



Benchmarking FENDL-2.1 with ENDF/B-VII.0 replacing ENDF/B-VI.8

Mohamed Sawan

Tim Bohm

Fusion Technology Institute
The University of Wisconsin-Madison

CSEWG Meeting
4–6 November 2008
BNL

FENDL-2.1 Background

- Revision to FENDL-2.0 (1995/96)
- Compiled November 2003, INDC(NDS)-451
- 71 elements/isotopes
- Working libraries prepared by IAEA/NDS, see INDC(NDS)-467 (2004)
- Processing performed using NJOY-99.90 at IAEA-NDS and resulting processed files are available in ACE format for MCNP and in MATXS format for multi-group transport calculations (175n-42g)
- New reference data library for ITER neutronics calculations

Data Source for FENDL-2.1

No.	Library	NMAT	Materials
1	ENDF/B-VI.8 (E6)	40	^2H , ^3H , ^4He , ^6Li , ^7Li , ^9Be , ^{10}B , ^{11}B , ^{16}O , ^{19}F , $^{28-30}\text{Si}$, ^{31}P , S , $^{35,37}\text{Cl}$, K , $^{50,52-54}\text{Cr}$, $^{54,57,58}\text{Fe}$, ^{59}Co , $^{61,62,64}\text{Ni}$, $^{63,65}\text{Cu}$, ^{197}Au , $^{206-208}\text{Pb}$, ^{209}Bi , $^{182-184,186}\text{W}$
2	JENDL-3.3 (J33)	18	^1H , ^3He , ^{23}Na , $^{46-50}\text{Ti}$, ^{55}Mn , $^{92,94-98,100}\text{Mo}$, ^{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 taken from ENDF/B-VI.8
- ENDF/B-VII.0 library officially released on December 15, 2006
- We examined changes made in data for these 40 isotopes/elements and assessed possible impact on nuclear analysis of ITER and other fusion system



Assessment of changes made in data for the 40 isotopes/elements taken from ENDF/B-VI.8

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 energy-angle 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 is reduced secondary particle production for new ENDF/B-VII release"

Assessment of changes made in data for the 40 isotopes/elements taken from ENDF/B-VI.8

Pb-206, Pb-207: ENDF/B-VII.0 data were taken from JEFF-3.1

Only minor change in cross sections above ~5 MeV

S-32, S-33, S-34, S-36, K-39, K-40, K-41: Only isotopic data provided in ENDF/B-VII.0 for S and K

Data for S and K isotopes taken from JENDL-3.3 with Large changes in cross sections

H-3: Large changes in elastic scattering and (n,2n) cross sections with expected impact on inertial confinement fusion (ICF) target neutronics

Li-6: Minor changes in (n,t) cross sections observed at very low and high energies that could lead to minor impact on predicting tritium production in breeding blankets

Be-9: Only minor change in elastic scattering

B-10: Only minor change in (n, α) and elastic scattering

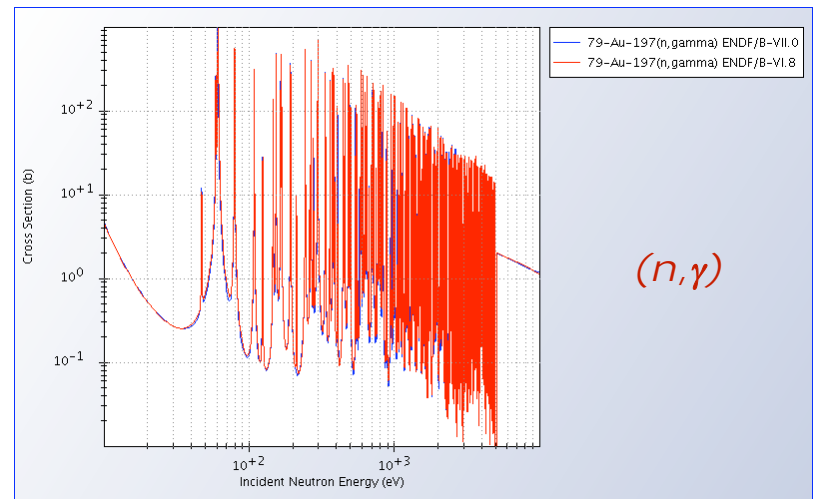
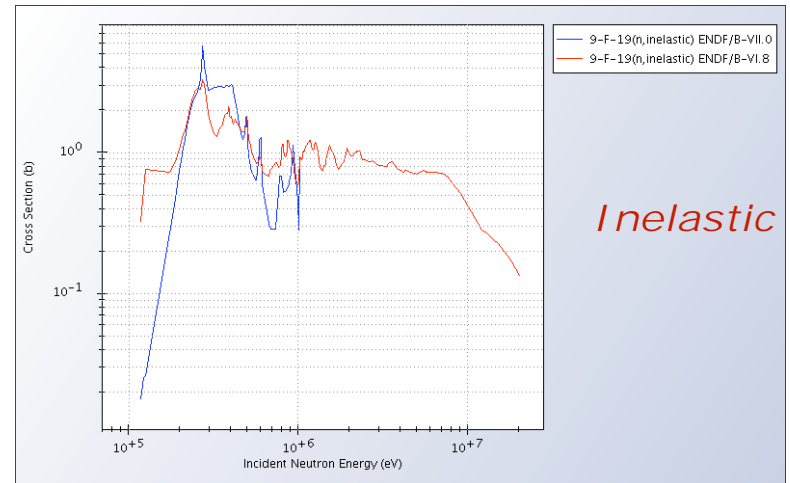
O-16: Only minor change in (n, α) and elastic scattering

