UW-Madison Nuclear Data Validation Activities for Fusion Applications

Tim Bohm, Jeremiah Oldenburg, Mohamed Sawan, and the CNERG team

CNERG
Computational Nuclear Engineering Research Group

UW Fusion Technology Institute (FTI)

U.S. National Nuclear Data Week
Brookhaven National Laboratory
4-8 November 2019

THE UNIVERSITY of WISCONSIN MADISON

Outline

1) Introduction
2) ITER-1D computational benchmark
3) MCNP model of Cf-252 source in iron sphere experimental benchmark (Sajo 1993)
4) Other Work
   - U.S. FNSF (3-D and 1-D computational benchmark)
   - ITER 3-D computational benchmark
   - JET experimental benchmark

References:

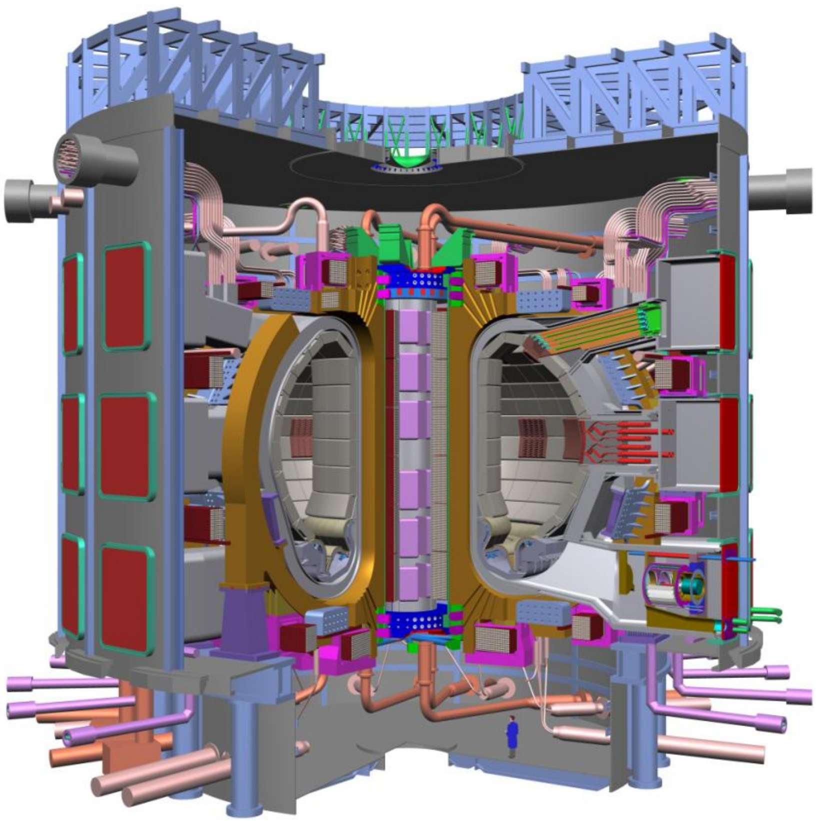
• T.D. Bohm, et al., “UW-Madison Neutronics Activities to Support FENDL”, IAEA presentation, September 2019.

• L. Packer, A. Trkov, “FENDL Library for Fusion Neutronics Calculations, Summary Report from the Consultants Meeting, IAEA report, INDC(NDS)-0769.

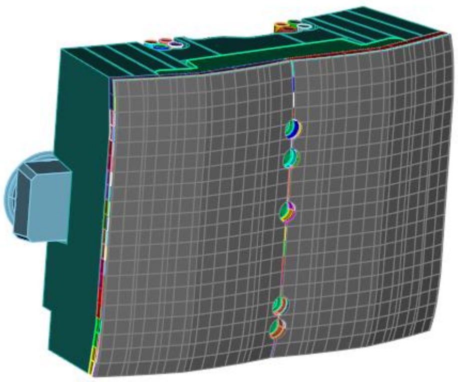
•T.D. Bohm, “The impact of ENDF/B-VIII.0 and FENDL-3.1d on fusion neutronics calculations”, IAEA presentation, October, 2018.

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



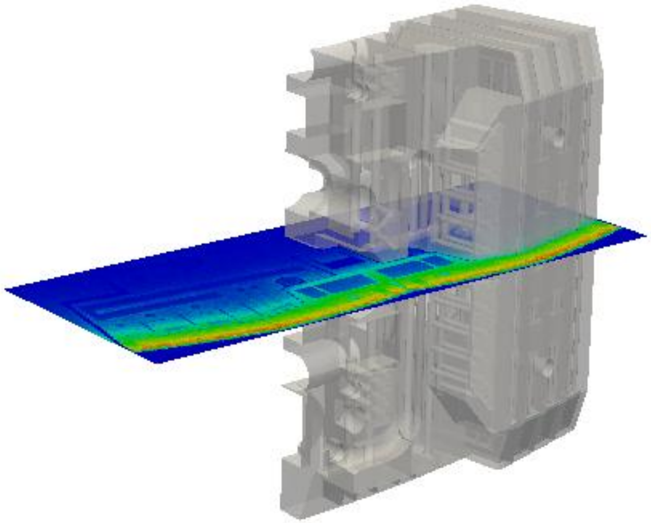
ITER



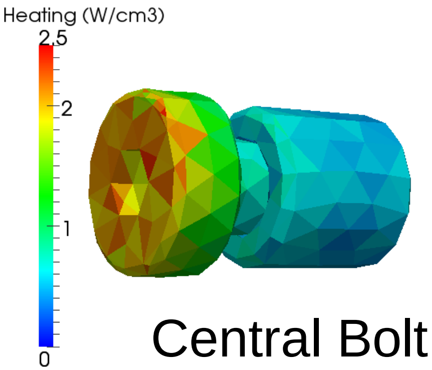
ITER Blanket (shield) Module

Important Fusion Neutronics Responses

- Neutron flux/fluence (**neutron**)
  - structure, magnets
- Radiation damage/dpa (**neutron**)
  - structural material, magnet degradation
- Helium production (**neutron**)
  - re-weldability
- Tritium production (**neutron**)
  - breeding, environmental concerns
- Radiation dose (**neutron+photon**)
  - insulators, electronics, personnel
- Total nuclear heating (**neutron+photon**)
  - coolant system design, thermal stress, etc. for structure, magnets
- Activation/shutdown dose (**photon**)
  - maintenance robotics, personnel
  - waste disposal



ITER Shield Block



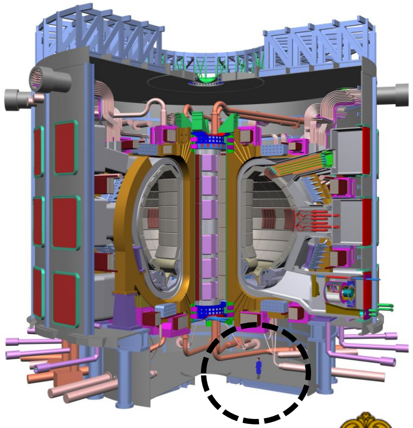
Central Bolt

Current D-T Fusion Experiments/Reactors

D + T -> He-4 (3.5 MeV) + n (14.1 MeV)

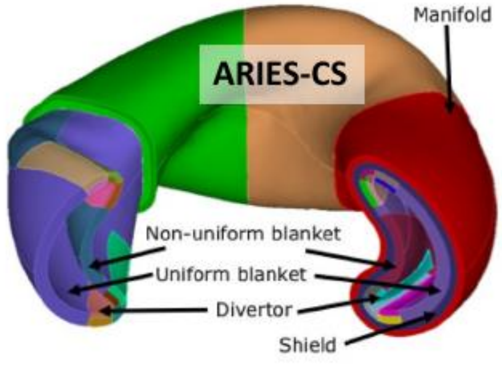
JET (UK)
- 1983-present
- R_{major}=3 m
- Vol_{plasma}=100 m^3
- pulse ~1 sec
- 16 MW_{fusion}

ITER (France)
- under construction
- R_{major}=6 m
- Vol_{plasma}=840 m^3
- pulse ~400-600 sec
- 500 MW_{fusion}



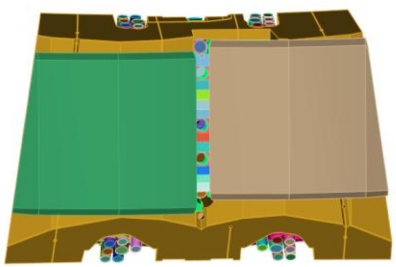
UW Neutronics Capabilities (3-D)

