Fusion-Relevant Changes in the ENDF/B-VIII.1 Library

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Methodology

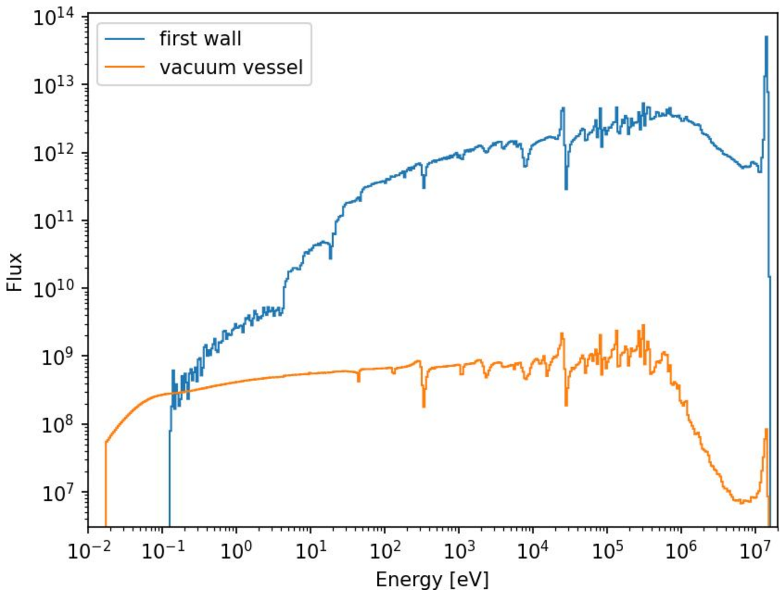
To assess fusion-relevant changes in ENDF/B-VIII.1, the following steps were carried out:

1. Go through draft ENDF/B-VIII.1 “big paper” to identify nuclides of interest
2. Computing reaction rates under a predetermined flux spectrum, comparing between VIII.0, VIII.1, and FENDL-3.2
3. OpenMC calculations on SINBAD benchmarks: FNG streaming, FNG W, Oktavian

Note: Analysis is limited to incident neutron sublibrary, but there are small changes in other sublibraries that should be studied

Methodology: reaction rate computation

- HDF5 cross section library generated for OpenMC
- Flux spectra obtained from CoNDERC:
  - 616-group DEMO HCPB spectrum for first wall (UKAEA)
  - 616-group DEMO HCPB spectrum for vacuum vessel (UKAEA)
- Reaction rates* computed for all nuclides in FENDL-3.2 using the `Nuclide.collapse_rate` function in OpenMC
- Looked at:
  - MT=2 (elastic scattering)
  - MT=16 (n,2n)
  - MT=103, 104, 105, 106, 107 (Production of p, d, t, 3He, a)
  - MT=301 (heating)
  - MT=444 (damage energy)



*Data: https://github.com/paulromano/nuclear-data-fusion-analysis

Reaction rate analysis

Tritium production and neutron multiplication

- **Tritium production**: Very minor changes in ^{6}Li and ^{7}Li, no appreciable difference in tritium production between VIII.0, VIII.1, and FENDL

Nuclide	E81/E80	E80/F32	E81/F32
Li6	0.999	1.000	0.999
Li7	1.000	1.000	1.000

- **Neutron multiplication**:
  - (n,2n) rate for ^{9}Be unchanged, agreement between VIII.0, VIII.1, and FENDL
  - (n,2n) cross section for ^{208}Pb went up slightly above 15 MeV, no difference in (n,2n) rate at 14 MeV and below
  - ^{208}Pb(n,2n) rate is within 2% between ENDF/B-VIII.1 and FENDL

Nuclide	E81/E80	E80/F32	E81/F32
Be9	1.000	1.000	1.000
Pb204	1.000	1.000	1.000
Pb206	1.062	1.000	1.062
Pb207	0.922	1.000	0.922
Pb208	1.018	0.999	1.018

Structural materials: Fe, Cr

- New INDEN evaluations for most isotopes of Fe and Cr

- **Fe**: ENDF/B-VIII.0 suffered from underestimation of fast neutron transmission through Fe between 1-10 MeV; this has been resolved in VIII.1
    - Overall better match to experiments

- **Cr**: significant improvement in angle-integrated cross sections, angular distributions, energy spectra, n/γ double-differential
    - Same INDEN evaluation adopted in FENDL 3.2b

Structural materials: Fe, Cr (capture rates)

