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FENDL Benchmark Calculations in Preparation for Upgrade to FENDL-3

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FENDL Background

- FENDL-2.1 released November 2003, INDC (NDS)-451
- 71 elements/isotopes with majority (40) taken from ENDF/B-VI.8
- Reference data library for ITER neutronics calculations
- Have been used in analysis of other fusion systems
- Since its release, updates of national libraries have been released (e.g., ENDF/B-VII.0 released December 2006)

Data Source for 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

FENDL-3 Development

- An effort was initiated by the IAEA in 2008 to update the FENDL library with the objective of improving the status of nuclear databases for fusion devices including IFMIF
- The library (FENDL-3) represent a substantial extension of FENDL-2.1 library toward higher energies, with inclusion of incident charged particles and the evaluation of related uncertainties
- FENDL-3 will be released at the end of the 3 years of the Coordinated Research Project (CRP) activities

FENDL-3/SLIB Starter Library

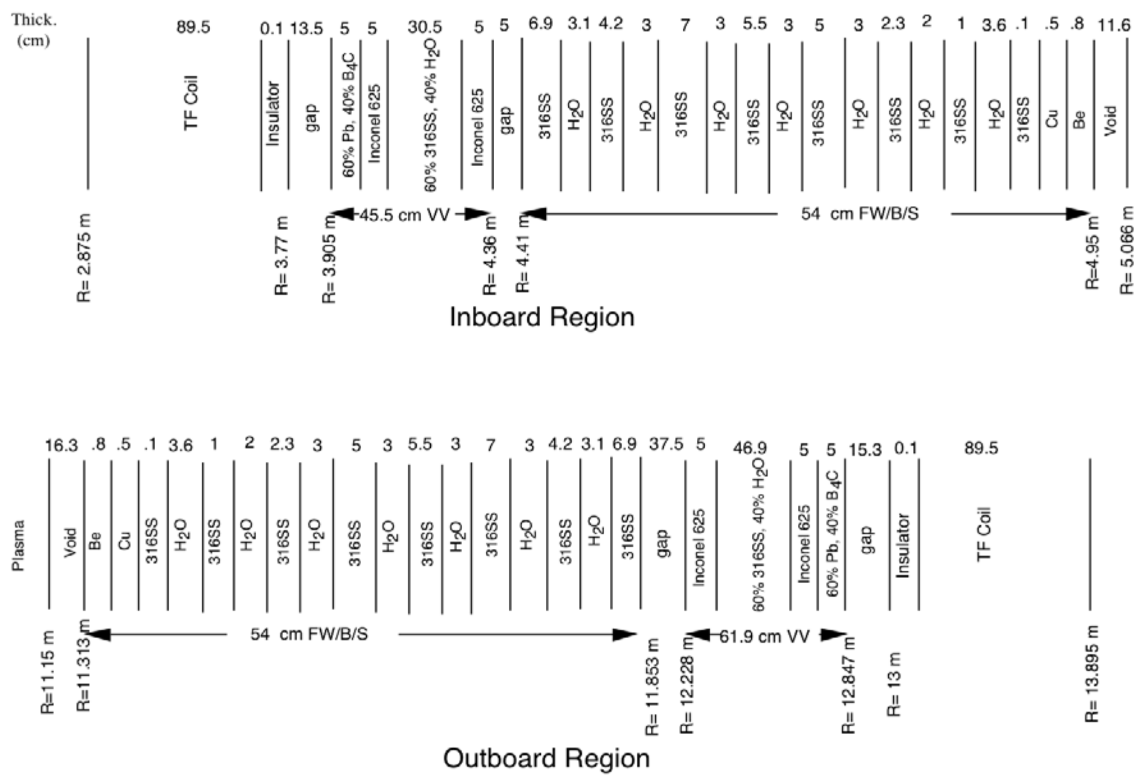
- A starter library (FENDL-3/SLIB) was generated based on several agreed upon rules of creation
  - Replace present evaluations with updates
  - Adopt evaluations from libraries that contain standards (H-1 from ENDF)
  - Use isotopic evaluations where available
- The library includes 88 isotopes with updated evaluations from ENDF/B-VII.0, JENDL-HE, JEFF-3.1, and BROND
- A noticeable change is for H-1, which switched from JENDL-3.3 to ENDF/B-VII.0 and is expected to impact analysis of systems with water-cooling like ITER
- We solicited input from the fusion neutronics community regarding additional materials to be included in the library
- 17 elements were identified for consideration to be added in the new library to enhance its usefulness for the different fusion applications

Findings of Data Comparison Between ENDF/B-VI.8 and ENDF/B-VII.0

- 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 impact of data changes, we performed MCNP calculations for a 1-D ITER calculational benchmark that was utilized during FENDL development process
- Three calculations carried out using FENDL-2.1 library, FENDL-2.1 with data for the 40 elements/isotopes replaced by ENDF/B-VII.0, and the FENDL-3/SLIB library
- Results for flux, heating, dpa, and gas production were compared

