The impact of updated Cr and Fe cross sections for fusion applications

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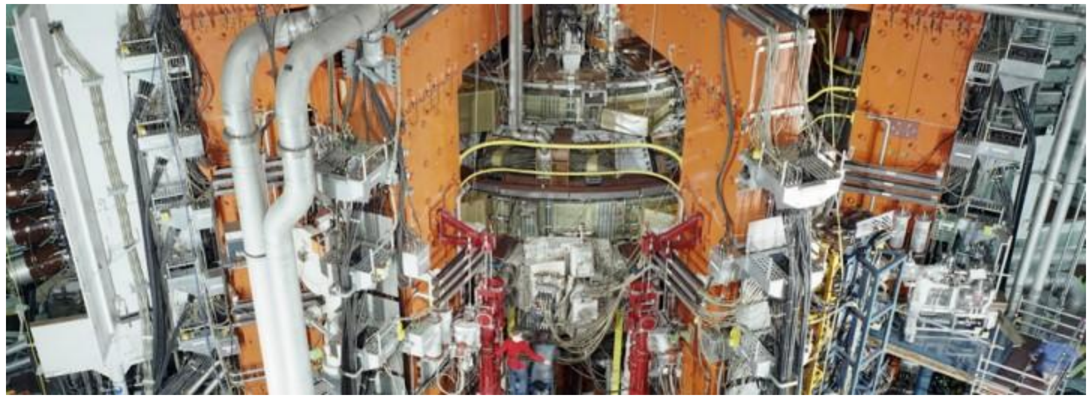
Outline

1) Introduction
2) Nuclear data libraries examined
3) Benchmark/Systems Analyzed:
    - ITER-1D computational benchmark
    - ITER-3D computational benchmark
    - FNSF-3D computational benchmark
    - Sajo1993 Cf-252 iron sphere experimental benchmark
4) Future Work

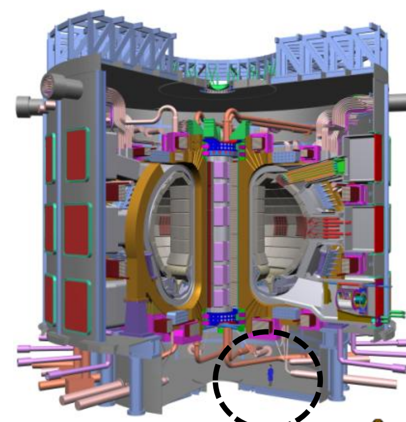
Current D-T Fusion Experiments/Reactors

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}

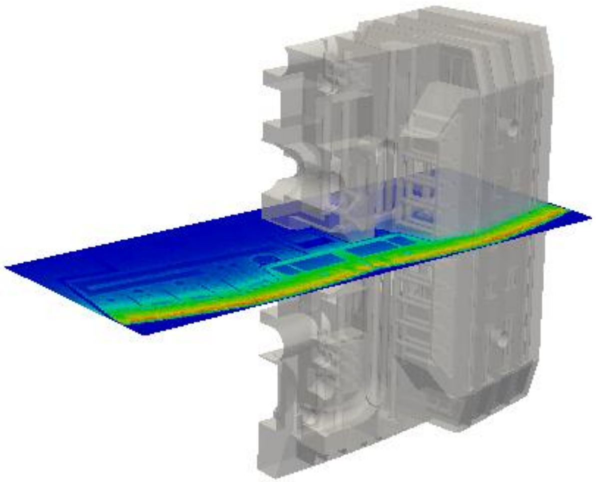


ITER (France)
- under construction
- R_{major}=6 m
- Vol_{plasma}=840 m^3
- pulse ~400-600 sec
- 500 MW_{fusion}