First wall spectrum

Nuclide	E81/E80	E80/F32	E81/F32
Cr50	1.305	0.766	1.000
Cr52	1.129	1.000	1.129
Cr53	1.666	0.600	1.000
Cr54	1.040	0.962	1.000
Fe54	1.127	0.897	1.011
Fe56	0.954	0.950	0.906
Fe57	1.000	1.000	1.000
Fe58	1.000	1.030	1.030

Vacuum vessel spectrum

Nuclide	E81/E80	E80/F32	E81/F32
Cr50	1.037	0.965	1.000
Cr52	1.034	1.000	1.034
Cr53	1.108	0.903	1.000
Cr54	1.000	1.000	1.000
Fe54	1.012	0.991	1.003
Fe56	0.984	1.003	0.987
Fe57	1.000	1.000	1.000
Fe58	1.000	1.002	1.002

Heating, damage, and gas production

- Heating, damage, and gas production cross sections rely heavily on **outgoing particle distributions**
- Many fixes and improvements made in ENDF/B-VIII.1
  - Updated gamma spectra from GRIN project for C13, O16, F19, Si28, S32, S34
  - Missing outgoing particle distributions for many nuclides/reactions were adopted from TENDL2019
  - CoH3 code was used to fill remaining missing distributions
- Note that NJOY makes its own approximations when data are missing

Structural materials: Fe, Cr (heating rates)

First wall spectrum

Nuclide	E81/E80	E80/F32	E81/F32
Cr50	1.144	0.909	1.039
Cr52	1.271	0.860	1.093
Cr53	1.190	1.034	1.231
Cr54	1.247	0.912	1.137
Fe54	1.000	1.017	1.017
Fe56	0.999	1.105	1.103
Fe57	1.011	1.263	1.277
Fe58	1.000	1.557	1.557

Vacuum vessel spectrum

Nuclide	E81/E80	E80/F32	E81/F32
Cr50	1.040	0.990	1.029
Cr52	1.002	1.018	1.020
Cr53	0.996	1.047	1.043
Cr54	1.070	0.948	1.014
Fe54	1.001	1.008	1.010
Fe56	1.005	1.034	1.040
Fe57	1.067	1.421	1.516
Fe58	1.001	0.893	0.894

Structural materials: Fe, Cr (damage rates)

First wall spectrum

Nuclide	E81/E80	E80/F32	E81/F32
Cr50	1.134	0.882	1.000
Cr52	1.018	0.982	1.000
Cr53	0.966	1.035	1.000
Cr54	1.043	0.959	1.000
Fe54	1.000	1.000	1.000
Fe56	0.997	1.008	1.005
Fe57	1.031	0.993	1.024
Fe58	1.000	1.434	1.434

Vacuum vessel spectrum

Nuclide	E81/E80	E80/F32	E81/F32
Cr50	1.009	1.015	1.024
Cr52	0.961	1.040	1.000
Cr53	0.977	1.050	1.025
Cr54	1.045	0.958	1.000
Fe54	1.002	1.000	1.002
Fe56	1.007	1.011	1.018
Fe57	1.101	0.963	1.060
Fe58	1.001	0.881	0.882

Gas production in steel (VV flux)

Proton production

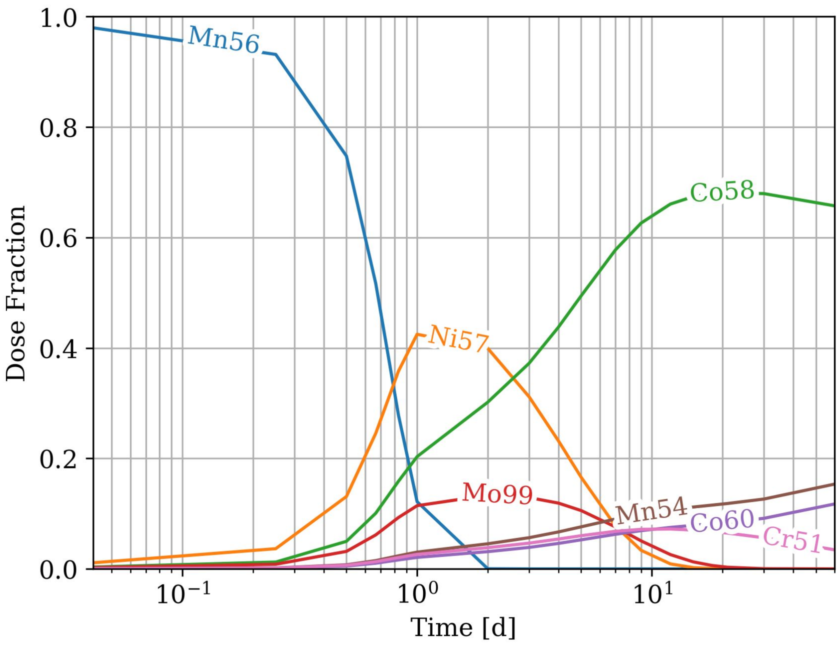
Nuclide	E81/E80	E80/F32	E81/F32
Co59	1.002	0.593	0.595
Cr50	0.908	1.101	1.000
Cr52	1.105	0.905	1.000
Cr53	1.058	0.945	1.000
Cr54	1.093	0.915	1.000
Fe54	1.000	1.000	1.000
Fe56	1.000	1.000	1.000
Fe57	1.000	1.000	1.000
Fe58	1.000	1.600	1.600
Mn55	1.000	1.000	1.000
Ni58	1.011	0.989	1.001
Ni60	0.959	1.022	0.980
Ni61	1.000	0.700	0.700
Ni62	1.000	1.116	1.116
Ni64	1.000	1.817	1.817