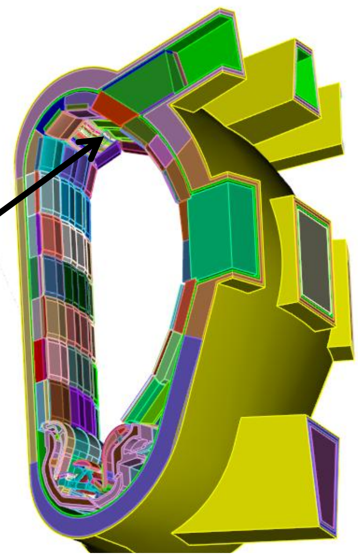
- DAGMC (detailed 3-D CAD based Monte Carlo transport)
  - Transports directly in the CAD model (not a translator)
  - Handles complex surfaces without simplification
  - Couples to MCNP, Geant4, FLUKA, SHIFT, OpenMC
  - Provides a common domain for coupling to other analysis
  - **http://fti.neep.wisc.edu/ncoe/**
  - **http://github.com/svalinn**



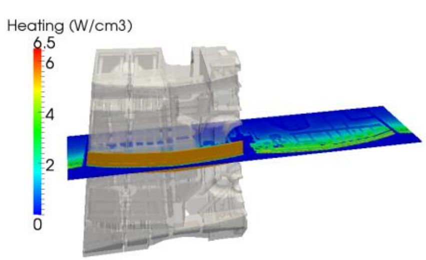
- 3-D CAD model based analysis:

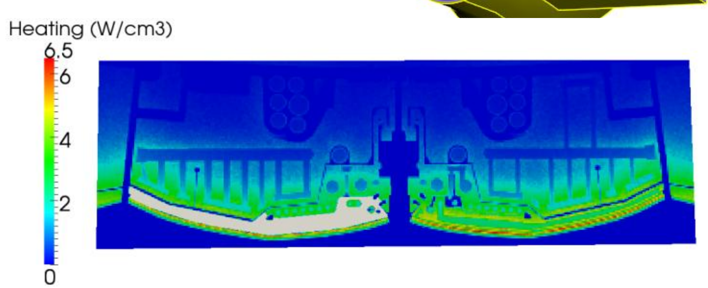
ITER BM08





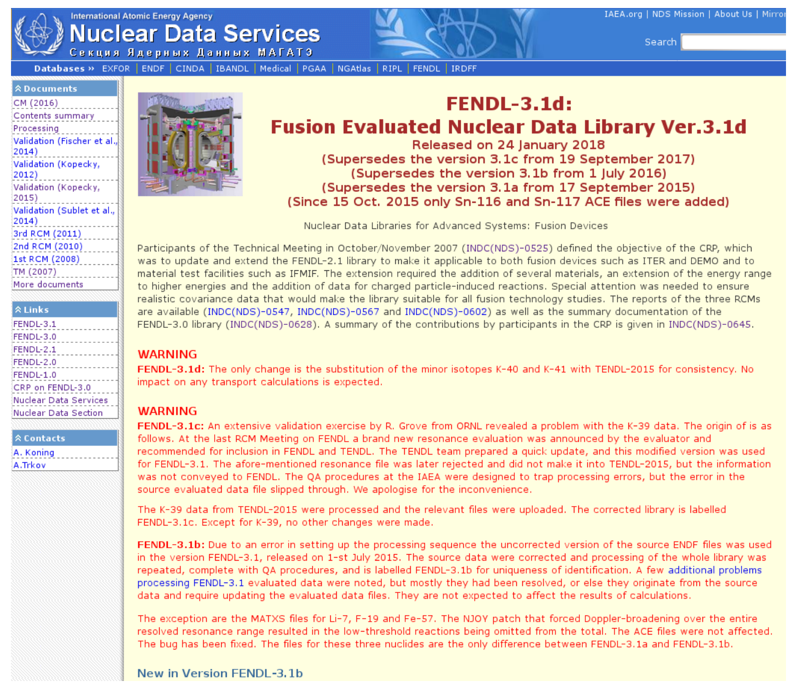
Nuclear heating mapped to ANSYS mesh for thermal analysis





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), TENDL (EU), RUSFOND/BROND (Russia)
- Process uses fusion specific experimental and calculational benchmarks to evaluate the data
- Data available on-line



Source of FENDL-3.1 Data

- 65/180 isotopes in FENDL-3 come from the ENDF/B-VII.1 library
  - See Table 1 in INDC(NDS)-0628
- Some key isotopes for this work:

Isotope	FENDL-2.1	FENDL-3.1
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

ENDF/B-VIII.0 Data

- Major new release of the ENDF/B neutron library
- ACE formatted data for MCNP distributed by LANL
  - https://nucleardata.lanl.gov
- Some key isotope updates for neutron sub-library (see Appendix A in reference* for comprehensive list):
  - H-1,2, Li-6, B-10, O-16, Fe-54,56,57,58, Ni-58-62,64, Cu-63,65, W-182-186, U-235,238, Pu-239

**D.A. Brown et al., "ENDF/B-VIII.0: The 8th major release of the nuclear reaction data library with CIELO-project cross sections, new standards, and thermal scattering data", Nuclear Data Sheets, vol 148, p. 1-142, 2018*

Goal of this work

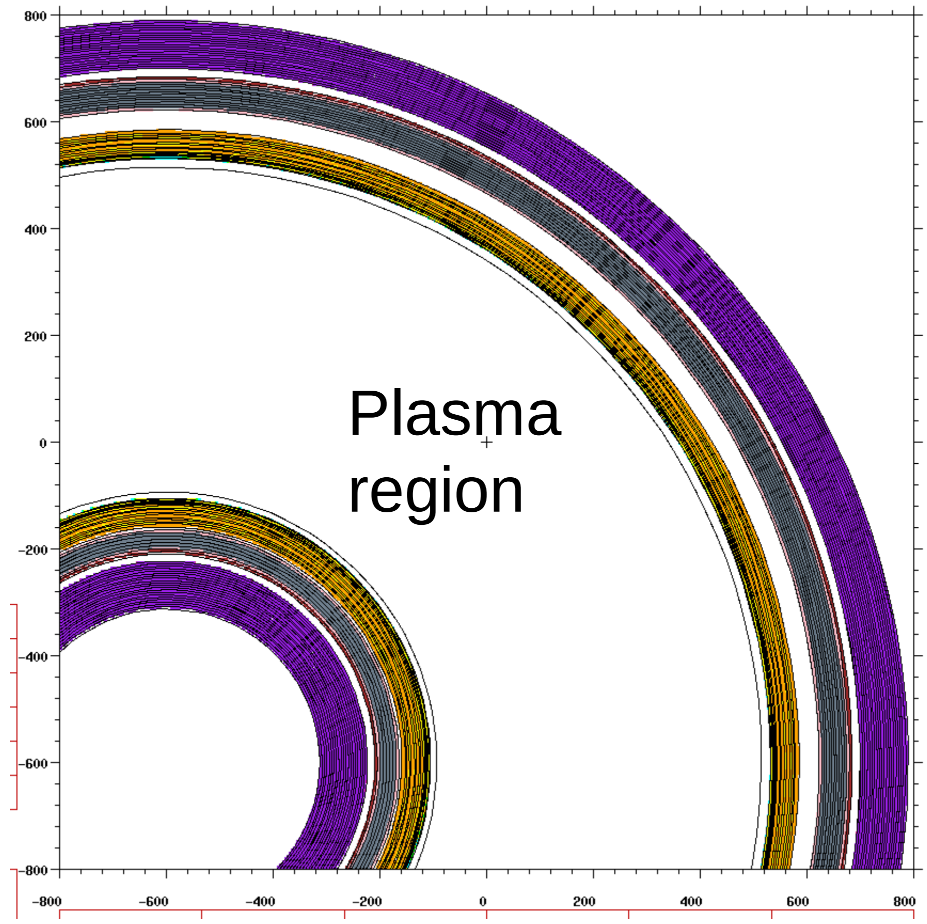
- Look at the impact of using the updated neutron libraries in a realistic model of fusion systems
- Libraries examined:
  - *Neutron:*
    1. FENDL-2.1 (21c)
    2. FENDL-3.1 (31b, 31d)-current version 3.1d
    3. ENDF/B-VII.1 (80c)
    4. ENDF/B-VIII.0 (00c)
  - *Photon*:*
    1. mcplib84 (84p)