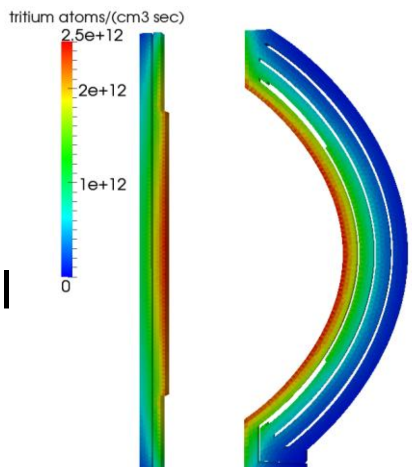
Important Fusion Neutronics Responses

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



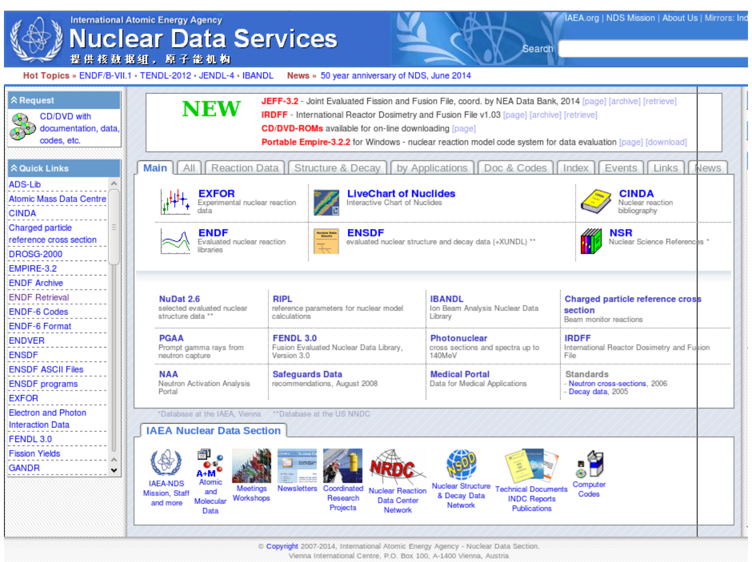
Nuclear heating in ITER FW/Shield Block

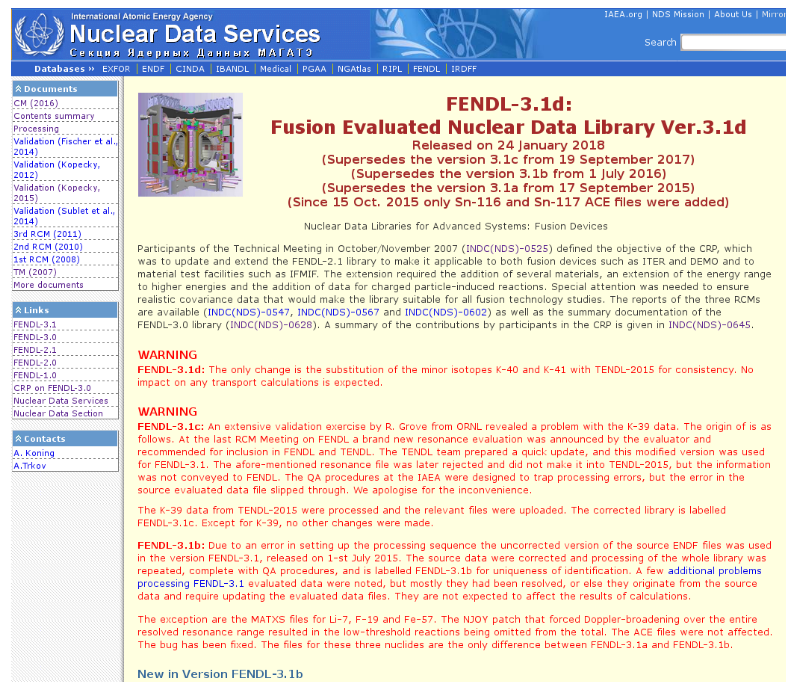
Tritium production in FNSF breeding channel



FENDL Library

- 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 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

*FENDL-2.1 is the reference library for ITER neutronics

ENDF/B-VIII.0 Library

- Released 2018, ACE formatted data available on-line:
  - https://nucleardata.lanl.gov
- Initial testing indicated deficiencies in XS for iron
  - revealed in iron transmission experiments with Cf-252 source
  - inelastic XS was too high
- Other structural elements' XS are being re-examined
  - Cr, Co, Ni, Ti, Pb
- Candidate replacements for some isotopes of Fe and Cr have been made available for this work* (*provided by A. Trkov*)

- A. Trkov, R. Capote, "INDEN (Post-CIELO) ^{56}Fe Evaluation", Consultants Meeting on the FENDL Library for fusion neutronics calculations, 15-18 Oct., IAEA, 2018.
- G.P.A Nobre, D.A. Brown, "Nuclear Data Evaluations of Structural Materials in BNL", INDEN Consultants Meeting on Evaluation of Structural Materials, Oct. 29-Nov. 1, IAEA, 2018.
- A. Trkov et al. "Improved evaluations of neutron induced reactions on ^{57}Fe and ^{56}Fe targets, Consultants Meeting of INDEN on Evaluated Nuclear Data of the Structural Materials, 2-5 Dec., IAEA, 2019.
- G.P.A. Nobre et al. "Status of Cr Evaluations", Consultants Meeting of INDEN on Evaluated Nuclear Data of the Structural Materials, 2-5 Dec., IAEA, 2019.
- * See the IAEA INDEN web site: https://www-nds.iaea.org/INDEN/

Goal of this work

- Look at the neutronics impact of using the updated neutron libraries in a **realistic model of fusion systems** using MCNP
- Libraries examined:
  - *Neutron:*

    standard MCNP id

    1. FENDL-2.1 (21c)
    2. FENDL-3.1 (31c)-current version 3.1d
    3. ENDF/B-VII.1 (80c)
    4. ENDF/B-VIII.0 (00c)
    5. New candidate evaluations for Fe, Cr

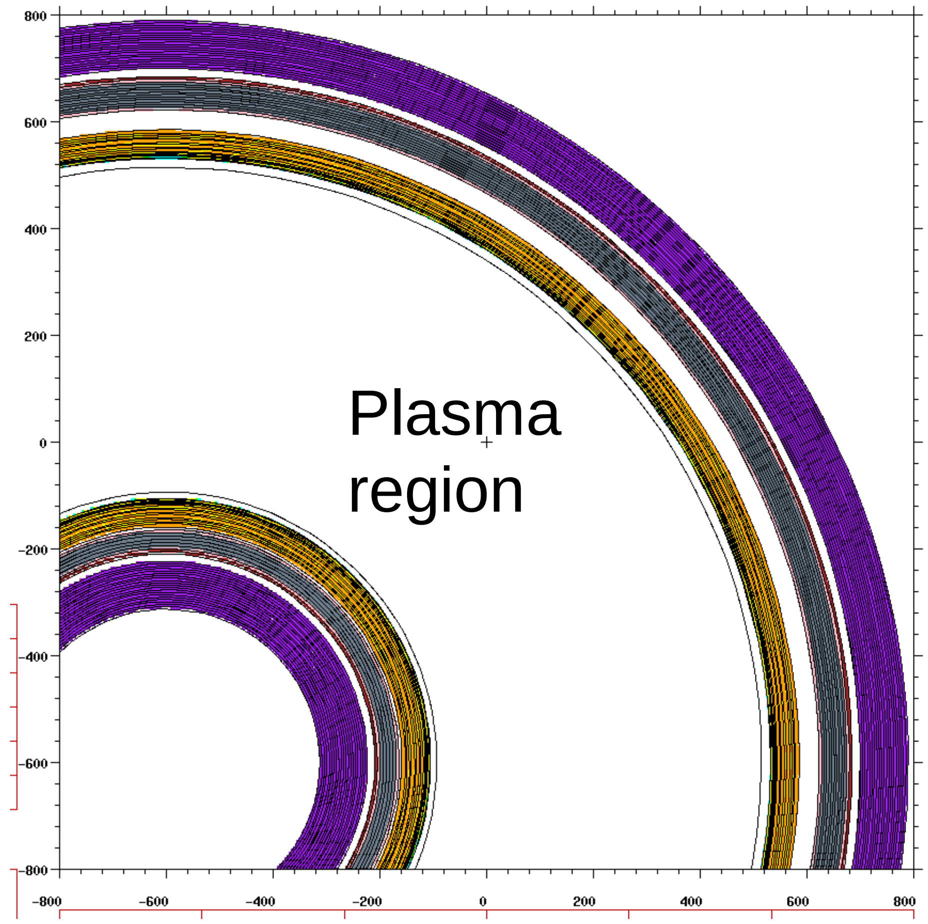
    New work
  - *Photon*:*
    1. mcplib84 (84p)