Alpha production

Nuclide	E81/E80	E80/F32	E81/F32
Co59	1.003	0.978	0.981
Cr50	1.543	0.648	1.000
Cr52	1.568	0.638	1.000
Cr53	0.736	1.358	1.000
Cr54	0.884	1.131	1.000
Fe54	1.000	1.000	1.000
Fe56	1.000	1.000	1.000
Fe57	1.000	1.000	1.000
Fe58	1.000	1.078	1.078
Mn55	1.001	1.000	1.001
Ni58	1.000	0.979	0.979
Ni60	1.000	0.969	0.969
Ni61	1.000	1.241	1.241
Ni62	1.000	1.171	1.171
Ni64	1.000	0.612	0.612

Activation in steel

- Typical breakdown of dose fraction by dominant radionuclide (previous calculation on FNG dose benchmark):



Activation in steel

- $^{58}Ni(n,2n)^{57}Ni$ tends to dominate dose from activated steel at 1–2 days
- No major differences in other reaction pathways for ^{56}Mn (shorter times) and ^{58}Co (longer times)

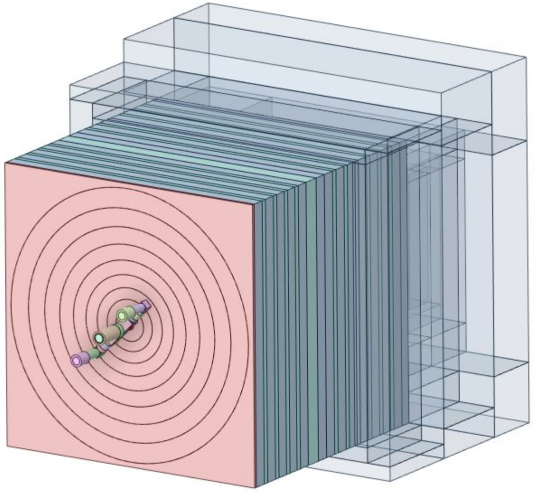
(n,2n) rate (VV flux)

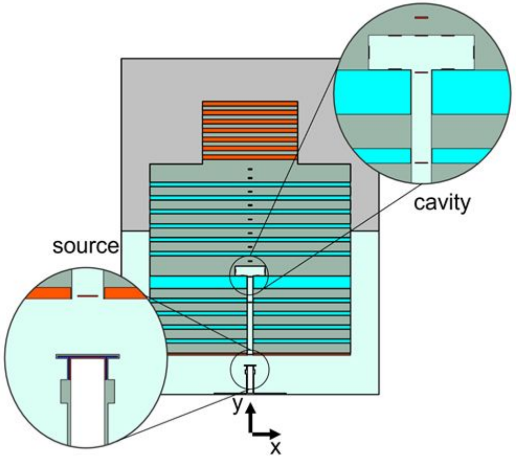
Nuclide	E81/E80	E80/F32	E81/F32
Co59	1.001	0.995	0.997
Cr50	0.794	1.260	1.000
Cr52	1.107	0.903	1.000
Cr53	0.973	1.028	1.000
Cr54	0.779	1.283	1.000
Fe54	1.000	1.000	1.000
Fe56	1.000	1.000	1.000
Fe57	1.000	1.000	1.000
Fe58	1.000	0.958	0.958
Mn55	1.062	1.000	1.062
Ni58	0.956	0.982	0.939
Ni60	1.000	1.130	1.130
Ni61	1.000	1.199	1.199
Ni62	1.000	1.018	1.018
Ni64	1.000	0.995	0.995

