11
VV	5.018E-03	0.12	5.035E-03	0.12	0.33

The peak radiation parameters in the inboard leg of the magnet were calculated and compared in Table IV. The peak fast neutron (E>0.1 MeV) fluence increased by ~1.4%, the insulator dose increased by ~0.9%, the Cu damage is ~1.8% higher, and the winding pack heating increased by ~0.9%. In general, these are small changes.

TABLE IV. PEAK IB MAGNET RADIATION PARAMETERS

	FENDL-2.1		FENDL-2.1 +ENDF/B-VII.0		
	Value	% Error	Value	% Error	% Change
Fast n fluence (n/cm^2/FPY)	6.27E+16	0.46	6.36E+16	0.46	1.42
Insulator dose (Gy/FPY)	5.59E+05	0.47	5.64E+05	0.46	0.87
Cu dpa/FPY	3.75E-05	0.49	3.82E-05	0.46	1.76
Nuclear heating (mW/cm^3)	3.66E-02	0.45	3.69E-02	0.45	0.87

The results presented in this work for the ITER calculational benchmark clearly show that the previously observed differences in nuclear heating and radiation damage are removed when the correctly processed ENDF/B-VII.0 data are used. Differences in all nuclear parameters are small implying that minimal impact is expected on ITER analysis and updating the FENDL-2.1 library is not urgently needed for ITER analysis.

III. RESULTS FOR ICF SYSTEM

As discussed in previous work [6], larger effects are expected in inertial fusion systems due to changes in data for H-3 and Au-197 that are used in ICF targets. We performed three-dimensional calculations for the chamber of a power plant concept that utilizes the Z-pinch driven inertial confinement technology [10]. The chamber has a diameter of 10 m and a height of 6 m. Double-layered recyclable transmission lines (RTL) drive the targets at the center of chamber. The imploded target radial build and composition with a ρR of 3 was included in the model at the lower tip of the RTL. 14.1 MeV source neutrons were sampled uniformly from the DT spherical target core. Thick PbLi jets are utilized to breed tritium, absorb energy, and shield the chamber wall. The chamber wall is made of the ferritic steel alloy F82H.

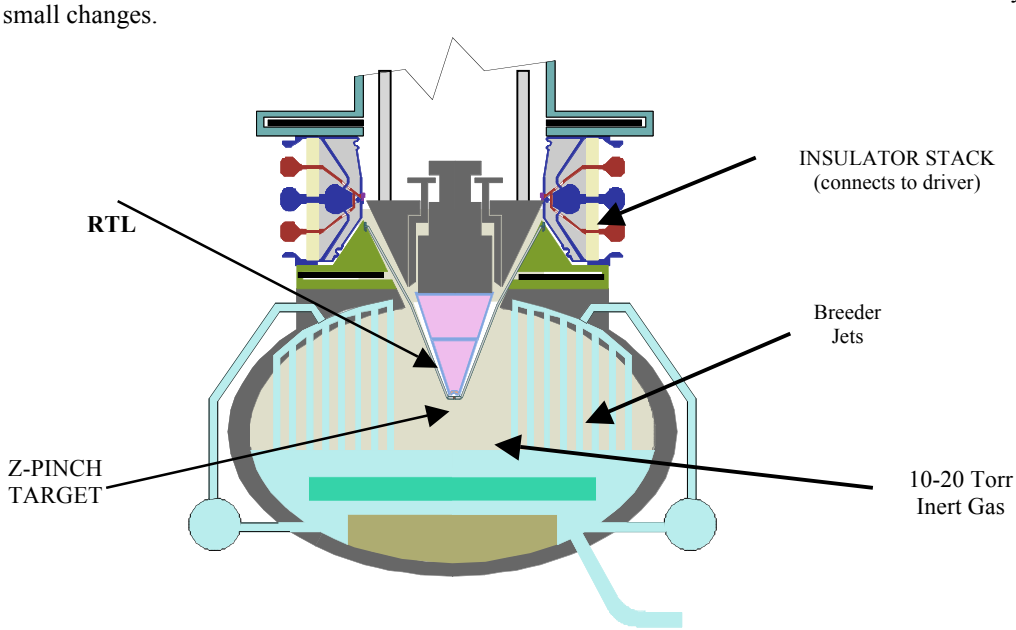

Figure 4. Schematic of ICF chamber.