Assessment of changes made in data for the 40 isotopes/elements taken from ENDF/B-VI.8

F-19: Large changes in (n,γ) and inelastic scattering cross sections observed with impact on nuclear analysis for breeding blankets that utilize Flibe

Cl-35, Cl-37: Large changes in (n,γ) , (n,p) and elastic scattering cross sections

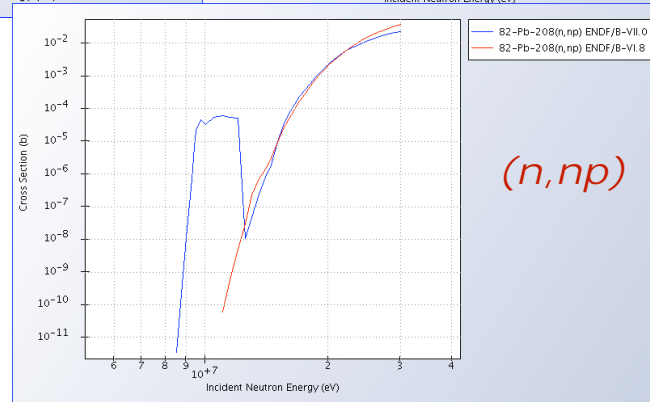
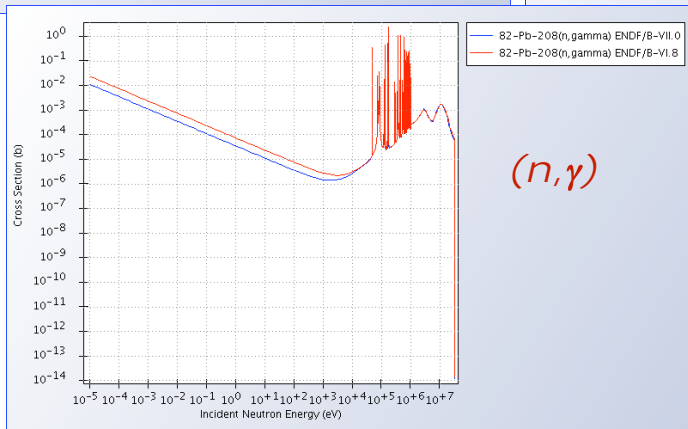
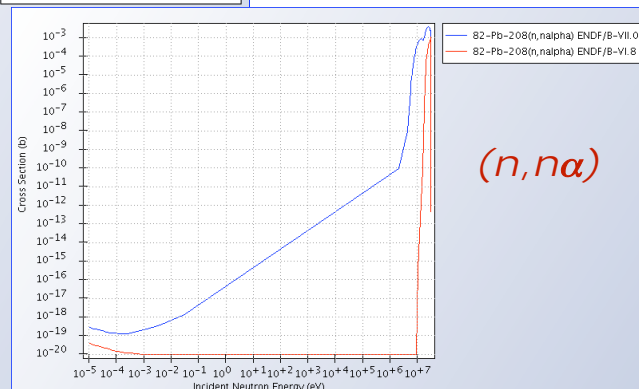
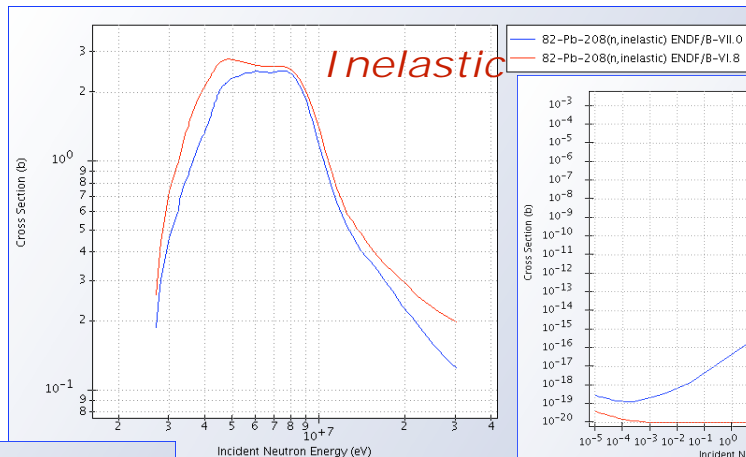
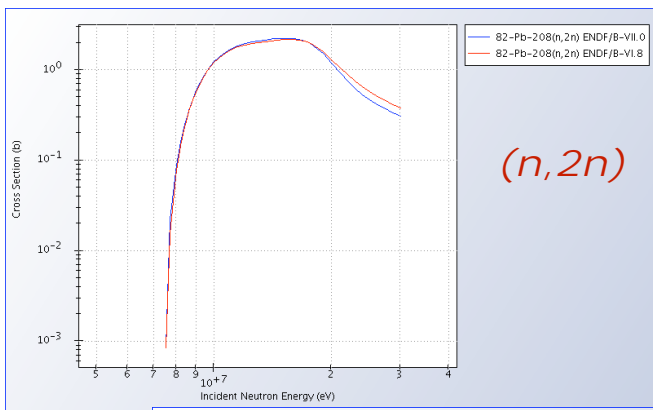
Au-197: Moderate changes in (n,γ) and elastic scattering cross sections in resonance region with possible impact on ICF target neutronics