Benchmark results

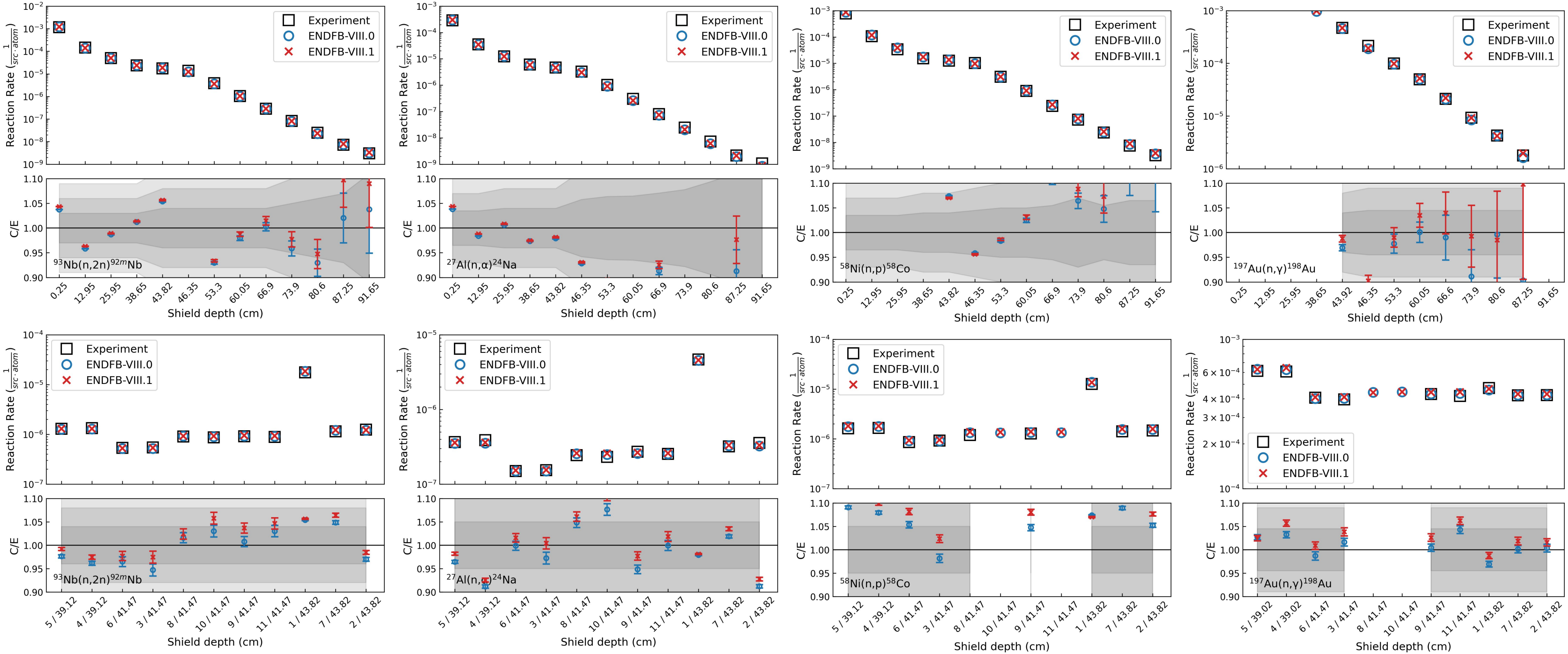
FNG-neutron streaming benchmark

- **14 MeV** neutrons
- Stainless steel (68% **Fe**, 17% **Cr**) and perspex/plexiglass layers
- High energy threshold **activation foils**:
  - Nb, ~10 MeV threshold
  - Al, ~8.5 MeV threshold
  - Ni, ~2.9 MeV threshold
  - Au, thermal neutrons