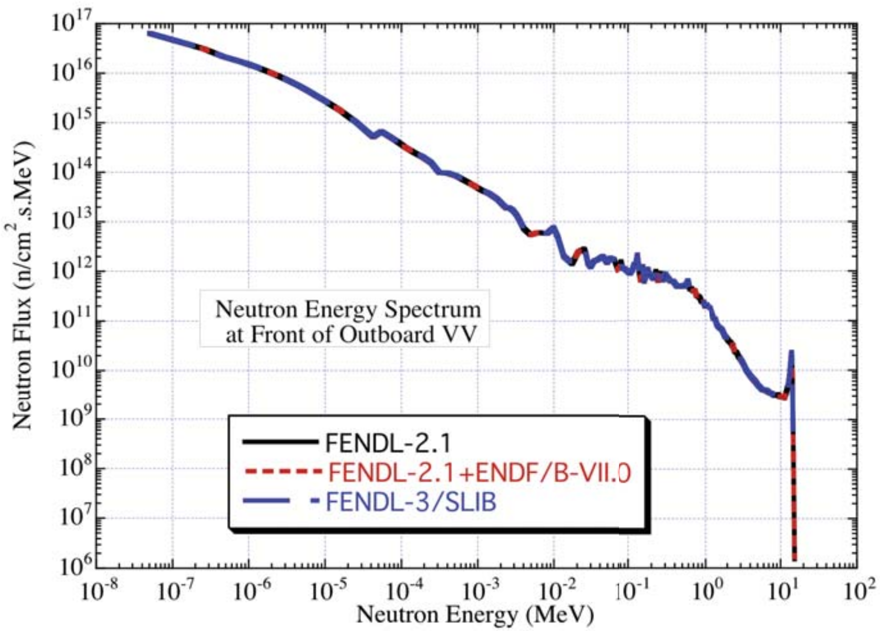


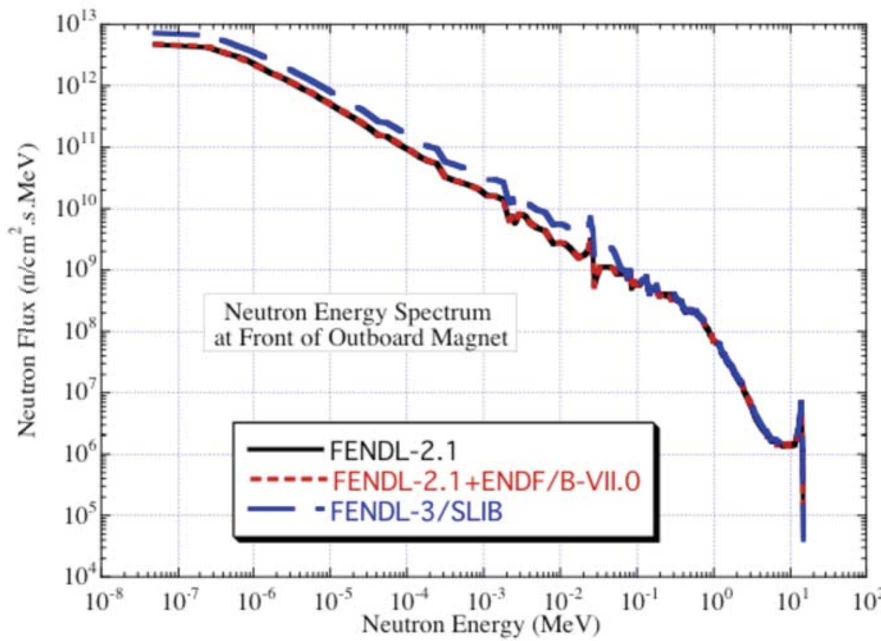
Peak Neutron and Gamma Flux Results

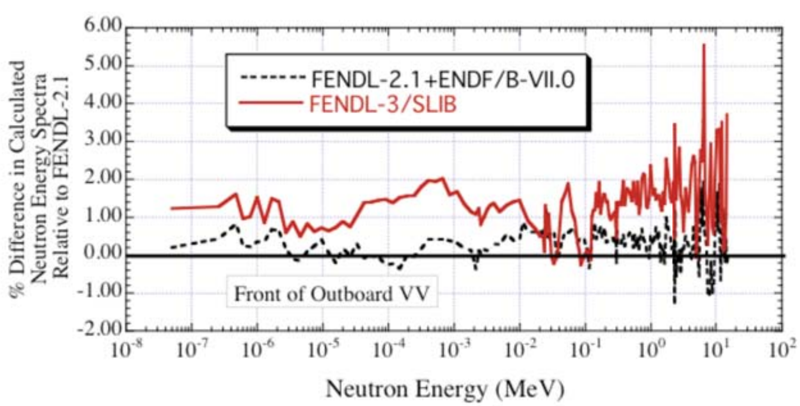
	FENDL-2.1		FENDL-2.1 +ENDF/B-VII.0		FENDL.3/SLIB		FENDL-2.1		FENDL-2.1 +ENDF/B-VII.0		FENDL.3/SLIB	
	Neutron Flux	1 σ % Error	Value	% Change	Value	% Change	Gamma Flux	1 σ % Error	Value	% Change	Value	% Change
IB												
FW												
Be	3.52E+14	0.05%	3.52E+14	0.05%	3.520E+14	0.07%	3.18E+14	0.05%	3.18E+14	0.12%	3.184E+14	0.14%
Cu	3.09E+14	0.05%	3.09E+14	0.08%	3.089E+14	0.03%	3.08E+14	0.05%	3.08E+14	0.10%	3.080E+14	0.11%
SS	2.96E+14	0.06%	2.96E+14	0.10%	2.960E+14	0.01%	3.07E+14	0.06%	3.07E+14	0.09%	3.071E+14	0.15%
VV	8.43E+11	0.19%	8.46E+11	0.29%	8.560E+11	1.52%	4.84E+11	0.17%	4.85E+11	0.26%	4.903E+11	1.32%
Magnet	3.42E+09	0.45%	3.45E+09	1.04%	3.619E+09	5.88%	9.34E+08	0.42%	9.41E+08	0.71%	9.687E+08	3.72%
OB												
FW												
Be	4.37E+14	0.03%	4.37E+14	0.12%	4.375E+14	0.15%	3.61E+14	0.04%	3.62E+14	0.15%	3.619E+14	0.20%
Cu	3.95E+14	0.03%	3.95E+14	0.13%	3.952E+14	0.18%	3.60E+14	0.04%	3.61E+14	0.14%	3.609E+14	0.15%
SS	3.80E+14	0.03%	3.80E+14	0.14%	3.804E+14	0.17%	3.66E+14	0.04%	3.66E+14	0.13%	3.664E+14	0.12%
VV	1.17E+12	0.09%	1.17E+12	0.34%	1.183E+12	1.31%	6.60E+11	0.08%	6.62E+11	0.27%	6.679E+11	1.19%
Magnet	4.93E+08	0.41%	4.97E+08	0.79%	6.695E+08	35.74%	1.38E+08	0.40%	1.39E+08	0.49%	1.632E+08	18.17%

- 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
- Using FENDL-3/SLIB results in much higher flux values particularly at the magnet that is heavily shielded by water-cooled shield and vacuum vessel

Neutron Spectra







- Using FENDL-3/SLIB results in significantly softer neutron energy spectrum at the heavily shielded outboard magnet that yields enhanced gamma generation
- At OB magnet E>0.1 MeV flux increases by only 3% while the E<0.1 MeV flux increases by 82%

Peak Nuclear Heating Results

	FENDL-2.1		FENDL-2.1 +ENDF/B-VII.0		FENDL-3/SLIB	
	Power Density	1 σ % Error	Value	% Change	Value	% Change
IB						
FW						
Be	1.008E+01	0.05	1.008E+01	-0.02	1.008E+01	0.02
Cu	2.017E+01	0.06	2.019E+01	0.07	2.021E+01	0.15
SS	1.783E+01	0.08	1.786E+01	0.16	1.787E+01	0.26
VV SS	2.619E-02	0.18	2.632E-02	0.51	2.657E-02	1.44
Magnet	3.659E-05	0.45	3.691E-05	0.87	3.789E-05	3.56
OB						
FW						
Be	1.391E+01	0.03	1.391E+01	-0.02	1.392E+01	0.05
Cu	2.474E+01	0.04	2.478E+01	0.13	2.478E+01	0.15
SS	2.230E+01	0.05	2.233E+01	0.10	2.233E+01	0.12
VV SS	3.573E-02	0.09	3.582E-02	0.24	3.614E-02	1.14
Magnet	5.376E-06	0.43	5.419E-06	0.79	6.361E-06	18.32

- While using ENDF/B-VII.0 data results in slightly higher heating values (<1%) using FENDL-3/SLIB results in much higher heating values particularly at the magnet
- Most of increase in outboard magnet heating is due to gamma heating increase (21% increase vs. 5% increase in neutron heating)