- **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.*

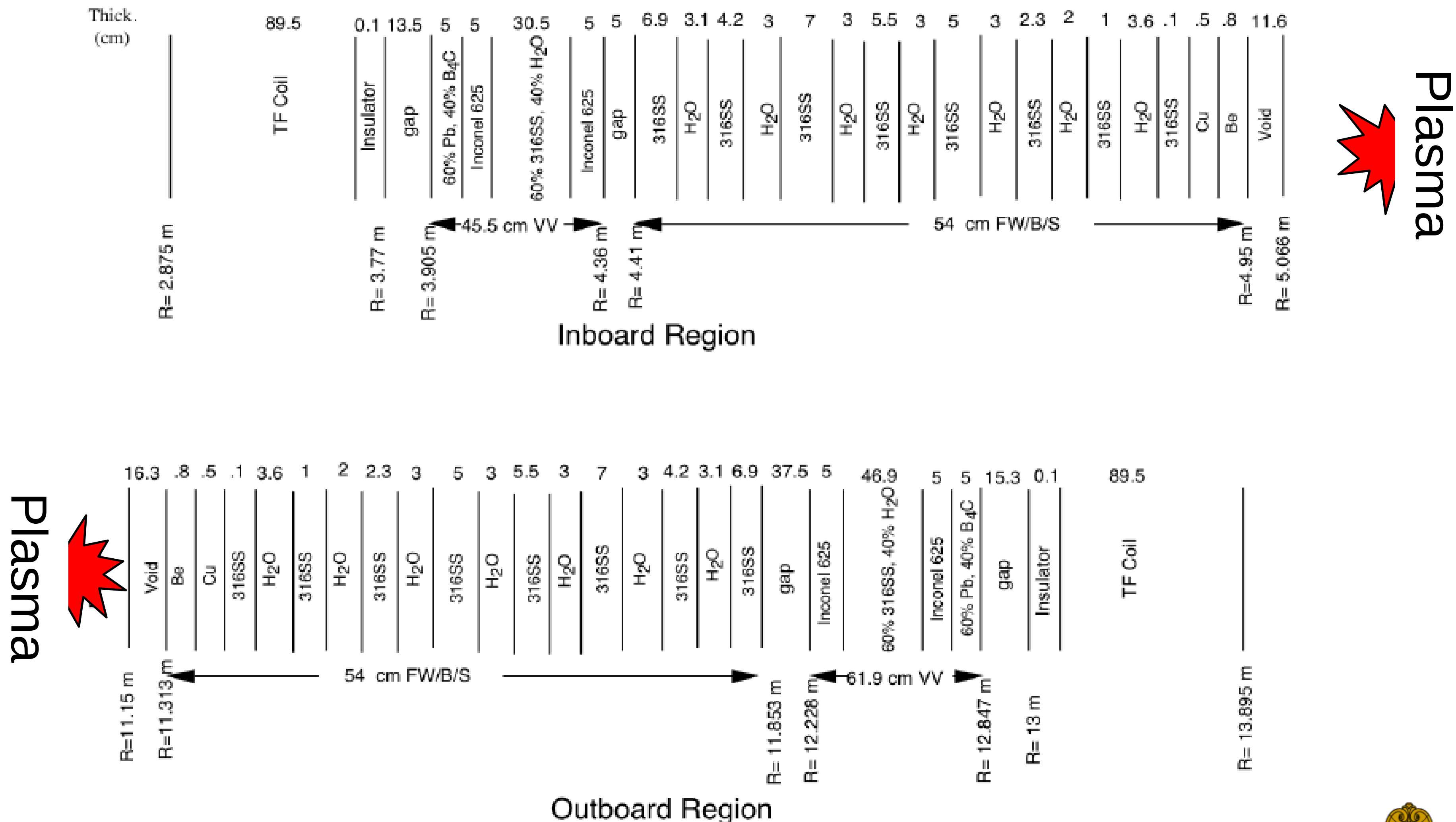
ITER 1-D Cylindrical Calculation Benchmark