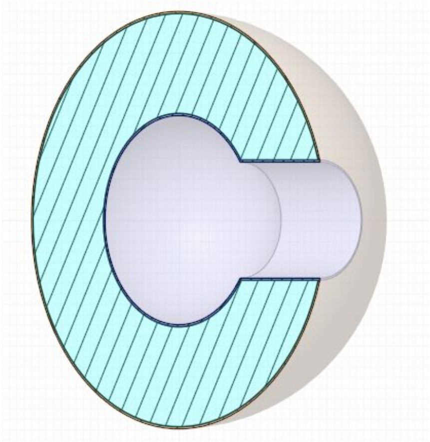


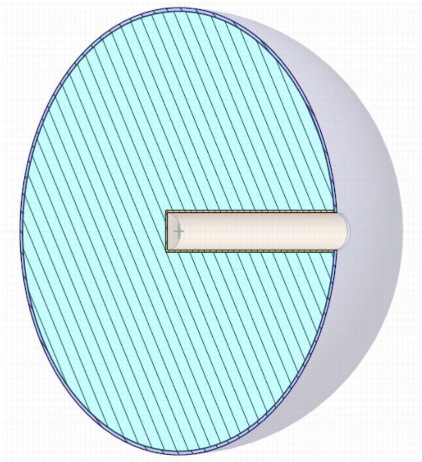
FNG-streaming foils E80 vs E81



Oktavian - Cr and Oktavian LiF

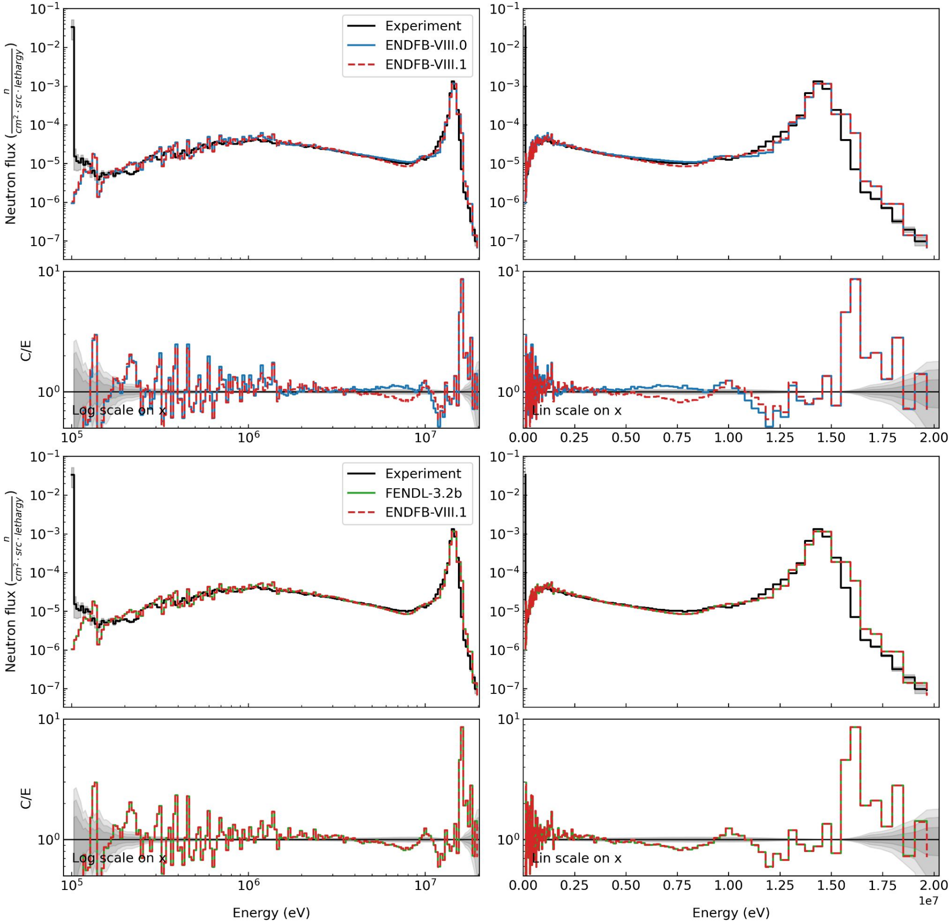
- **14 MeV** neutrons
- Bulk **Cr** and bulk **LiF** experiments
- **Neutron** spectrometers





Oktavian - Chromium E80/E81 & F32/E81

- E80/E81 good agreement in thermal-epithermal region
- E81 up to 2× better agreement w/ experiment in ~0.5-12 MeV range
  - C/E between 1–2× closer to unity
- E81 perfect agreement with F32



Summary and conclusions

- Carried out reaction rate analysis in fusion first wall/vacuum vessel fluxes and ran OpenMC on several SINBAD benchmarks
- No major differences in tritium production and neutron multiplication observed between B80, B81, and F32
- Analysis of elements in steel show several areas that are in need of further study with significant differences between E81 and F32:
  - Fast transmission in ^{56}Fe (10%)
  - Heating in Fe and Cr (10-20%)
  - Damage in ^{58}Fe (40%)
  - p and α production in Ni isotopes (up to 80%)
  - $^{58}Ni(n,2n)^{57}Ni$ reaction for activation (6%)
- Simulations of FNG and Oktavian experiments show good agreement with measurements and small improvements with E81 data

Acknowledgments

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Questions?