Assessment of changes made in data for the 40 isotopes/elements taken from ENDF/B-VI.8

Pb-208

Many cross sections changed



Large changes in several cross sections

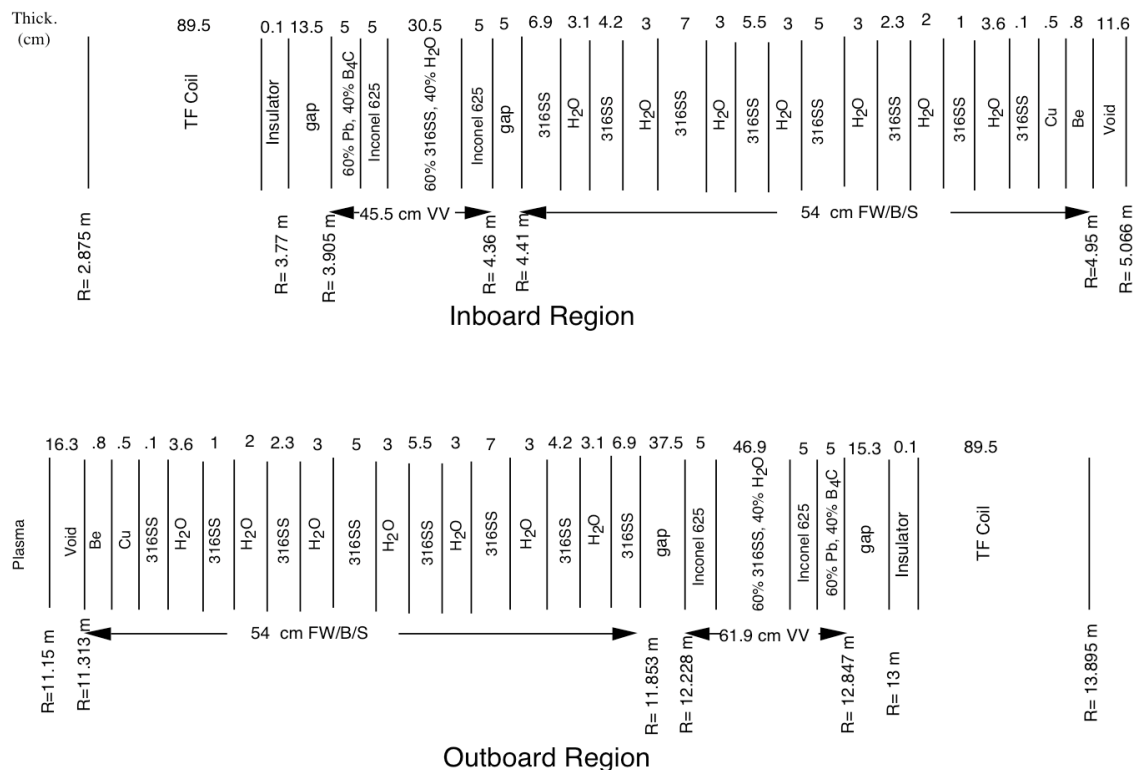
Possible impact on analysis for breeding blankets with PbLi