- 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

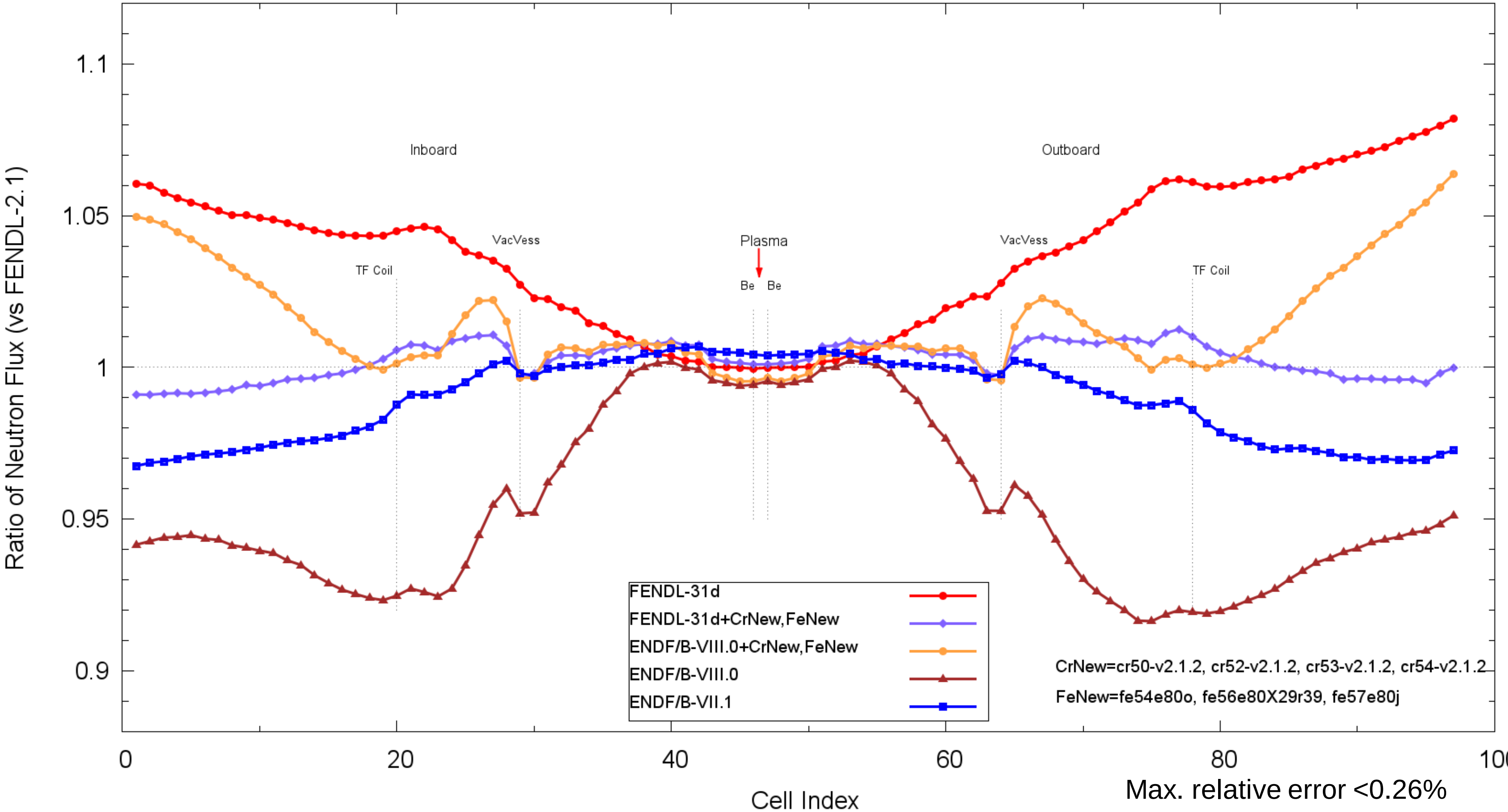


M. Sawan, FENDL Neutronics Benchmark: Specifications for the calculational and shielding benchmark, INDC(NDS)-316, December 1994

ITER 1-D Cylindrical Benchmark continued



Results: Neutron Flux



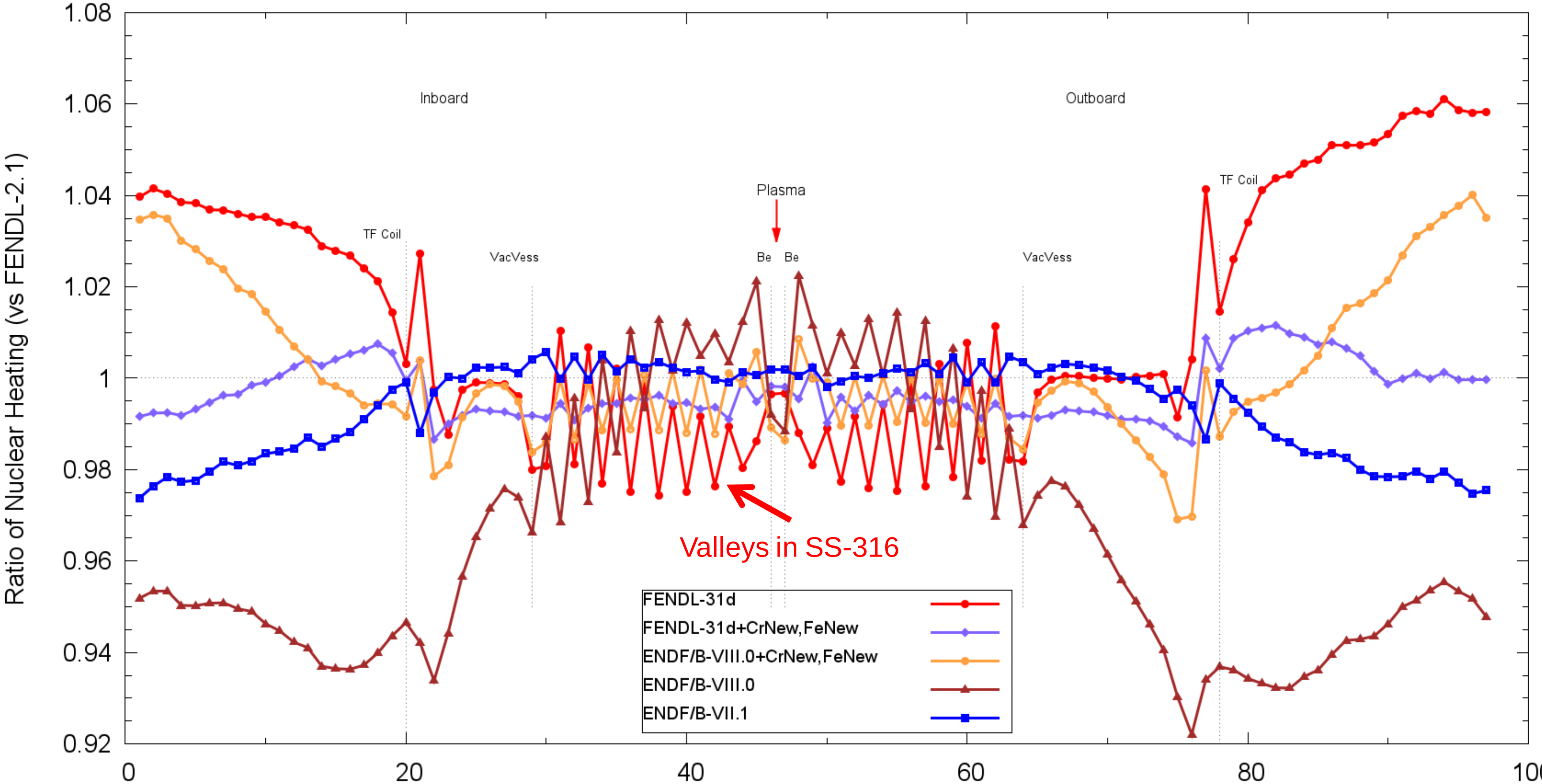
Max. relative error <0.26%

- With FENDL-3.1, we see neutron fluxes up to 8% higher than FENDL-2.1
- With ENDF/B-VIII.0 we see neutron fluxes up to 8% lower than FENDL-2.1

➢ ENDF/B-VIII.0+CrNew,FeNew closer to FENDL-2.1 but see structure at VV, TFC

➢ FENDL-3.1+CrNew,FeNew quite close to FENDL-2.1 but structure at VV

Results: Total Nuclear Heating



Max. relative error <0.27%

CrNew=cr50-v2.1.2, cr52-v2.1.2, cr53-v2.1.2, cr54-v2.1.2
FeNew=fe54e80o, fe56e80X29r39, fe57e80j

- With FENDL-3.1, we see heating up to 6% higher than FENDL-2.1
- With ENDF/B-VIII.0 we see heating up to 8% lower than FENDL-2.1