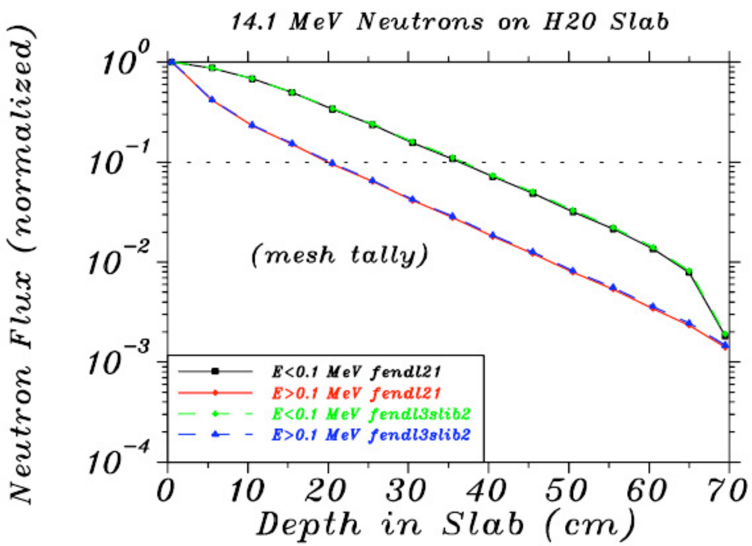
Peak Magnet Nuclear Parameters

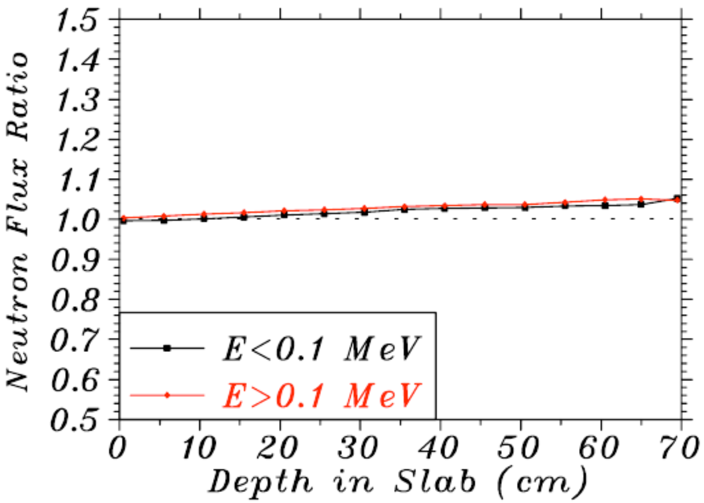
	FENDL-2.1		FENDL-2.1 +ENDF/B-VII.0		FENDL-3/SLIB	
	Value	1 σ % Error	Value	% Change	Value	% Change
IB						
Fast n fluence (n/cm^2/FPY)	6.27E+16	0.46	6.36E+16	1.42	6.47E+16	2.82
Insulator dose (Gy/FPY)	5.59E+05	0.47	5.64E+05	0.87	5.72E+05	2.33
Cu dpa/FPY	3.75E-05	0.49	3.82E-05	1.76	3.87E-05	3.11
Nuclear heating (mW/cm^3)	3.66E-02	0.45	3.69E-02	0.87	3.79E-02	3.55
OB						
Fast n fluence (n/cm^2/FPY)	9.1E+15	0.42	9.21E+15	1.20	9.39E+15	3.18
Insulator dose (Gy/FPY)	8.15E+04	0.44	8.18E+04	0.38	8.87E+04	8.91
Cu dpa/FPY	5.48E-06	0.43	5.56E-06	1.46	5.81E-06	6.09
Nuclear heating (mW/cm^3)	5.38E-03	0.43	5.42E-03	0.80	6.36E-03	18.32

- While using ENDF/B-VII.0 data results in slightly higher magnet parameters using FENDL-3/SLIB results in much higher parameters with the largest increase in magnet heating due to enhanced gamma production

FENDL-3/SLIB in H_2O Slab

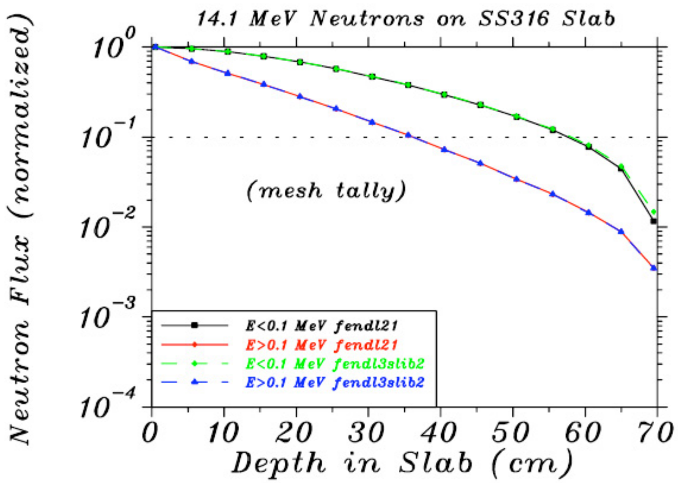
- To further investigate the increase in low energy (E<0.1 MeV) neutron flux observed in the ITER 1-D calculational benchmark with FENDL-3/SLIB we performed simple calculations for slabs with all water, all SS316, and SS316/H_2O mixture
- Compared neutron fluxes in the various slabs calculated with MCNPX using FENDL-2.1 versus FENDL-3/SLIB
- Used isotropic 14.1 MeV neutron source