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 Computational Benchmark

- To quantify these observations, we performed calculations for a 1-D cylindrical geometry calculation 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).



Analysis for ITER Computational Benchmark

- This benchmark problem has been mainly used in discrete ordinate calculations using FENDL multi-group data
- FZK prepared MCNP geometry input and compared nuclear responses using the different versions of FENDL, namely FENDL-1.0, 2.0 and 2.1
- 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		% Change	FENDL-2.1		FENDL-2.1 +ENDF/B-VII.0		% Change
	Neutron Flux	% Error	Neutron Flux	% Error		Gamma Flux	% Error	Gamma Flux	% Error	
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

- Excellent agreement obtained for neutron and gamma fluxes implies excellent agreement in response parameters as well
- 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
- This 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 (WHEN??)
- 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

Peak He appm/FPY

	FENDL-2.1		FENDL-2.1 +ENDF/B-VII.0		% Change
	He Prod.	% Error	He Prod.	% Error	
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 Magnet Radiation Effects

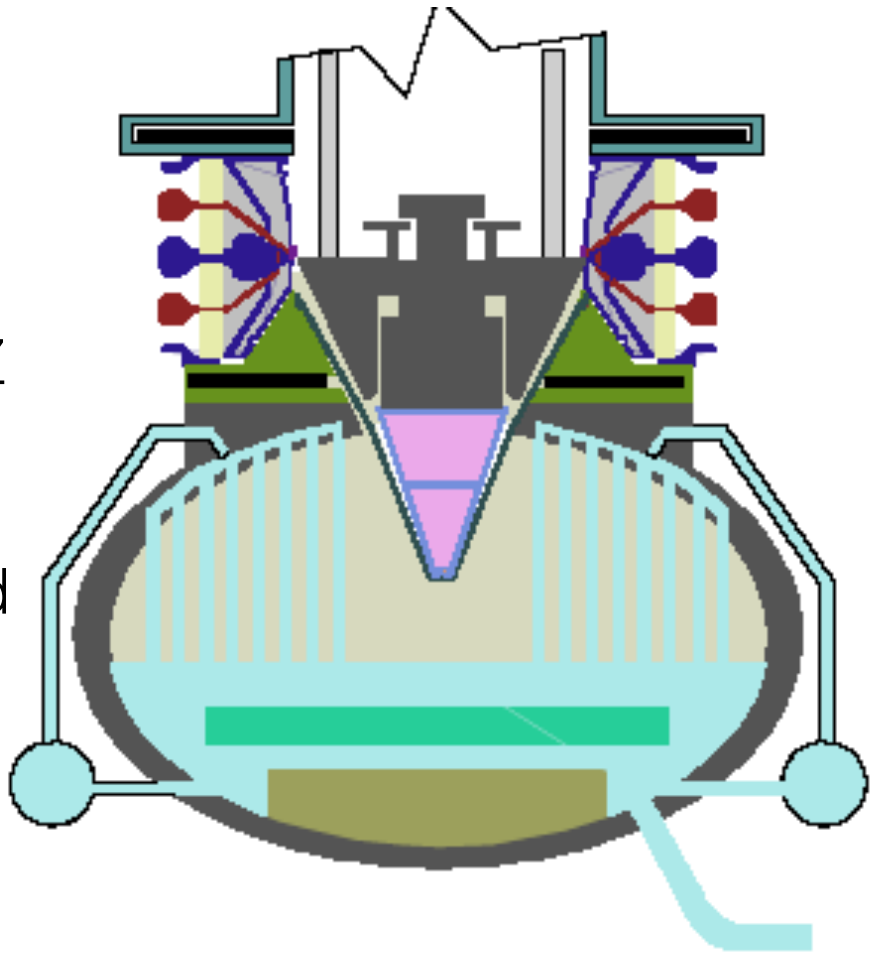
⌘

	FENDL-2.1		FENDL-2.1 +ENDF/B-VII.0		
	Value	% Error	Value	% Error	% Change
INBOARD					
Fast n fluence, $E > 0.1$ MeV (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%	5.49E+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/cm ³)	3.66E-02	0.45%	3.59E-02	0.45%	-1.87%
OUTBOARD					
Fast n fluence, $E > 0.1$ MeV (n/cm ² /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/cm ³)	5.38E-03	0.43%	5.26E-03	0.43%	-2.13%