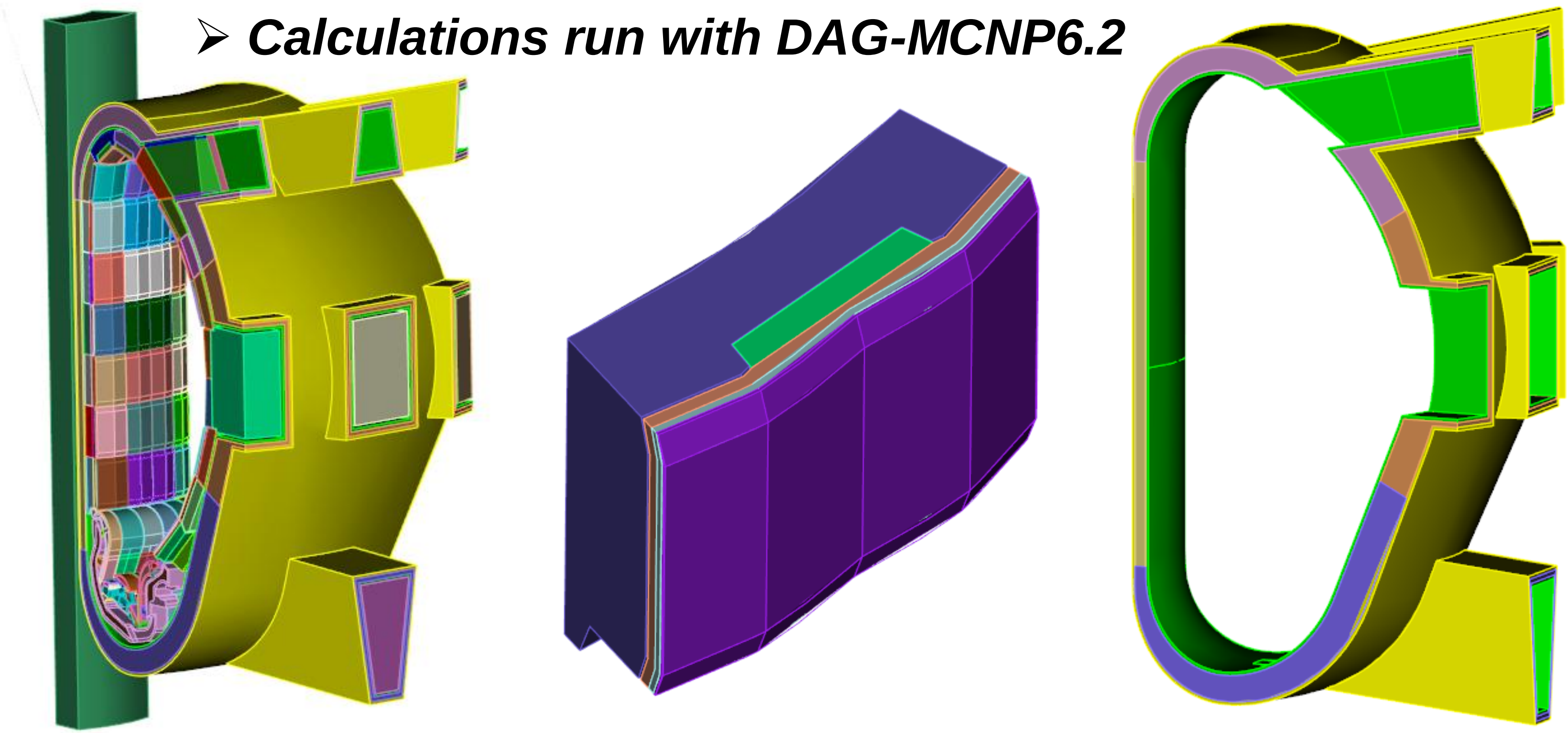
➢ ENDF/B-VIII.0+CrNew,FeNew closer to FENDL-2.1 but see structure at VV, TFC

➢ FENDL-3.1+CrNew,FeNew quite close to FENDL-2.1 but structure at TFC

3-D ITER CAD Model

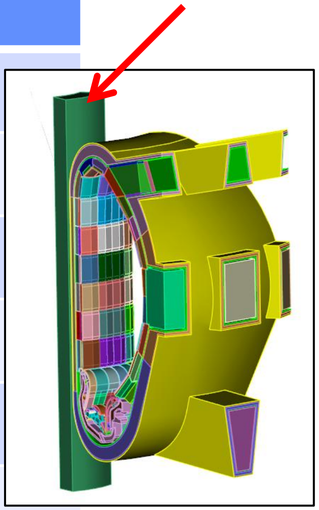
- Based on UW BL-Lite model with added IB Toroidal Field Coil (TFC) volume
- All BMs homogenized and consist of 5 volumes (Be layer, Cu layer, SS finger layer, Beam layer, SB)
- VV consists of 3 homogenized parts (inner shell, body, outer shell)
- Model has 723 volumes, 12067 surfaces, 29467 curves

➢ ***Calculations run with DAG-MCNP6.2***



Results- total nuclear heating IB TFC

Library	Tally IB TFC (W/cm^3)	Ratio
FENDL-2.1	3.72244E-05	1
FENDL-3.1	3.73618E-05	1.004
ENDF/B-VII.1	3.62283E-05	0.973
ENDF/B-VIII.0	3.44391E-05	0.925
ENDF/B-VIII.0 + CrNew,FeNew	3.61820E-05	0.972
FENDL-3.1 + CrNew,FeNew	3.70739E-05	0.996



Max. relative error <0.66%

- With FENDL-3.1, we see heating the same as FENDL-2.1 at IB TFC
- With ENDF/B-VIII.0 we see heating 7% lower than FENDL-2.1

➢ With ENDF/B-VIII.0+CrNew,FeNew we see heating 3% lower than FENDL-2.1

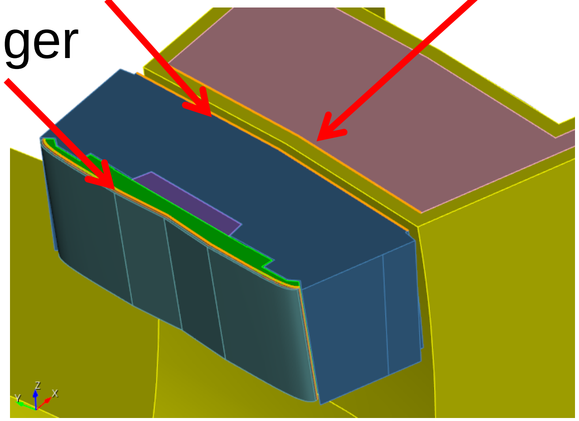
➢ With FENDL-3.1+CrNew,FeNew we see heating the same as FENDL-2.1