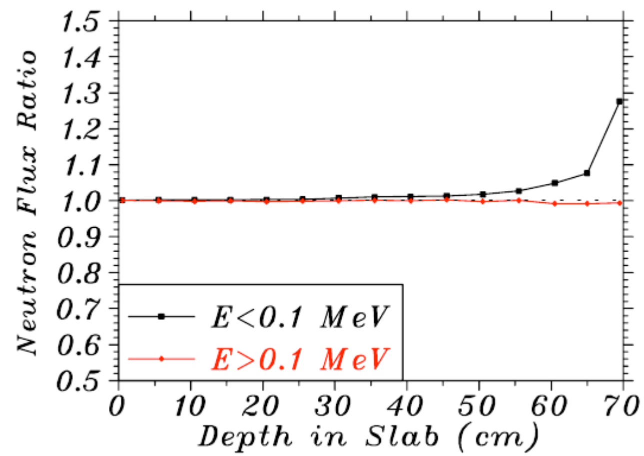




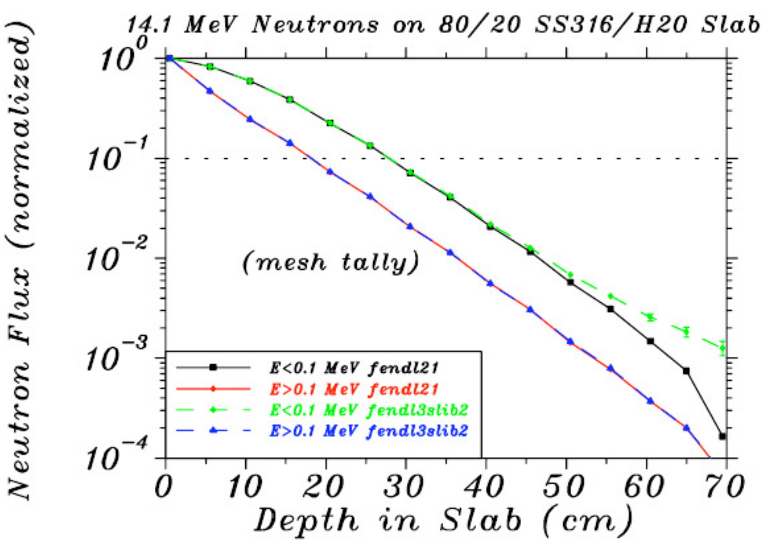
5% increase

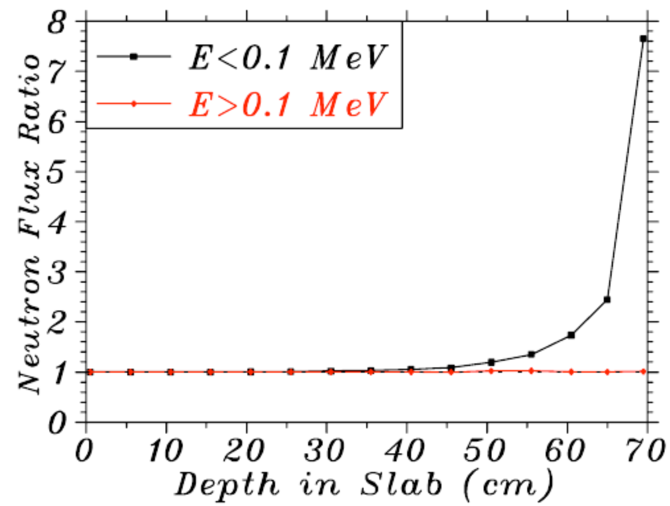
FENDL-3/SLIB in SS316 and SS/H_2O (80/20)





30% increase

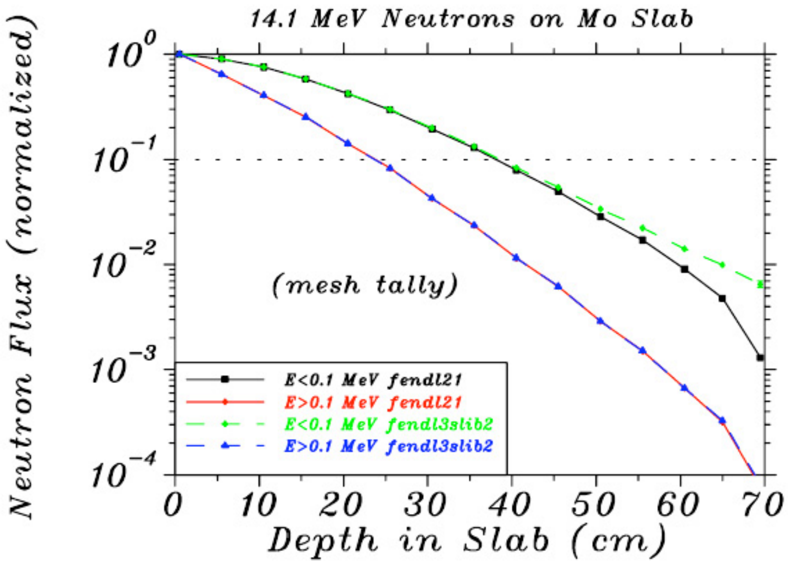


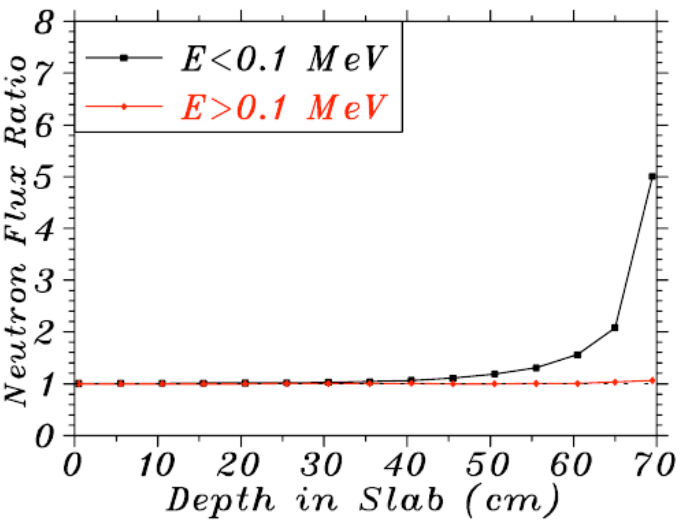


750% increase

FENDL-3/SLIB in Mo Slab

Largest difference in Mo (JENDL-3.3→JENDL-HE)



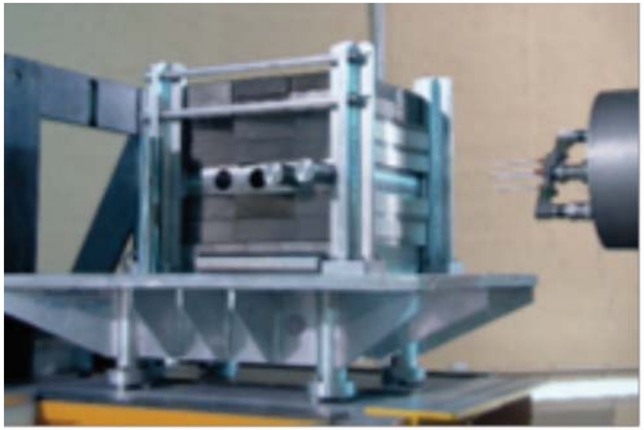


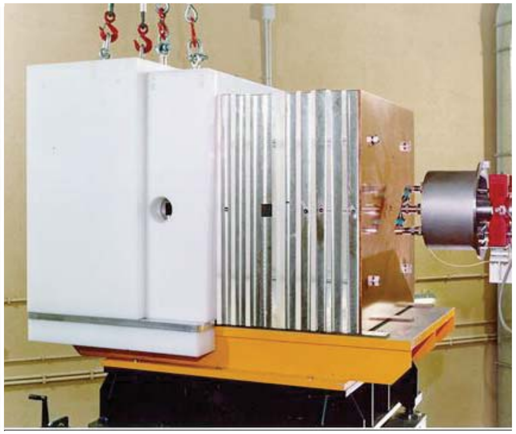
500% increase

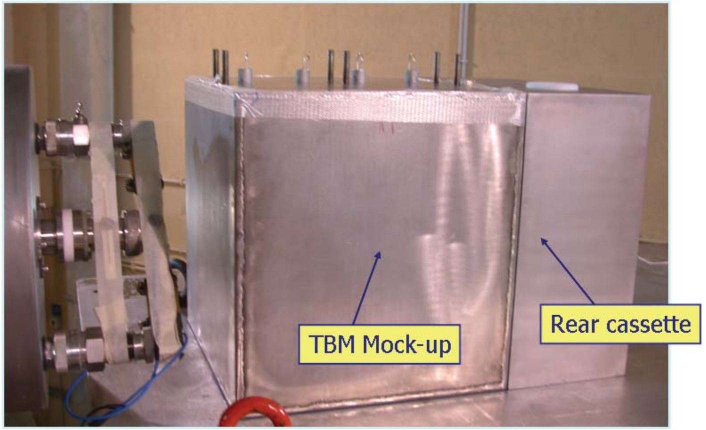
- Mo resonances are below 0.1 MeV compared to higher energy resonances for Fe
- Resonance data might have changed or data processing might have an error (used NJOY-99.90?)
- Existence of water enhances differences since it slows down neutrons into resonance region