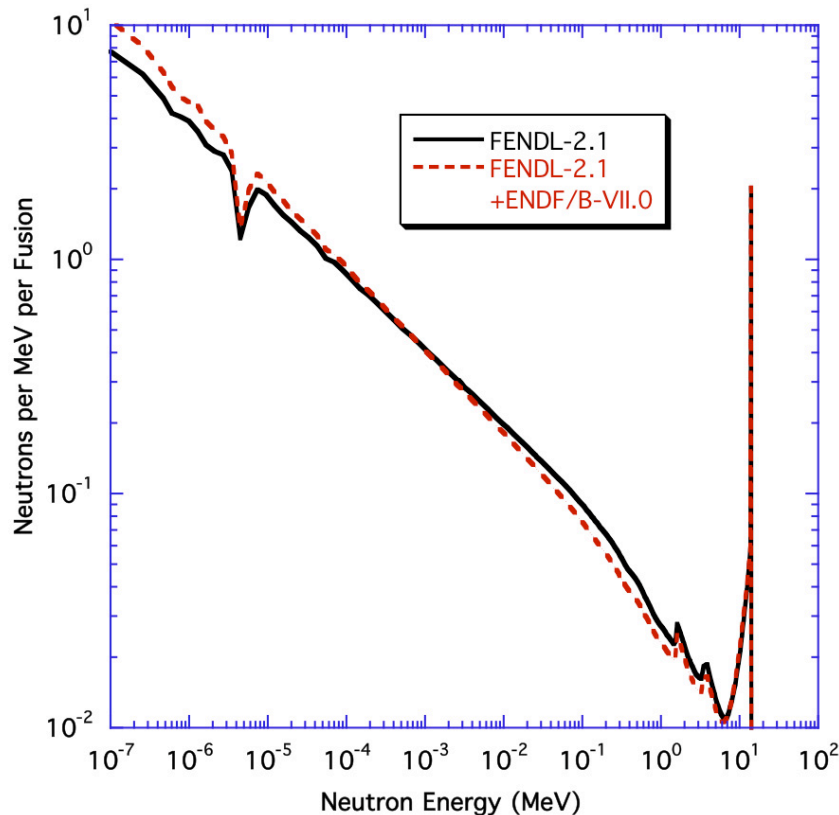
- The peak fast neutron ($E > 0.1$ MeV) fluence increased by ~1.4%, the insulator dose was reduced by ~1.6%, and the winding pack heating decreased by ~1.9% and stabilizer damage rate decreased by 27%
- Despite the error in processing neutron heating data, heating changes are small since heating is dominated 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



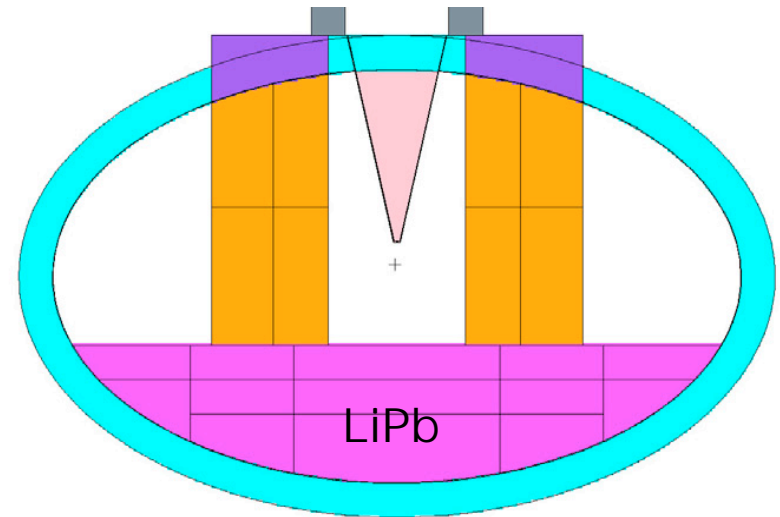
Neutron Spectrum Emitted from Target



- 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 4.73×10^{-3} to 4.75×10^{-3}