➢ *This is consistent with what we saw in 1-D model at the* ***front of the TFC***

Results: Iron dpa near BM14 (ratios)

Location	F-2.1	E-VII.1	F-3.1	E-VIII.0	E-VIII.0 + CrNew,FeNew	F-3.1 + CrNew,FeNew
Finger	1.000	1.062	0.997	1.000	0.997	0.997
SBback	1.000	1.015	1.009	0.964	1.000	0.995
VVshell	1.000	1.019	1.010	0.968	1.004	0.998

Maximum relative error <0.10%



- For ITER, the main concern for dpa is at the VV shell
- With ENDF/B-VIII.0 we see 3-4% lower dpa than the other libraries
  - In general, close agreement among the other libraries at all locations
- With ENDF/B-VII.1 we see an outlier at the BM Finger

Results: He production near BM14 (ratios)

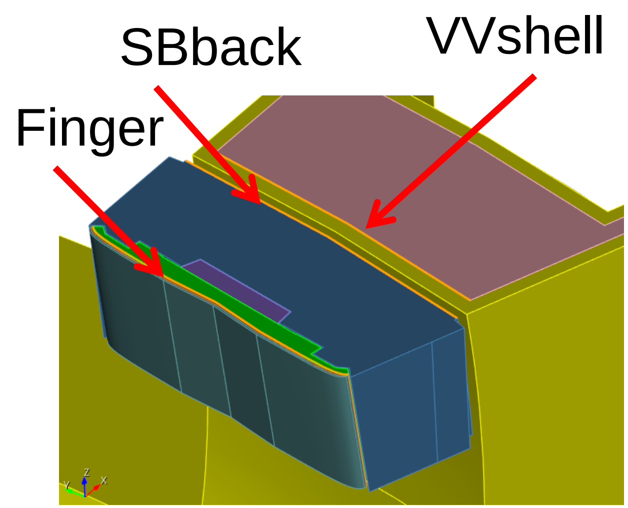
Location	F-2.1	E-VII.1	F-3.1	E-VIII.0	E-VIII.0 + CrNew,FeNew	F-3.1 + CrNew,FeNew
Finger	1.000	1.081	1.042	1.078	1.136	1.157
SBback	1.000	1.048	1.056	1.037	1.095	1.108
VVshell	1.000	1.079	1.057	1.066	1.127	1.144

Maximum relative error <0.13%

- For ITER, the main concern for He production is at the back of the SB and the VV shell for re-welding
- Overall, He production is 4-8% higher with previous libraries

➢ Libraries using the new Cr and Fe evaluations are 10-16% higher than that calculated with FENDL-2.1

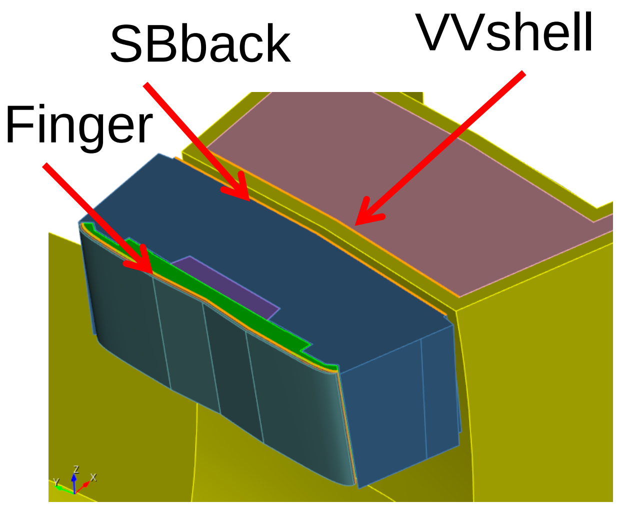
  - We will need to check the He production XS and spectra to determine the underlying cause



Results: He production near BM14 (ratios)

➢ Calculate He production using FENDL-2.1 for transport, and various libraries for He production response function (mt 207) in SS-316 L(N)-IG (17.5 w/o Cr)

Mt 207 Library	Finger	SBback	Vvshellback
FENDL-2.1	1.000	1.000	1.000
ENDF/B-VII.1	1.071	1.048	1.073
FENDL-3.1d	1.041	1.032	1.037
ENDF/B-VIII.0	1.080	1.057	1.086
E-VIII.0 + CrNew,FeNew	1.134	1.082	1.129
F-3.1 + CrNew,FeNew	1.149	1.098	1.141

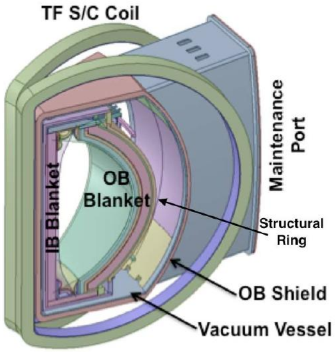


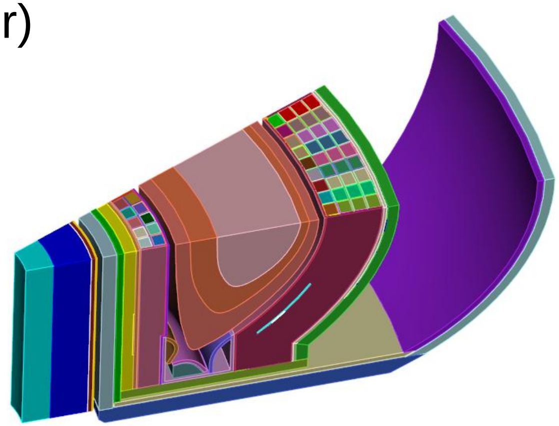
Maximum relative error <0.13%

➢With the CrNew,FeNew evaluations, we see most of the differences in He production at these locations are due to the change in He production XS