ITER Relevant Benchmark Experiments

- ENEA, Frascati Research Centre (Italy)
- 14-MeV Frascati Neutron Generator (FNG)
  - Accelerator based
  - T(d,n)α E_d=300 keV
- Operating since 1992
- 14-MeV neutron intensity 10^{11} n/s
- Variety of mockups:

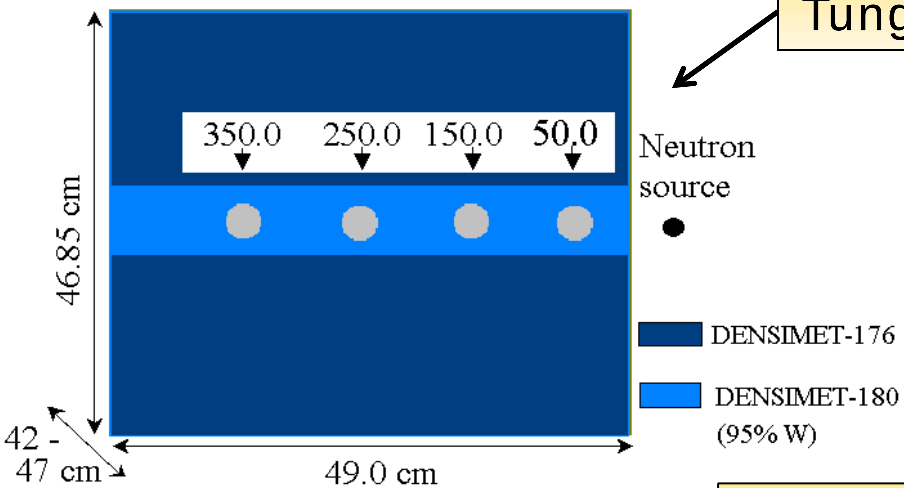




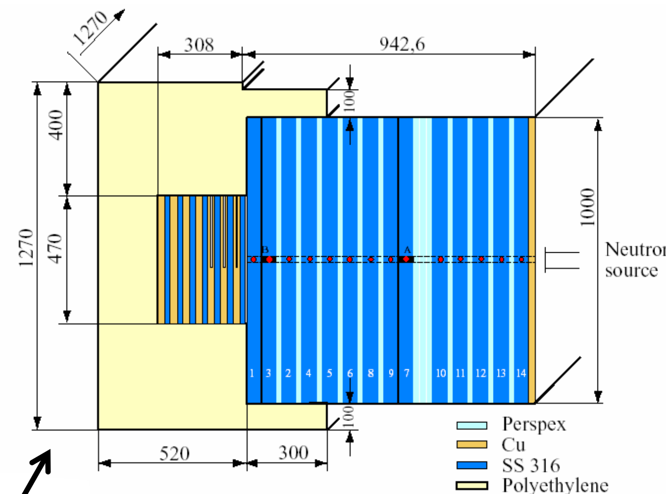


Schematic of ITER Relevant Experiments

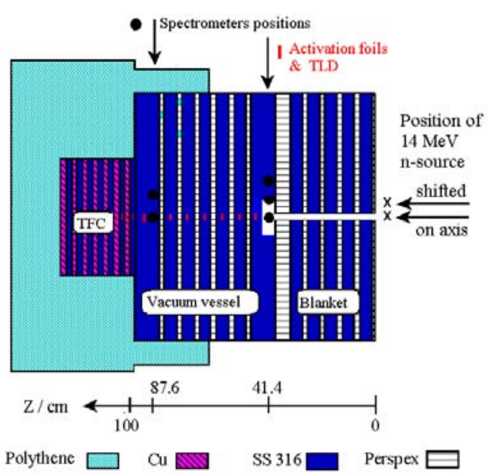
Tungsten



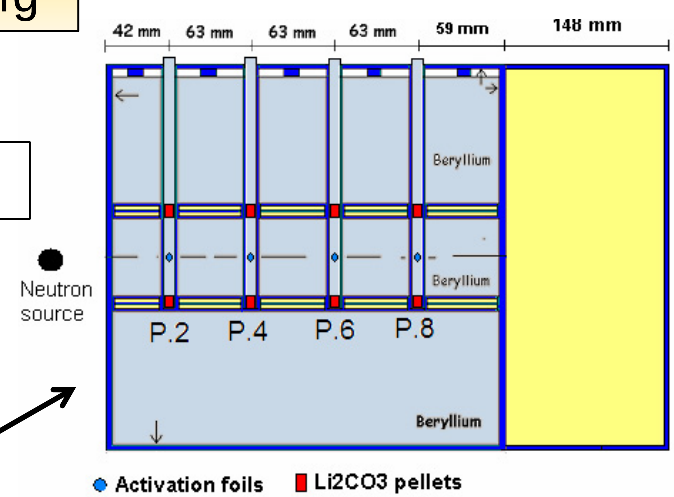
Bulk shielding



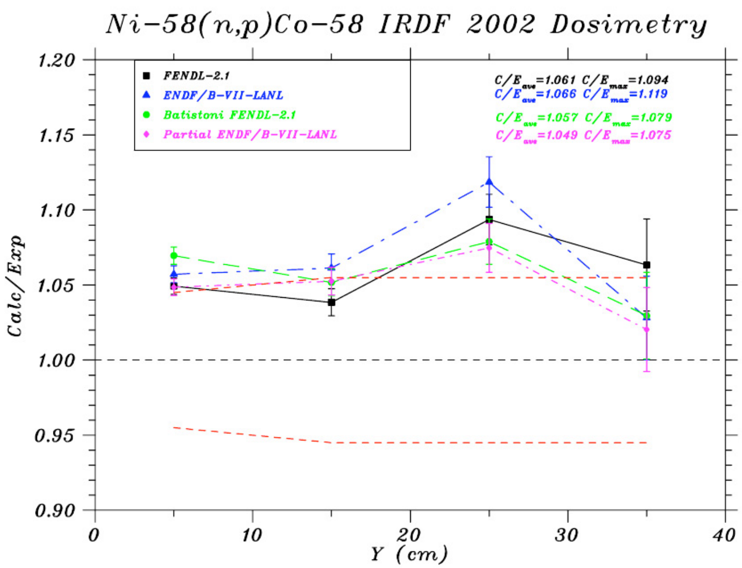
Streaming

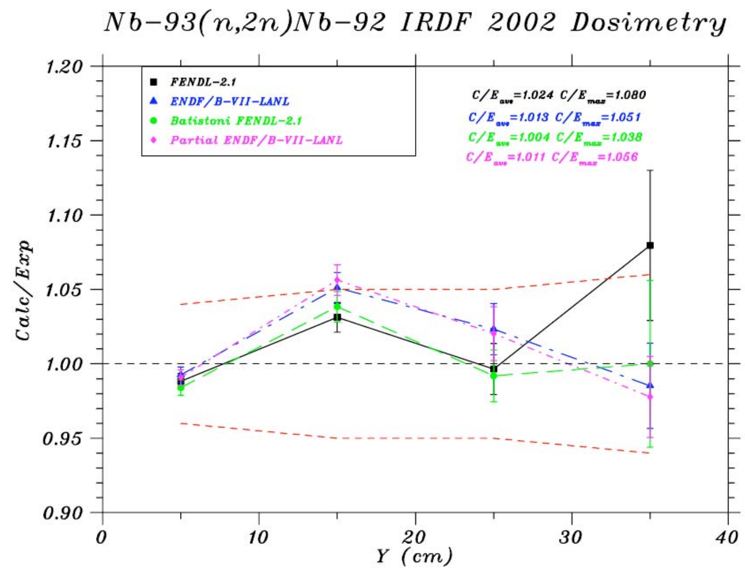


HCPB breeder



Tungsten experiment activation foils

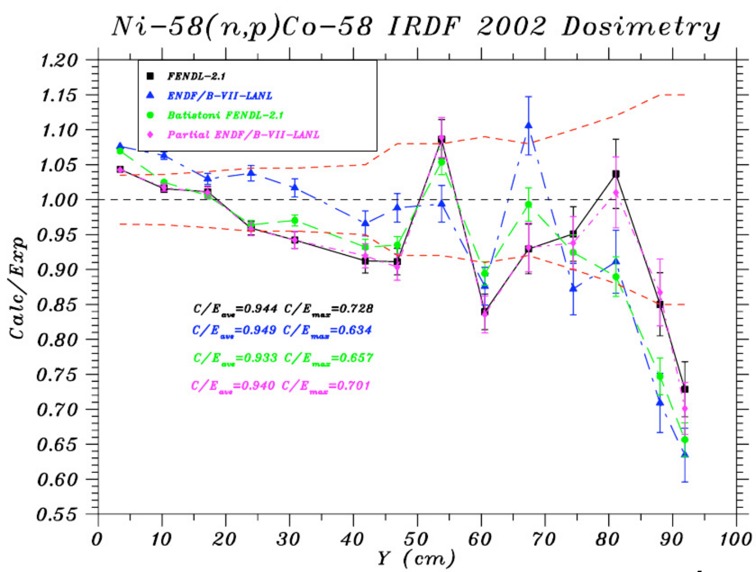