Tritium Breeding in ICF Chamber

	FENDL-2.1		FENDL-2.1+ENDF/B-VII.0		% Change
	Tritons per fusion	% error	Tritons per fusion	% error	
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%

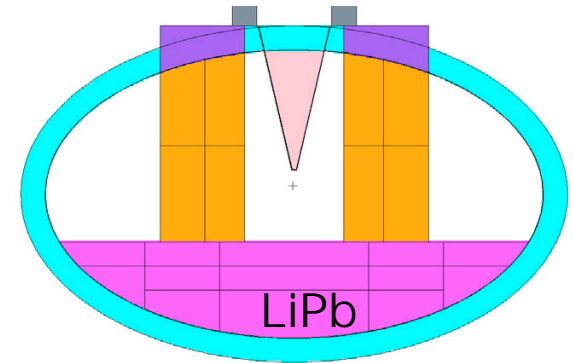


- Tritium breeding in different PbLi zones was calculated
- The overall TBR increased by 1.32%

Nuclear Heating in ICF Chamber

21

	FENDL-2.1		FENDL-2.1+ENDF/B-VII.0		
	MeV per fusion	% Error	MeV per fusion	% Error	% Change
Jets	9.51E+00	0.12%	5.62E+00	0.14%	-40.93%
Pool	2.93E+00	0.30%	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%



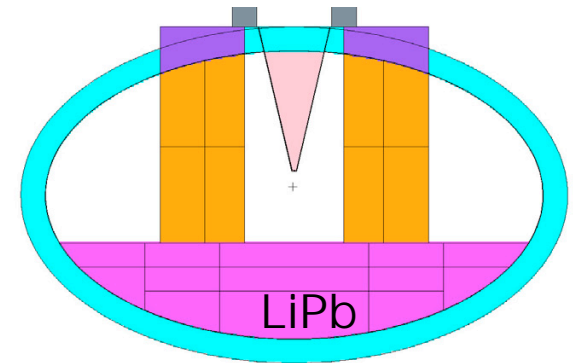
- Changes in nuclear heating are much higher (up to ~70%) and are caused by the bug in the NJOY version used for processing ENDF/B-VII.0
- Differences are smaller in steel chamber wall and support structure where heating is dominated by gamma heating

Peak Damage and Helium Production in ICF Chamber

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

21

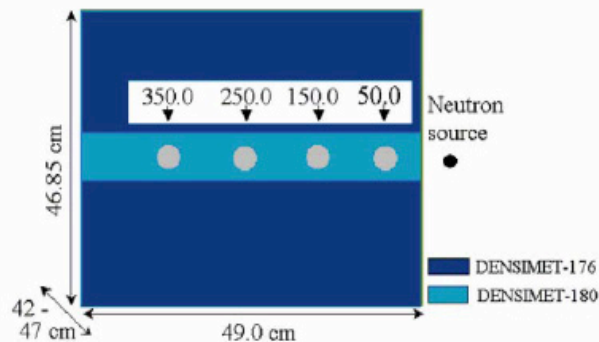
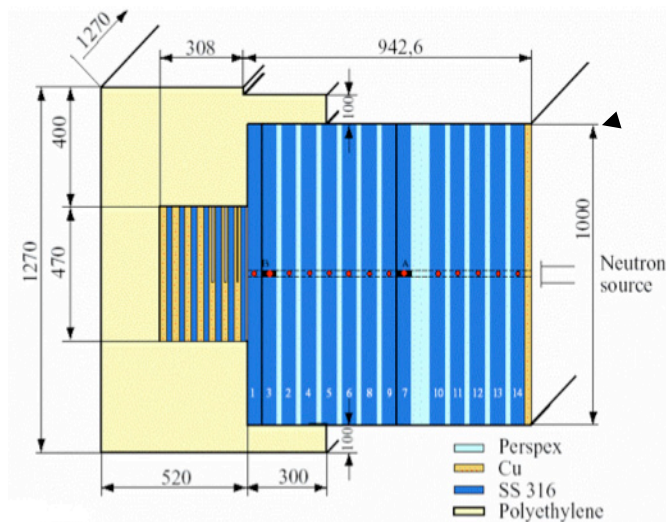
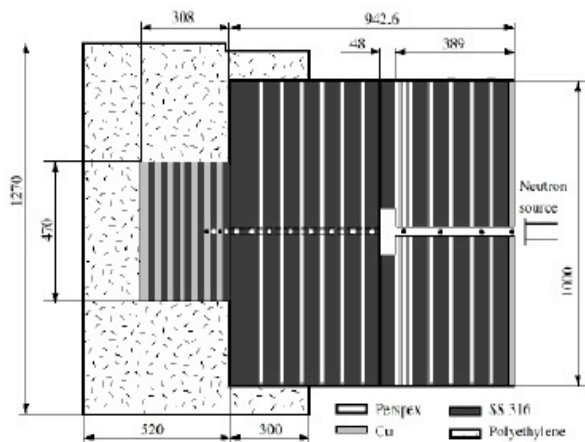
	FENDL-2.1		FENDL-2.1+ENDF/B-VII.0		
	Value	% Error	Value	% Error	% Change
dpa	1.23E+03	0.49%	1.20E+03	0.45%	-2.30%
He appm	3.85E+03	1.71%	3.85E+03	1.71%	-0.08%