Calculations were performed using the FENDL-2.1 library with the data for the 40 isotopes/elements taken from ENDF/B-VI.8 replaced by the recent data from ENDF/B-VII.0. The results were compared to the previous results obtained using the FENDL-2.1 library [11]. Changes in ENDF/B-VII.0 resulted in a softer neutron spectrum emitted from the target similar to the total number of neutrons emitted from the target per fusion, reducing from 1.047 to 1.039 [6].

Tritium breeding in the different PbLi zones was calculated per fusion and the results were similar to those given in previous work [6]. The overall tritium breeding ratio (TBR) increased by 1.32%. Table V gives nuclear heating per fusion in the target layers and chamber components. Total target heating decreased by ~3% and total chamber heating reduced by ~2%. While changes in nuclear heating in the previous analysis [6] were as large as ~70%, the recent calculations with the correctly processed ENDF/B-VII.0 data show much smaller differences. However, these differences are larger than those obtained for the ITER benchmark. Table VI provides the peak structure cumulative atomic displacements (dpa) and He production (appm) after 40 FPY plant lifetime.

TABLE V. NUCLEAR HEATING IN TARGET AND CHAMBER

	FENDL-2.1		FENDL-2.1+ENDF/B-VII.0		% Change
	MeV per fusion	% error	MeV per fusion	% error	
Target					
DT	1.469E+00	0.22	1.426E+00	0.22	-2.94
Be	9.636E-03	0.07	9.688E-03	0.07	0.54
CH	2.953E-04	0.06	2.962E-04	0.06	0.30
Au	4.387E-04	1.38	4.330E-04	1.40	-1.30
Chamber					
Jets	9.507E+00	0.12	9.134E+00	0.11	-3.93
Nozzle	9.342E-01	0.34	9.480E-01	0.33	1.48
Pool	2.928E+00	0.30	2.899E+00	0.29	-0.97
Wall	1.875E+00	0.15	1.951E+00	0.15	4.04
RTL	6.719E-01	0.53	6.678E-01	0.53	-0.62

TABLE VI. PEAK END-OF-LIFE STRUCTURE RADIATION DAMAGE

	FENDL-2.1		FENDL-2.1+ENDF/B-VII.0		% Change
	Value	err%	Value	err%	
dpa	1.233E+03	0.49	1.251E+03	0.48	1.48
He appm	3.848E+03	1.71	3.826E+03	1.71	-0.56

IV. SUMMARY AND CONCLUSIONS

The most recent version of the Fusion Evaluated Nuclear Data Library, FENDL-2.1, includes 71 elements or isotopes. Data for most of the isotopes/elements (40) were taken from ENDF/B-VI.8. Following the release of ENDF/B-VII.0 we performed MCNP calculations for a 1-D calculational benchmark representative of an early ITER design that was utilized during the FENDL development process. Calculations were carried out using FENDL-2.1 with the data for the 40 isotopes/elements replaced by the recent data from ENDF/B-VII.0 and the results for flux, heating, dpa, and gas production were compared to those obtained using the FENDL-2.1 library.

The results presented in this work for the ITER calculational benchmark clearly show that the previously observed differences in nuclear heating and radiation damage are removed when we use the recent correctly processed ENDF/B-VII.0 data. Differences in all nuclear parameters are very small implying that minimal impact is expected on ITER analysis and updating the FENDL-2.1 library is not urgently needed for ITER analysis.

However, a larger effect is expected when used in analysis of other fusion systems with breeding blankets (Demo and power plants). Calculations for an inertial fusion power plant showed relatively large changes in nuclear parameters due to the large changes in the H-3 and Au-197 data that affect the energy spectrum of neutrons emitted from the ICF target. The results confirm the need for updating FENDL-2.1 for use in analysis of fusion systems beyond ITER.

Additional calculations are in progress for three integral experimental benchmarks to fully understand the impact of data changes introduced in ENDF/B-VII.0 as compared against experimental data.

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