- **Previous work has shown that mcplib84 produces results similar to the newer MCNP eprdata12 library*
- *The latest MCNP photon library (eprdata14) has not been tested yet*

**Bohm T.D, Sawan M.E. "The impact of updated cross section libraries on ITER neutronics calculations", Fusion Science and Technology, Vol 68 p. 331-335, 2015.*

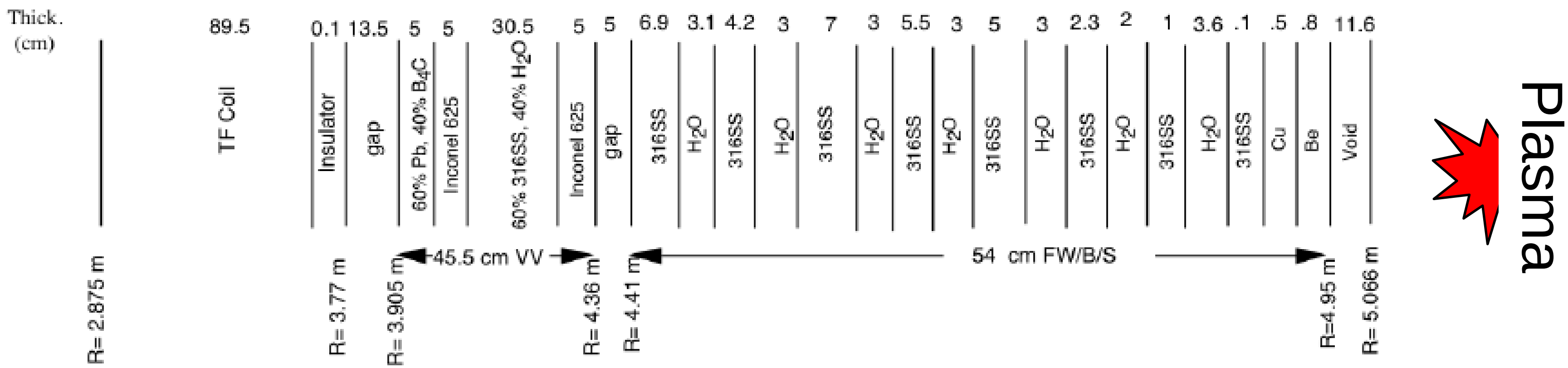
ITER 1-D Cylindrical Calculation Benchmark

- 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

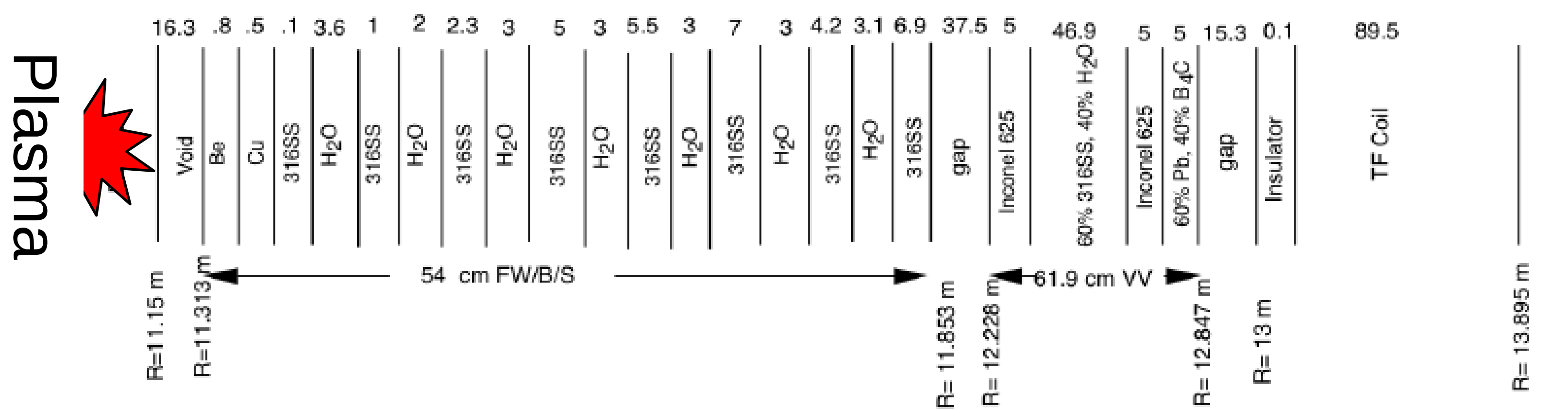


M. Sawan, FENDL Neutronics Benchmark: Specifications for the calculational and shielding benchmark, INDC(NDS)-316, December 1994