- 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



Started Calculations for Three Benchmark Experiments



Tungsten Experiment

Streaming Experiment

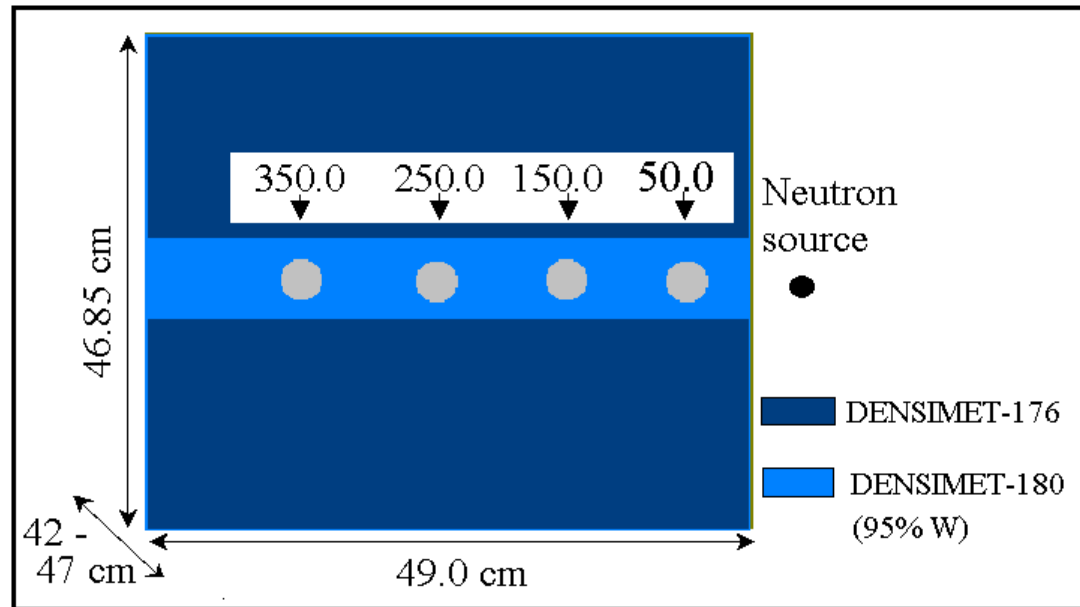
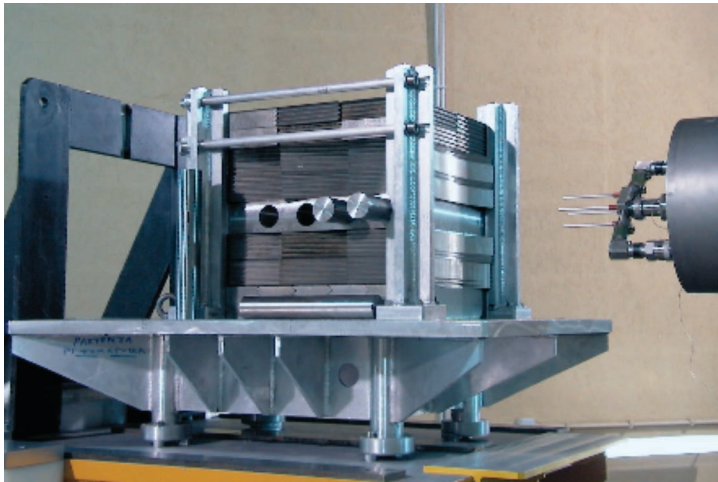
Bulk Shielding Experiment

Frascati 14-MeV Neutron Generator (FNG)