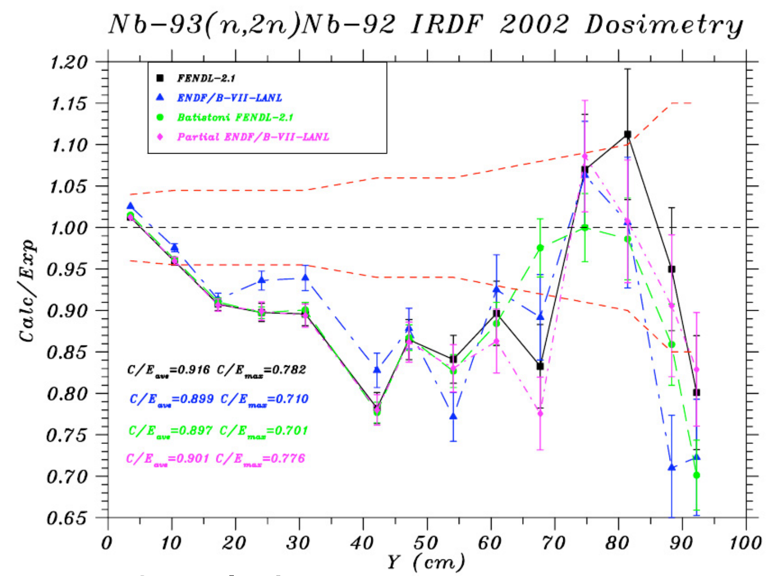


Average/Maximum of Calc/Exp

Reaction	$E_{threshold}$ (MeV)	FENDL-2.1	ENDF/B-VII	Partial ENDF/B-VII
Mn-55(n,γ)Mn-56	0	1.454/1.785	1.450/1.748	1.453/1.771
Au-197(n,γ)Au-198	0	0.981/0.905	0.984/1.097	0.982/1.093
Ni-58(n,p)Co-58	0.8	1.061/1.094	1.066/1.119	1.049/1.075
In-115(n,n')In-115m*	0.8	0.929/0.869	0.923/0.864	0.924/0.862
Al-27(n,α)Na-24	3	1.030/1.055	1.041/1.058	1.031/1.047
Fe-56(n,p)Mn-56	3	0.961/0.945	0.962/0.941	0.958/0.930
Ni-58(n,2n)Ni-57	10	1.020/1.034	1.040/1.069	1.036/1.049
Zr-90(n,2n)Zr-89	10	1.034/1.049	1.036/1.055	1.043/1.057
Nb-93(n,2n)-Nb92	10	1.024/1.080	1.013/1.051	1.011/1.056