ITER 1-D Cylindrical Benchmark continued

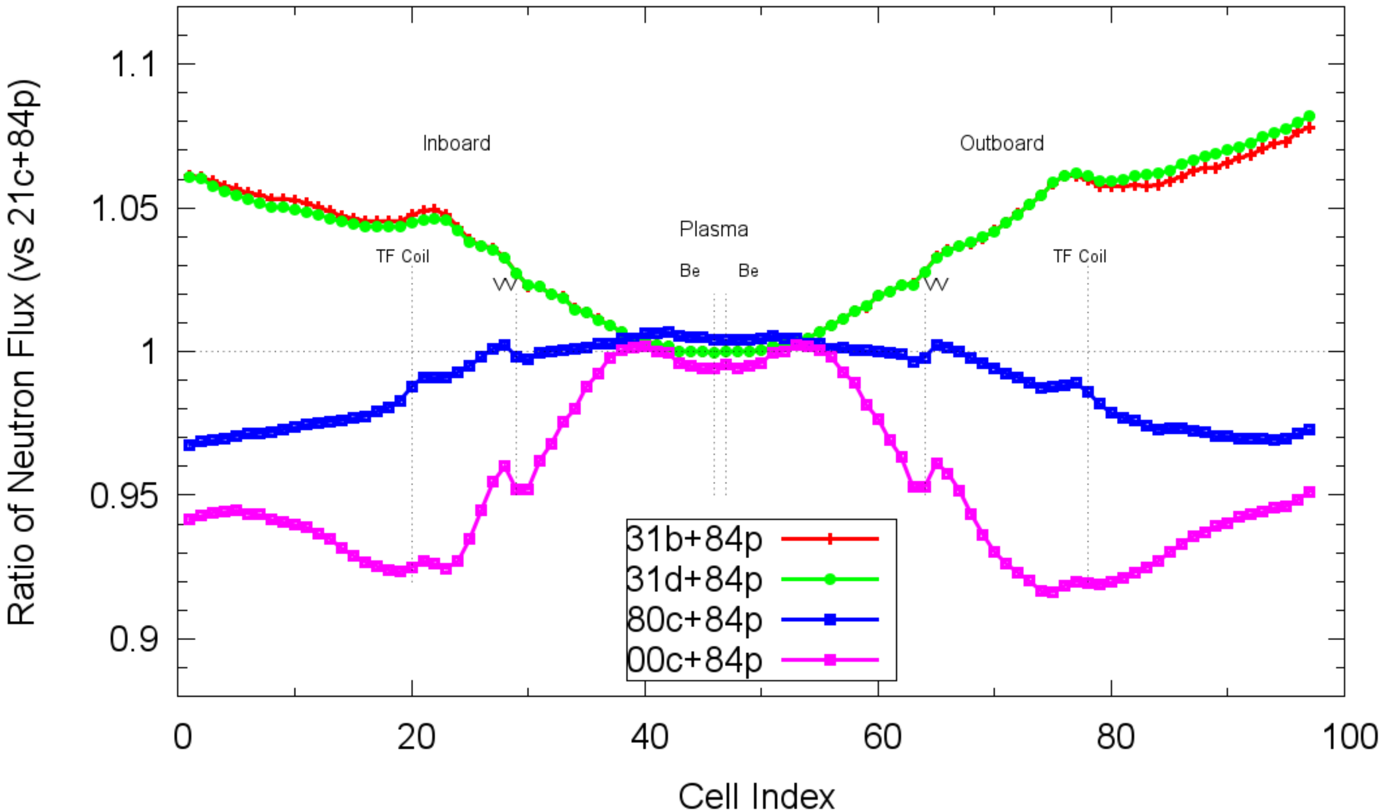


Inboard Region



Outboard Region

Previous Results: Neutron Flux

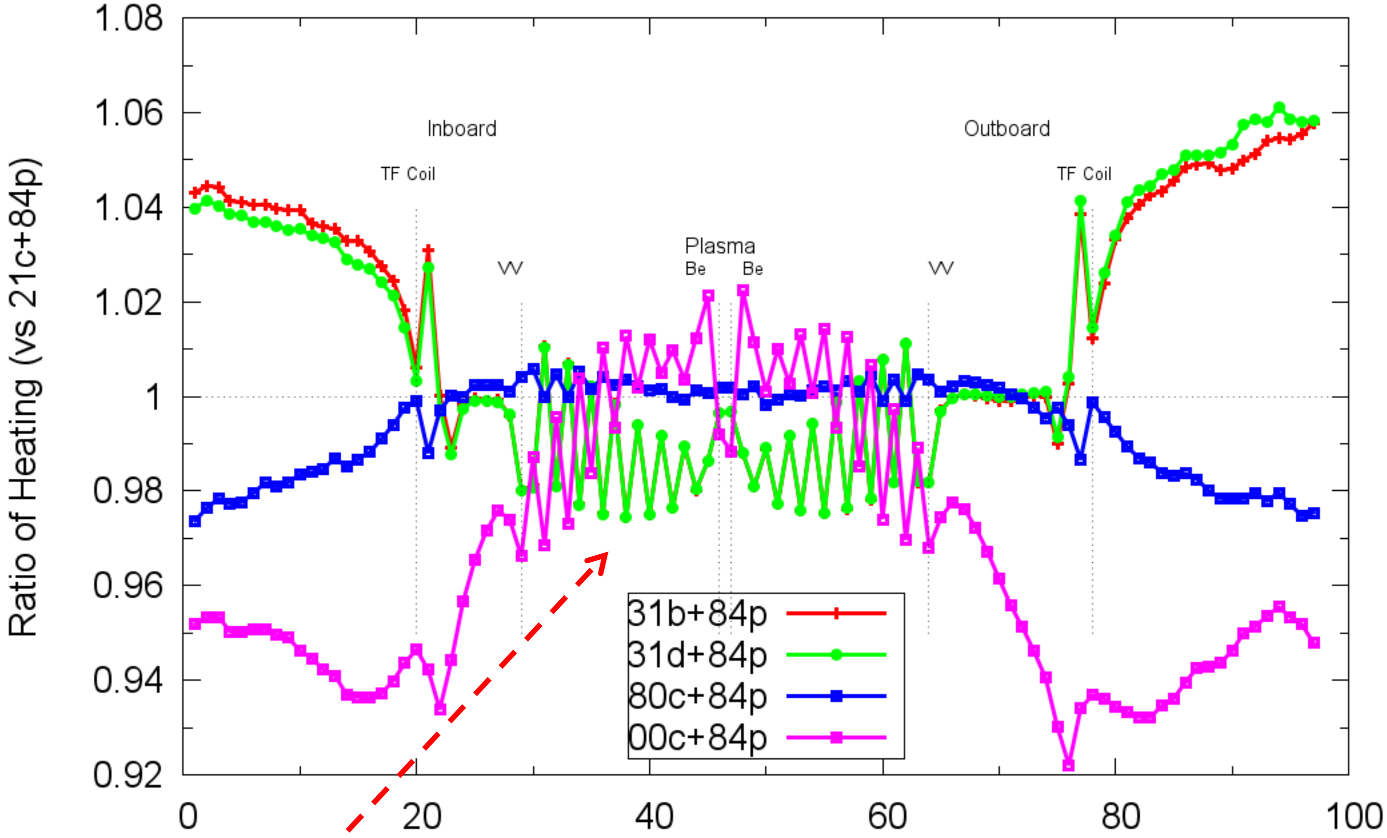


21c=FENDL-2.1
31b=FENDL-3.1b
31d=FENDL-3.1d
70c=ENDF/B-VII.0
80c=ENDF/B-VII.1
00c=ENDF/B-VIII.0
84p=mcnp photon library

Max. relative error <0.26%

- With ENDF/B-VIII.0 (00c) see neutron fluxes up to 10% lower than FENDL-3.1
- In FENDL-3.1, Fe-56 and Cu data come from JEFF-3.1.1 and ENDF/B-VII.0

Previous Results: Total nuclear heating



Valleys are in SS 316

Max. relative error <0.27%

• With ENDF/B-VIII.0 (00c) see total heating up to 10% lower than FENDL-3.1

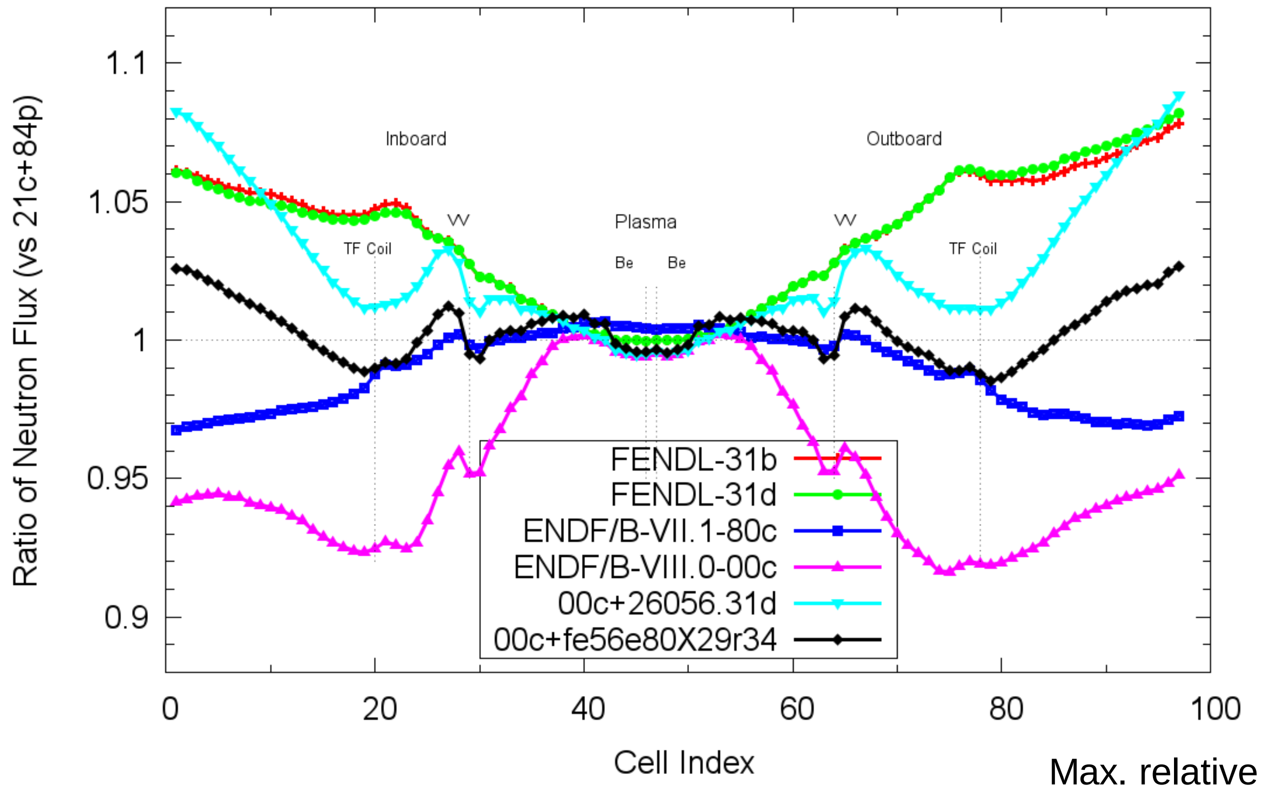
Isotope substitution study

- There is likely a deficiency in the XS data for the structural elements in ENDF/B-VIII.0:
  - A. Trkov, R. Capote “INDEN (Post-CIELO) ^{56}Fe Evaluation”, presented at IAEA FENDL Consultants Meeting, Oct. 2018.
- Repeat the ITER 1-D calculation with ENDF/B-VIII.0 neutron data, **but replace certain XS with those from FENDL-3.1d**:
  - Fe-56, Ni-58, Ni-60, Cr-52, Cr-53, Cu-63, Cu-65

- **Results**: these isotopes were the main cause of the differences observed in previous work (for more details, see the slides at the end of this presentation)

Replace 25056.00c w/ fe56e80X29r34 in ENDF/B-VIII.0

Test a candidate replacement for fe-56 in ENDF/B-VIII:

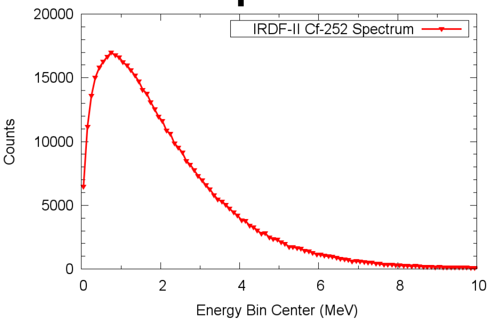


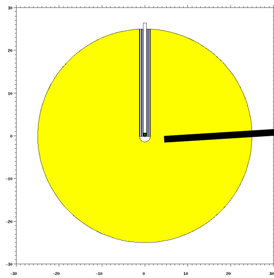
Max. relative error <0.26%

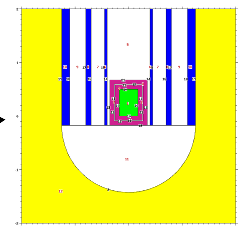
- We see the fe56e80X29r34 has a similar shape to ENDF/B-VIII.0
- We see the fe56e80X29r34 results does not show the large decrease in flux in steel region
- *We need to consider any Cu, Ni, and Cr updates to see the full impact*

MCNP model of Iron Sphere Benchmark Experiment

- Encapsulated Cf-252 source in 25 cm iron sphere

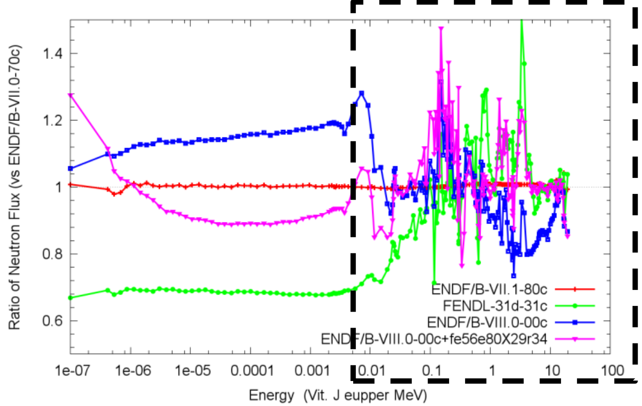


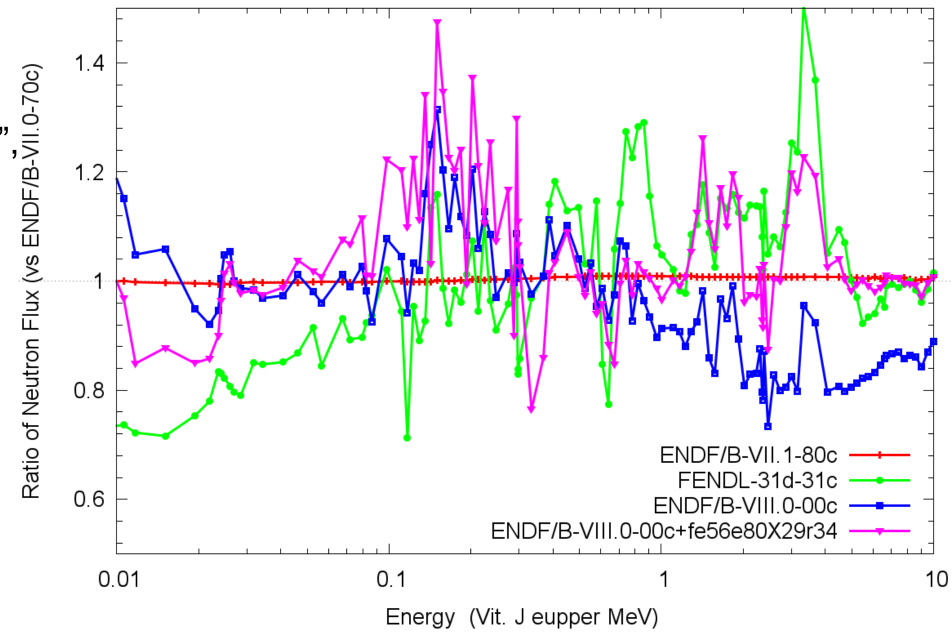




Yellow=iron (99.42 w/o Fe)
Blue=AlCu alloy (93.9 w/o Al)
Pink=SS304
Green=Cf

E. Sajo, et al, “Comparison of Measured and Calculated Neutron Transmission Through Steel for a 252-Cf Source”, Ann. Nucl. Energy, Vol. 20, No. 9, page 585-604, 1993



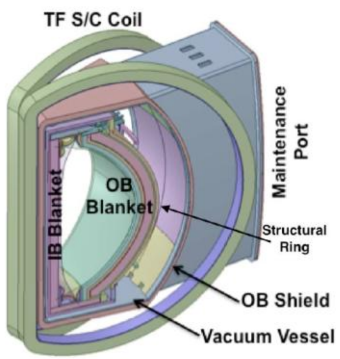


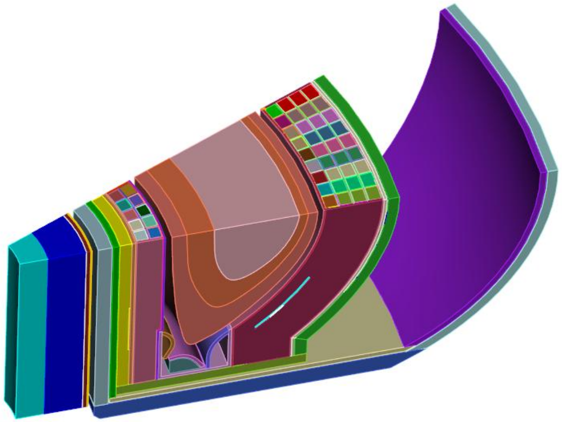
- With FENDL-3.1d, we see highest fluxes in the E=0.4 to 5 MeV region
- With ENDF/B-VIII.0, we see lowest fluxes in the E=0.7 to 10 MeV region
- With fe56e80X29r34, we see results similar to FENDL-3.1d in the E=1.0-10.0 MeV region, but not the big peak at E=0.7-1.0 MeV seen with FENDL-3.1d

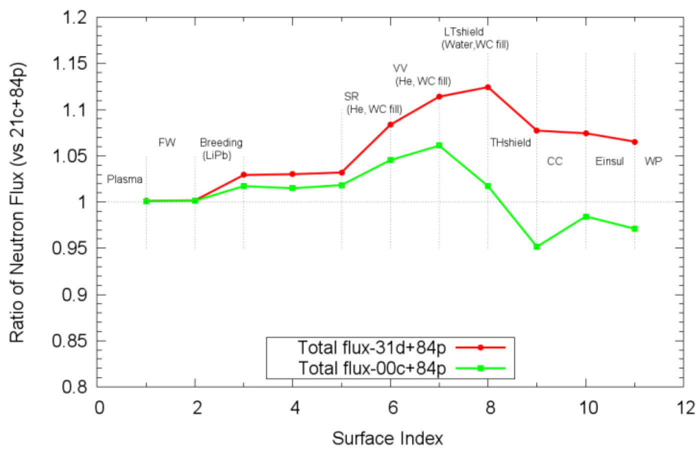
Other Work-FNSF Computational Benchmarking

➢ Need to test on fusion designs other than ITER
  - use different structural materials and tritium breeding materials

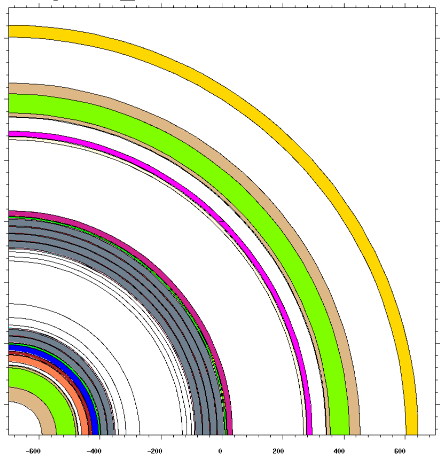
- 3-D neutronics model of U.S. Fusion Nuclear Science Facility (FNSF)







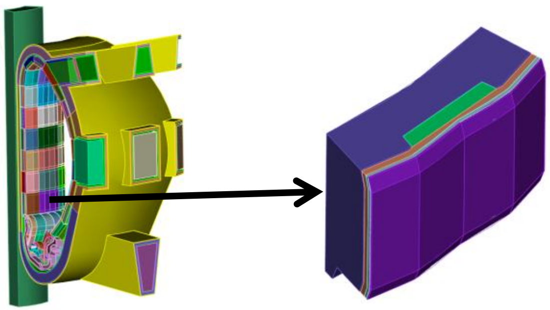
- Developing 1-D model for rapid testing of nuclear data:



- Currently 49 radial zones
- Need to add shell plates for SR, VV, Ltshield
- MCNP materials created with PyNE

Other Work-ITER and JET

- 3-D partially detailed model of ITER:

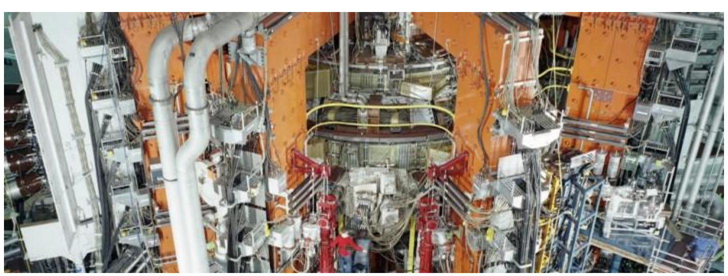


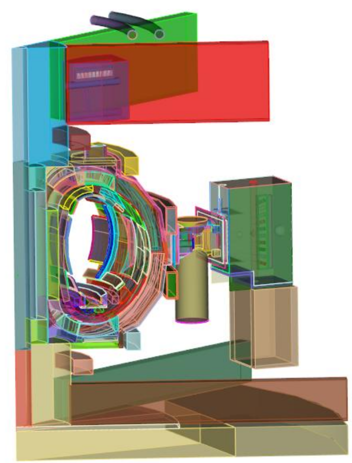
Blanket Shield Module

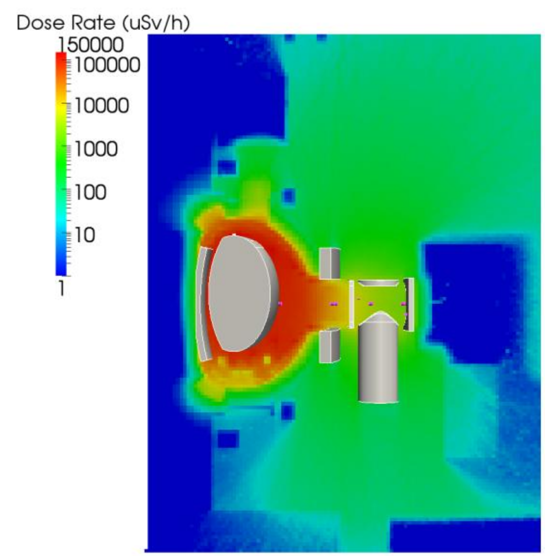
Library	Tally IB TFC (W/cm^3)	Ratio
21c+84p	3.72074E-05	1
31d+84p	3.73618E-05	1.00
80c+84p	3.62283E-05	0.97
00c+84p	3.44389E-05	0.93

Example: Nuclear heating in magnet

- Experimental measurement based benchmarking at JET:
  - Prompt measurements
  - Shutdown dose rate measurements
  - EU-US collaboration







DTE2 SDR results

Questions

Questions?

(For those interested, there are more details in the following slides)

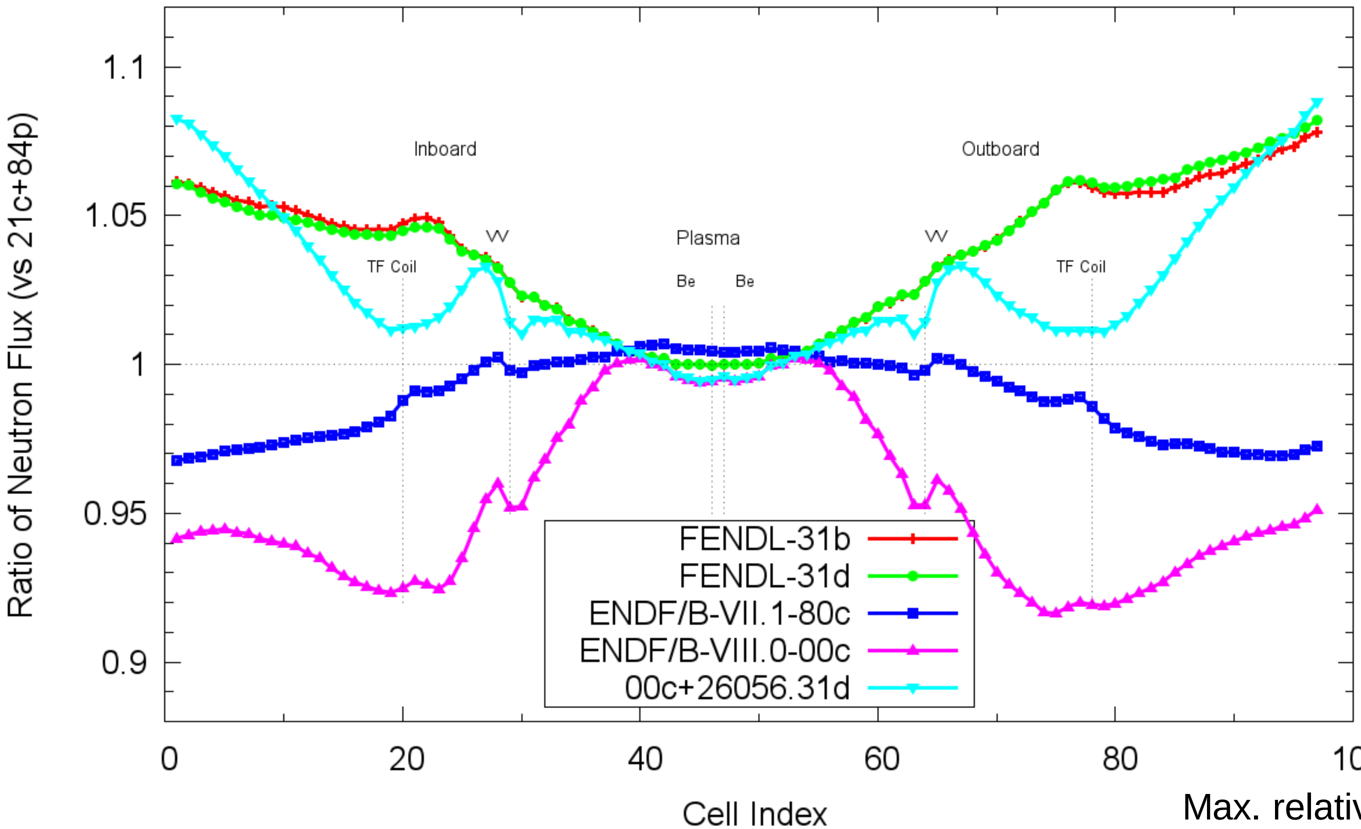
FENDL continued

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

Source of FENDL-2.1 data:

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

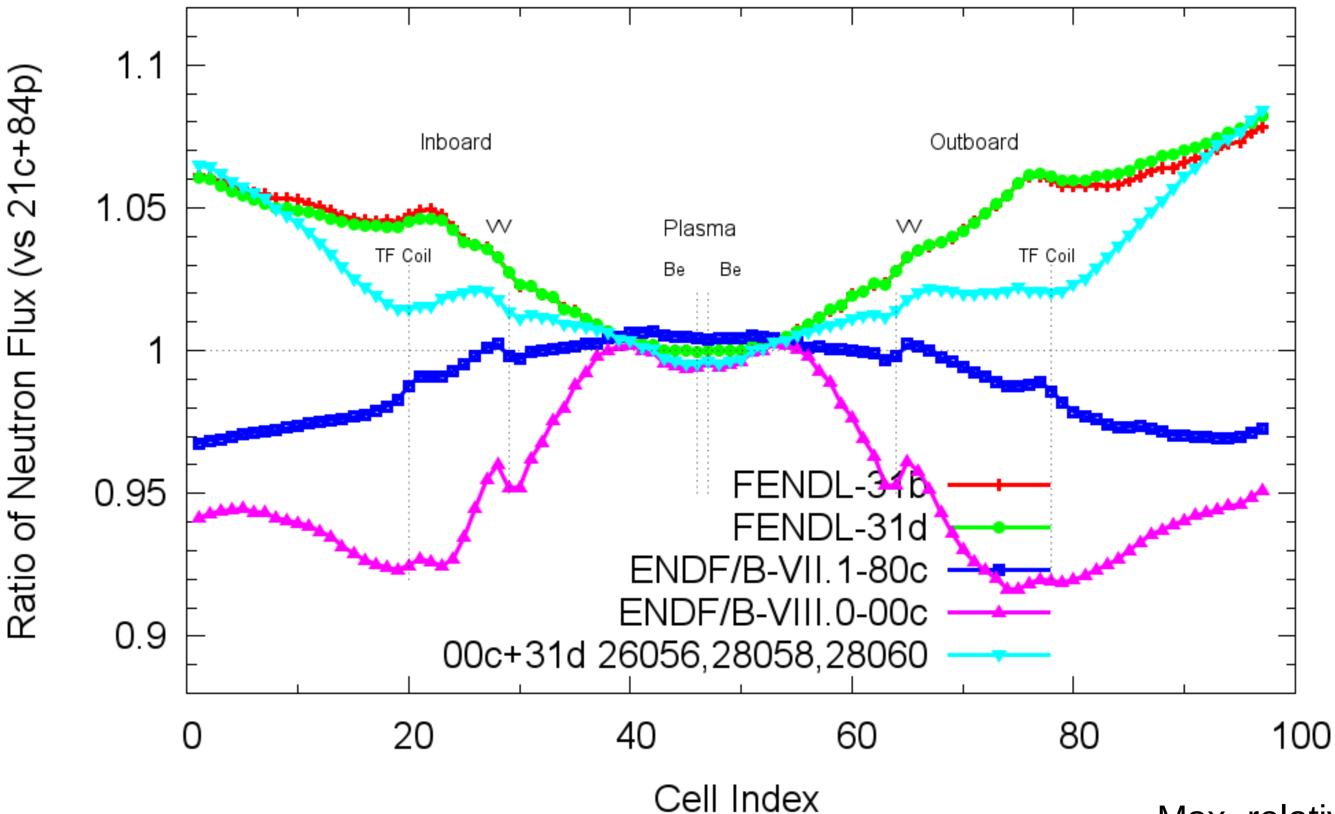
Substitution Results: Fe-56



Max. relative error <0.26%

- With ENDF/B-VIII.0 (00c)+26056.31d, we see neutron fluxes more closely match those of FENDL-3.1d until deep in the FW/Blanket Shield and nearing the VV (Inconel shells) and TF coil (significant Cu content)
- Recall that the ITER 1-D benchmark is composed of alternating SS and water for the FW/Blanket Shield, then a VV composed of an Inconel shell with water cooled SS filler. Cu is present near the Be layer and in the TF coil

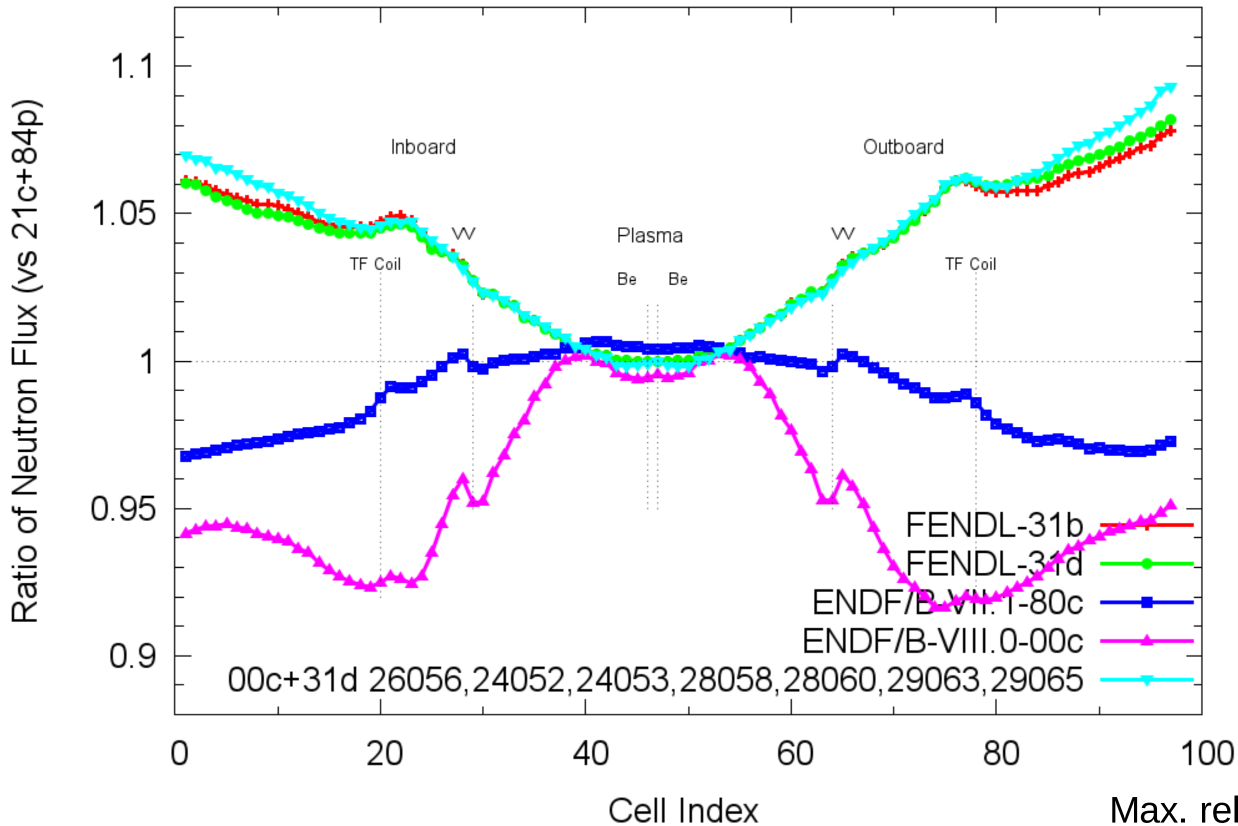
Substitution Results: Fe-56, Ni-58, Ni-60



Max. relative error <0.26%

- Now we see neutron fluxes more closely match those of FENDL-3.1d near the VV shell (the large peak at the VV shell seen on previous slide is no longer present)
- We still see a large difference at the TF coil

Substitution Results: Fe-56, Ni-58, Ni-60, Cr-52, Cr-53, Cu-63, Cu-65



Max. relative error <0.26%

- Now we see neutron fluxes closely match those of FENDL-3.1d (both near the FW Cu layer and the TF coil which has significant Cu content)

MCNP model of Iron Sphere Benchmark Experiment

- Measurements of neutron transmission in iron spheres from a Cf-252 source were performed by the Czech. National Research Institute (NRI) and the Skoda Company
- This work uses the r=25 cm sphere case described by E. Sajo.
- Some of this work was completed by an undergraduate student as a project for the NE 506 Monte Carlo Radiation Transport class

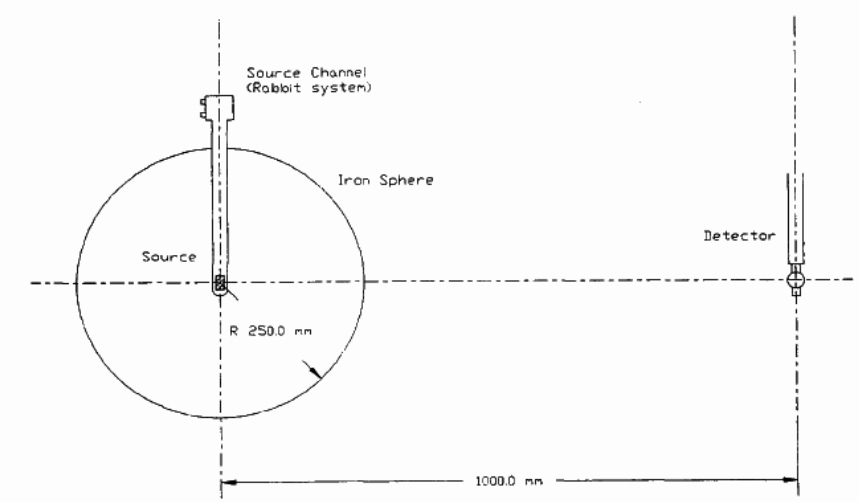
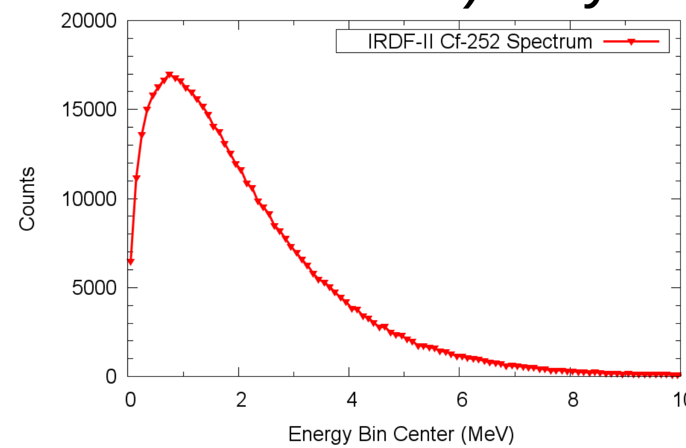


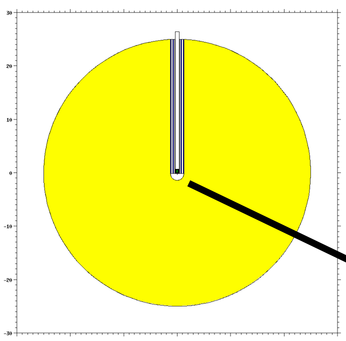
Fig. 1. Experimental setup.