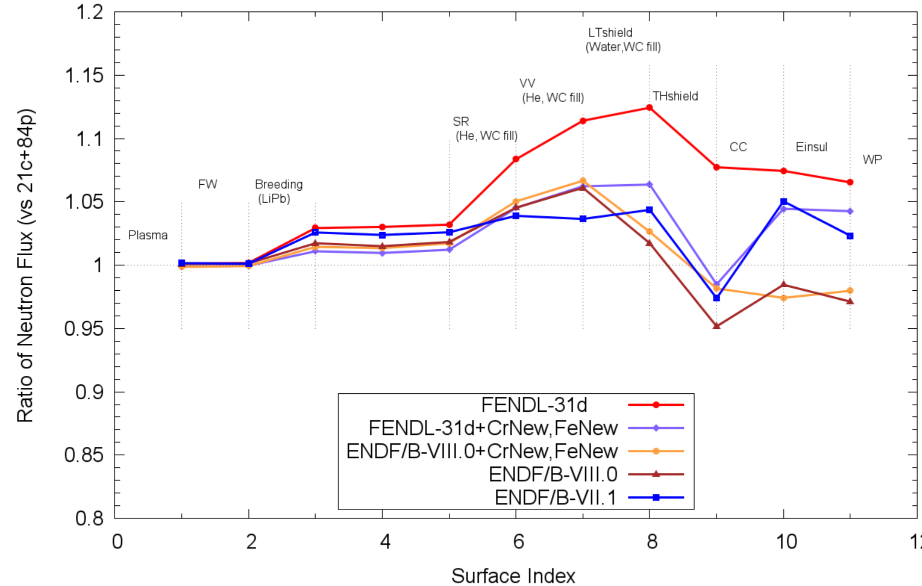
Other Work-FNSF Computational Benchmarking

➢Need to test on fusion designs other than ITER (different structural materials and tritium breeder)





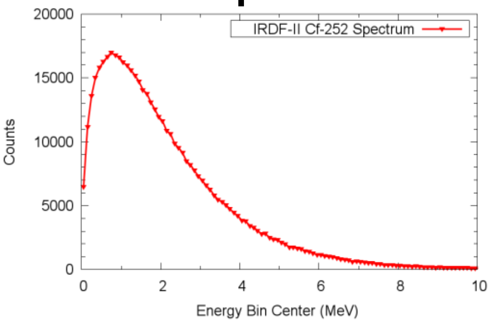
Neutron flux:

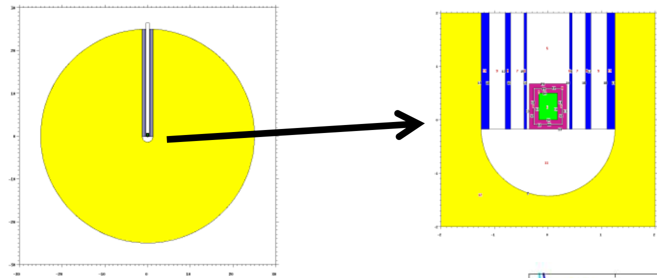


Nuclear heating at VV and Magnet coil case:

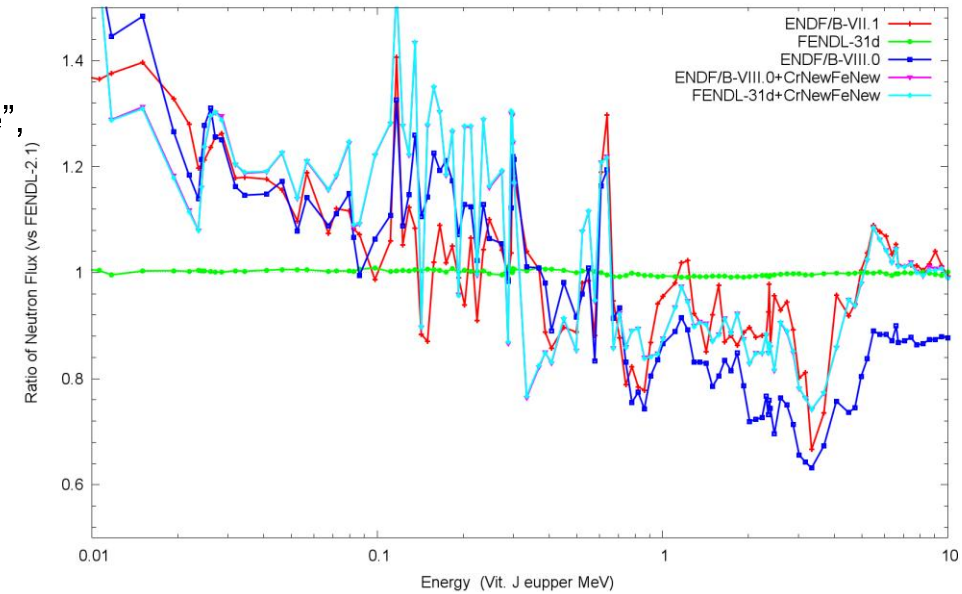
Library	IB VV (MW)	Ratio	IB Coil Case (MW)	Ratio
FENDL-2.1	1.7573E-01	1	7.1836E-05	1
ENDF/B-VIII.0	1.8418E-01	1.048	7.7464E-05	1.08
FENDL-3.1	1.8521E-01	1.054	8.1532E-05	1.14
ENDF/B-VII.1	1.8038E-01	1.026	7.7310E-05	1.08
E-VIII.0+CrNew,FeNew	1.8439E-01	1.049	7.7924E-05	1.09
F-3.1+CrNew,FeNew	1.8384E-01	1.046	7.8837E-05	1.10