Bulk Shielding experiment activation foils

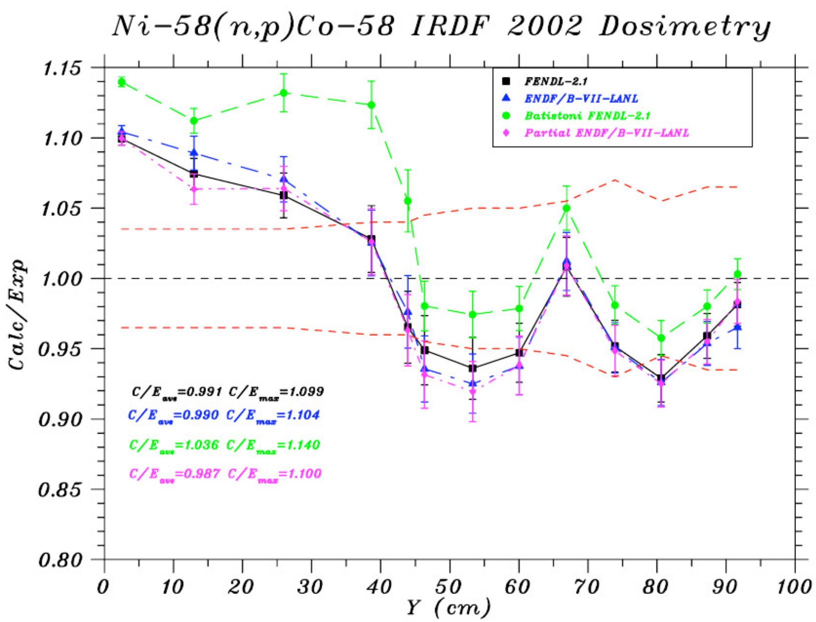


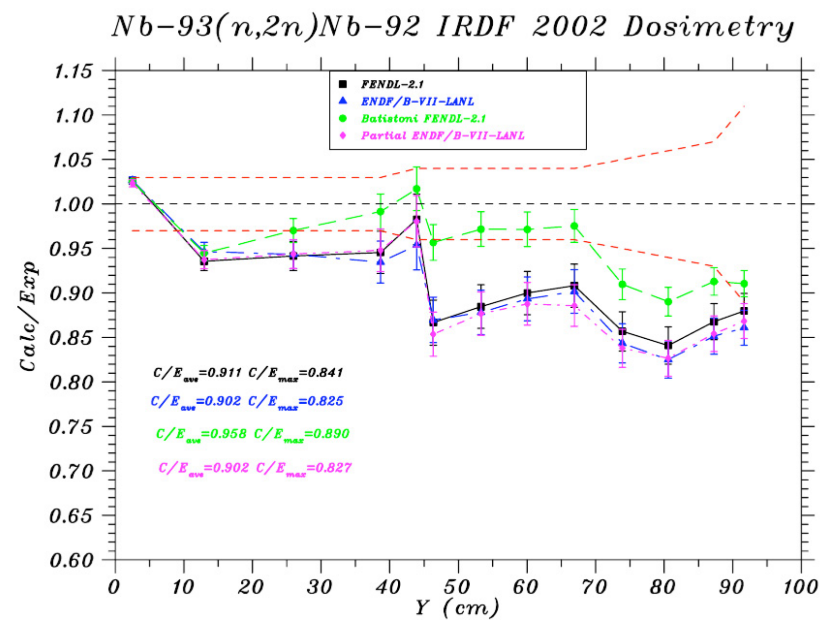


Average/Maximum of Calc/Exp

Reaction	$E_{threshold}$ (MeV)	FENDL-2.1	ENDF/B-VII	Partial ENDF/B-VII
Mn-55(n,γ)Mn-56	0	0.902/0.763	0.890/0.722	0.903/0.743
Au-197(n,γ)Au-198	0	0.910/0.789	0.908/0.790	0.922/0.802
Ni-58(n,p)Co-58	0.8	0.944/0.728	0.949/0.634	0.940/0.701
In-115(n,n')In-115m*	0.8	0.751/0.501	0.748/0.450	0.751/0.500
Al-27(n,α)Na-24	3	0.912/0.848	0.917/0.741	0.903/0.787
Fe-56(n,p)Mn-56	3	0.897/0.827	0.921/0.805	0.890/0.786
Ni-58(n,2n)Ni-57	10	0.923/0.873	0.933/0.889	0.924/0.876
Zr-90(n,2n)Zr-89	10	-	-	-
Nb-93(n,2n)-Nb92	10	0.916/0.782	0.899/0.710	0.901/0.776

Streaming experiment activation foils

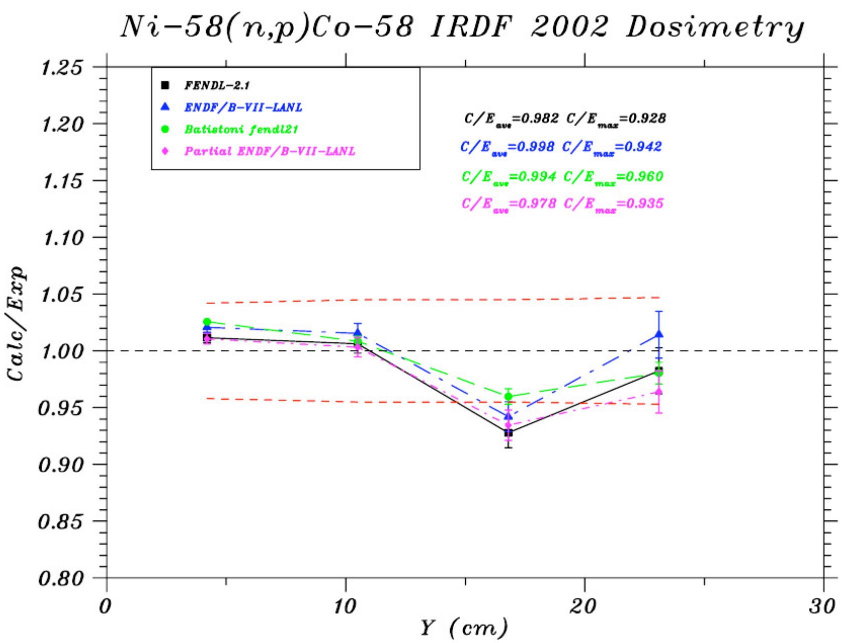


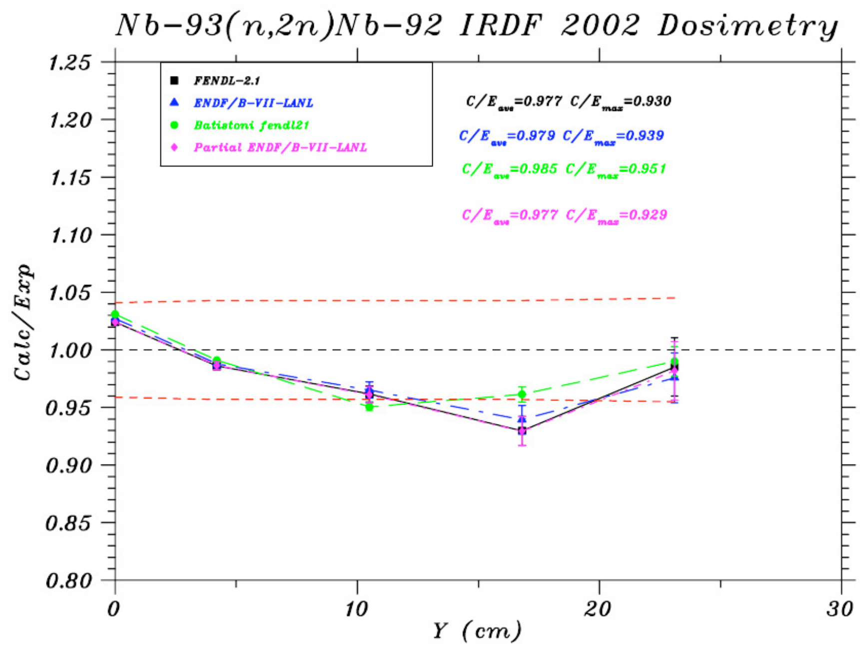


Average/Maximum of Calc/Exp

Reaction	$E_{threshold}$ (MeV)	FENDL-2.1	ENDF/B-VII	Partial ENDF/B-VII
Ni-58(n,p)Co-58	0.8	0.991/1.099	0.990/1.104	0.987/1.100
Al-27(n,α)Na-24	3	0.869/0.703	0.888/0.712	0.877/0.713
Nb-93(n,2n)-Nb92	10	0.911/0.841	0.902/0.825	0.902/0.827