- ENEA, Frascati Research Centre (Italy)
- Accelerator based
 - $T(d, n)\alpha$
 - $E_d = 300 \text{ keV}$
- Operating since 1992
- 14-MeV neutron intensity 10^{11} n/s

Tungsten Experiments

Tungsten block (armor material for plasma facing components)

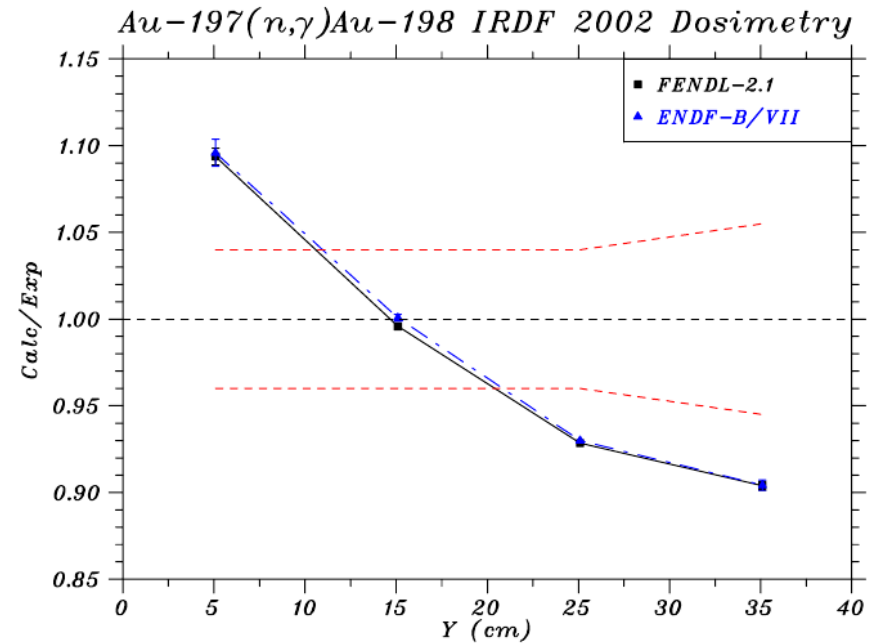
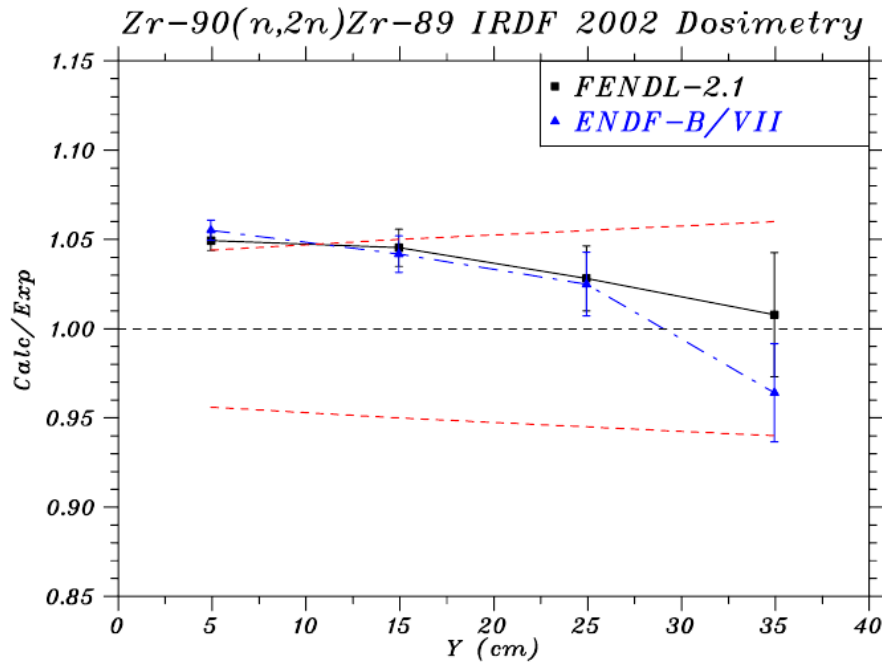


DENSIMET-176 (93.2%w W, 2.6%w Fe, 4.2%w Ni, 17.70 g/cm³).

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

Sample Results for Tungsten Experiments



ENDF-B/VIII.0 results in minor changes (within statistical error in MCNP calculations) except for high energy flux deep in the block

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 3 integral experimental benchmarks to fully understand the impact of data changes introduced in ENDF/B-VII.0 as compared against experimental data