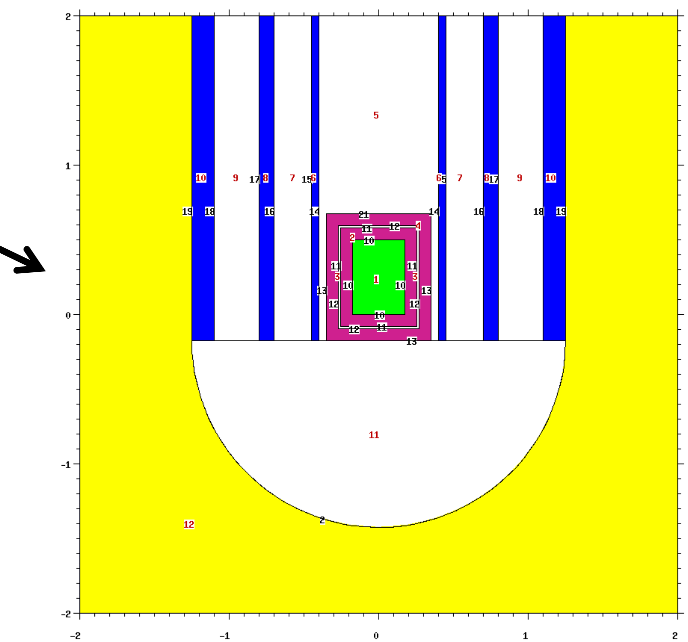
E. Sajo, et al, "Comparison of Measured and Calculated Neutron Transmission Through Steel for a 252-Cf Source", Ann. Nucl. Energy, Vol. 20, No. 9, page 585-604, 1993

MCNP model of Iron Sphere Benchmark Experiment

- ➢ Modeled and calculated with native MCNP-6.2
- ➢ Encapsulated Cf-252 source with guide tubes in the iron sphere
- ➢ Used detailed dimensions, material compositions, and source spectrum provided in the Sajo paper, (r_{sphere}=25 cm)
- ➢Results determined with a ring f5 (next event estimator) tally at r=100 cm (position of measurement)







Yellow=iron (99.42 w/o Fe)
Blue=AlCu alloy (93.9 w/o Al)
Pink=SS304
Green=Cf

Results Neutron Flux (preliminary)

Library	E<0.1 MeV	E=0.1-1 MeV	E=1-10 MeV	Total
70c (ENDF/B-VII.0)	1	1	1	1
80c (ENDF/B-VII.1)	0.9972	1.0060	1.0080	1.0054
31c (FENDL-3.1d)	0.8547	1.0201	1.0722	1.0105
00c (ENDF/B-VIII.0)	1.0266	1.0204	0.8940	1.0054
fe56e80X29r34+00c	1.0164	0.9929	1.0575	1.0032

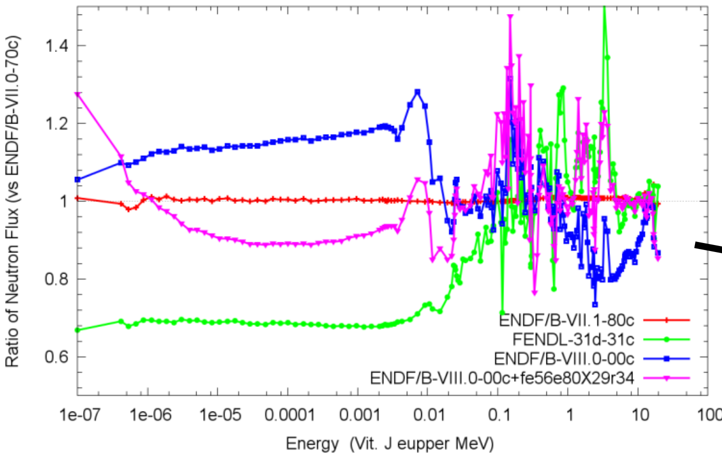
relative error negligible

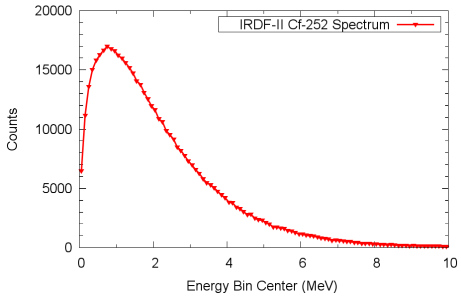
For the total flux:

- With FENDL-3.1d, we see the highest total neutron flux
- With ENDF/B-VIII.0, we see neutron fluxes closely match those of ENDF/B-VII.1
- With fe56e80X29r34, we see neutron fluxes slightly less than those of ENDF/B-VIII.0

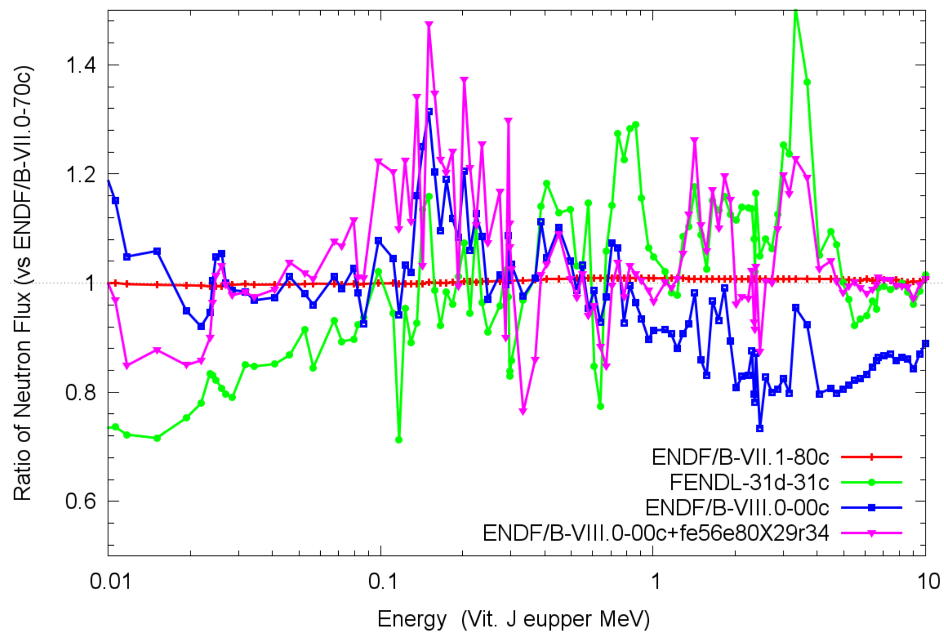
(Recall this is essentially a 25 cm iron sphere with little other materials)

Results Spectrum (preliminary)





Cf-252 source spectrum



- **Looking at the E=.01 to 10 MeV range:**

- With FENDL-3.1d, we see lowest fluxes in the E=.01 to 0.1 MeV region and highest in the E=0.4 to 5 MeV region
- With ENDF/B-VIII.0, we see lowest fluxes in the E=0.7 to 10 MeV region
- With fe56e80X29r34, we see results similar to FENDL-3.1d in the E=1.0-10.0 MeV region, but not the big peak at E=0.7-1.0 MeV seen with FENDL-3.1d
- Recall this is essentially a 25 cm iron sphere with little other materials

Future Work for Sajo Iron Sphere Benchmark

- Compare calculated neutron spectrum to measurements performed by NRI and Skoda
  - Calculations have already been completed (but not plotted)
  - Note that these two measurements have been performed with different energy group structures
- Other?