HCPB Breeder activation foils

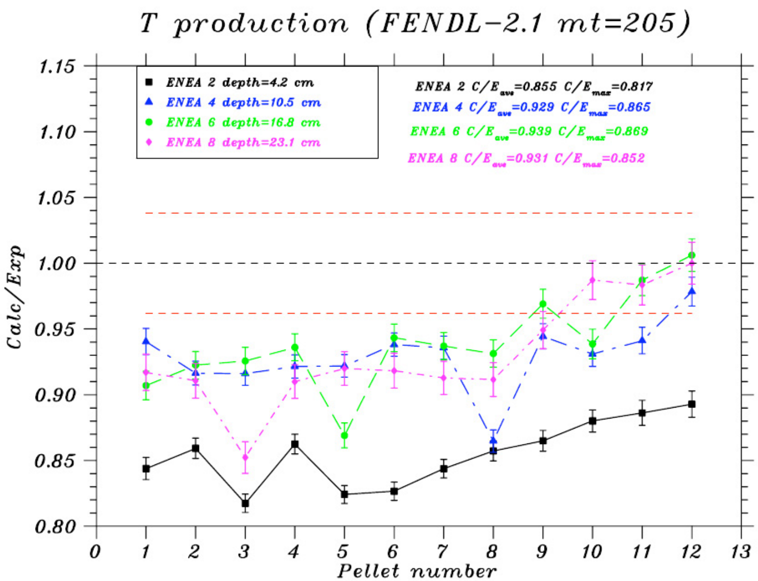


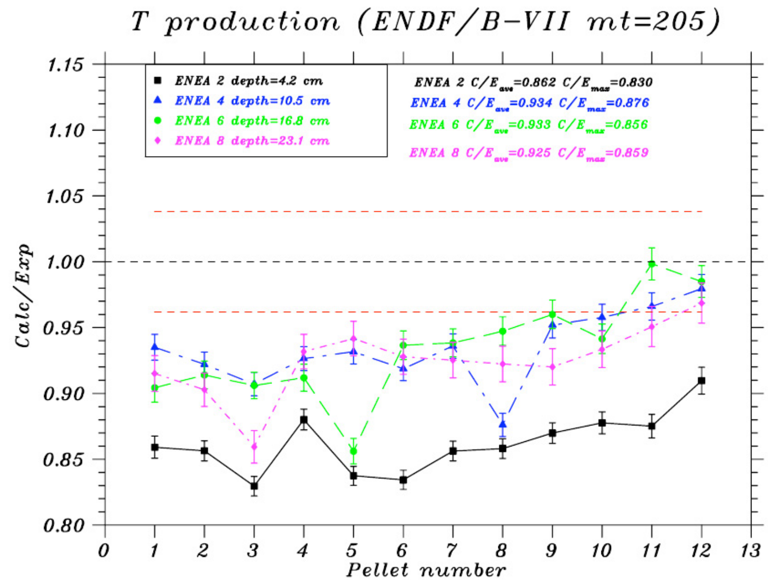


Average/Maximum of Calc/Exp

Reaction	$E_{threshold}$ (MeV)	FENDL-2.1	ENDF/B-VII	Partial ENDF/B-VII
Au-197(n,γ)Au-198	0	0.904/0.829	0.921/0.875	0.928/0.853
Ni-58(n,p)Co-58	0.8	0.982/0.928	0.998/0.942	0.978/0.935
Al-27(n,α)Na-24	3	1.001/1.034	1.008/1.037	0.998/1.034
Nb-93(n,2n)-Nb92	10	0.977/0.930	0.979/0.939	0.977/0.929

HCPB Breeder tritium production





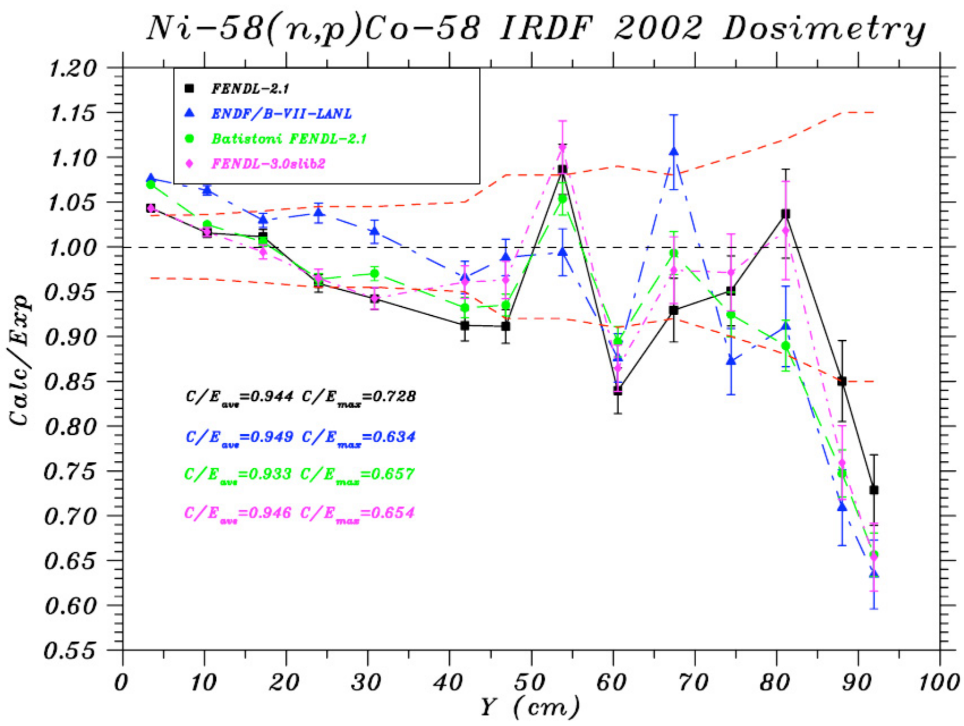
Average/Maximum of C/E values at each 12 pellet ENEA group

Depth (mm)	FENDL-2.1	ENDF/B-VII	Partial ENDF/B-VII
42	0.855/0.817	0.862/0.830	0.853/0.815
105	0.929/0.865	0.934/0.876	0.928/0.870
168	0.939/0.869	0.933/0.856	0.938/0.863
231	0.931/0.852	0.925/0.859	0.919/0.838

FENDL-3/SLIB calculations for ITER relevant experiments

- Work is underway to validate FENDL-3/SLIB using these ITER relevant experiments
- Initial results indicate similar results to those with FENDL-2.1

Bulk Shielding experiment with FENDL-3/SLIB:



Conclusions

- Replacing the ENDF/B-VI.8 data in FENDL-2.1 by ENDF/B-VII.0 while keeping data from other evaluations unchanged resulted in minor change (<1%) in nuclear parameters for ITER relevant calculations
- However, larger changes in calculated ICF target neutronics parameters and tritium breeding were observed in previous analysis
- Calculations of foil activation and tritium breeding for ITER relevant integral experiments yield nearly similar results for FENDL-2.1 and ENDF/B-VII.0
- Using FENDL-3/SLIB instead of FENDL-2.1 for ITER or other systems with water cooling results in much larger increase in nuclear parameters particularly behind the thick water-cooled shield. This is under investigation and could be related to steel resonance data (particularly Mo) that is enhanced by existence of water
- Results confirm the need for updating and validating FENDL for analysis of ITER and future fusion systems as national evaluations get updated