➢ Encapsulated Cf-252 source in 25 cm iron sphere

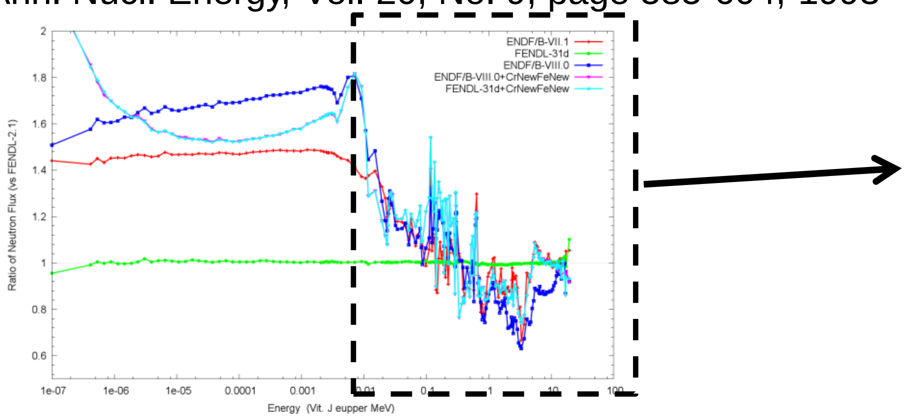




Yellow=iron (99.42 w/o Fe)
Blue=AlCu alloy (93.9 w/o Al)
Pink=SS304
Green=Cf



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

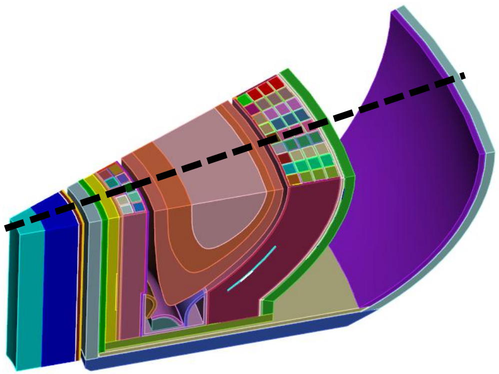


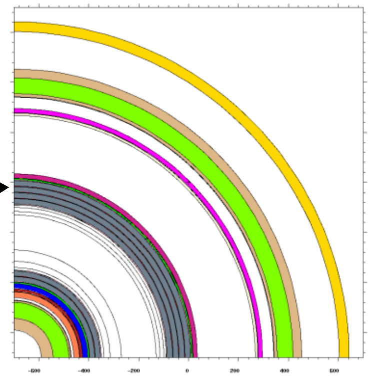
- With FENDL-3.1d, we see a close match to fluxes calculated with FENDL-2.1
- With ENDF/B-VIII.0, we see lowest fluxes in the E=1 to 10 MeV region vs. FENDL-2.1

➢ With new evaluations added, see results similar to FENDL-3.1 in E=1-10 MeV

Future Work

- ***Repeat previous calculations with updated O-16, O-17 XS***
- ***Create an FNSF-1D model:***
  - The current 3-D model is too computationally expensive for XS studies





- Currently 85 radial zones
- Includes SiC flow channel inserts in breeding zone
- Includes face plates for SR, VV, Ltshield
- MCNP materials created with PyNE

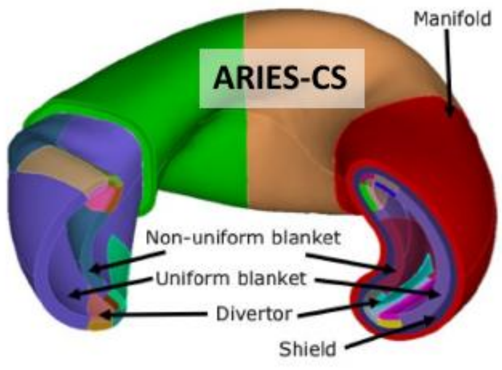
- ***Create an updated ITER-1D model:***
  - The current 1-D model is an early design so it needs to be updated to the current design

Questions?

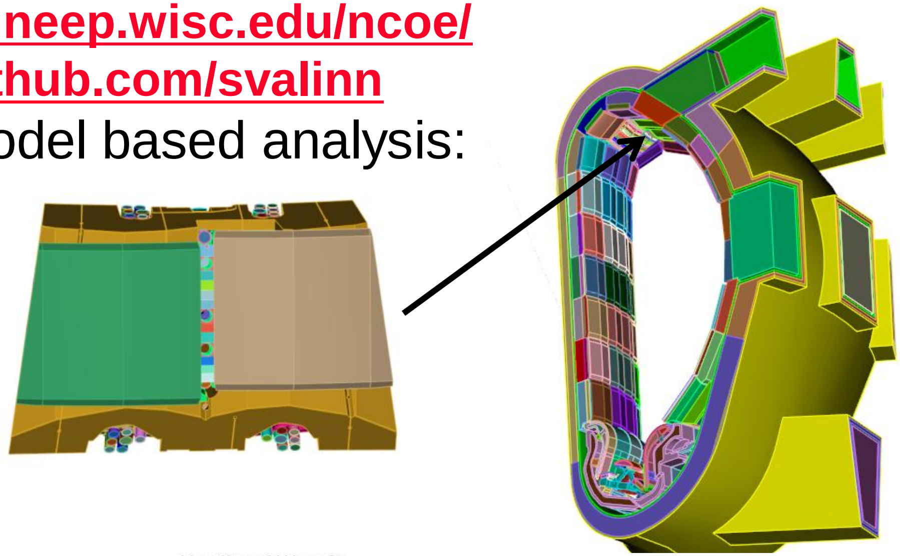
Backup slides

UW Neutronics Capabilities (3-D)

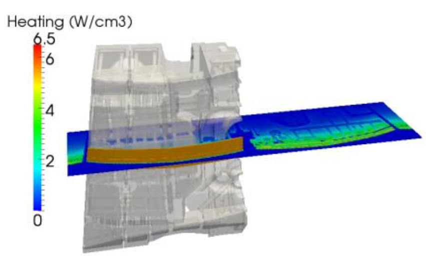
- DAGMC (detailed 3-D CAD based Monte Carlo transport)
  - Transports directly in the CAD model (not a translator)
  - Handles complex surfaces without simplification
  - Couples to MCNP, Geant4, FLUKA, SHIFT, OpenMC
  - Provides a common domain for coupling to other analysis
  - http://fti.neep.wisc.edu/ncoe/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

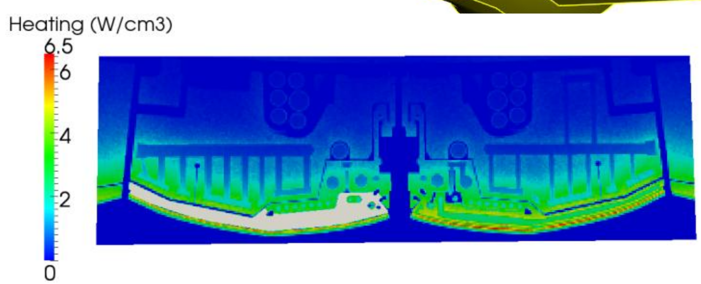


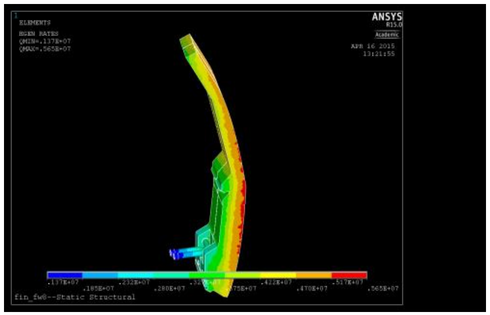
ITER BM08



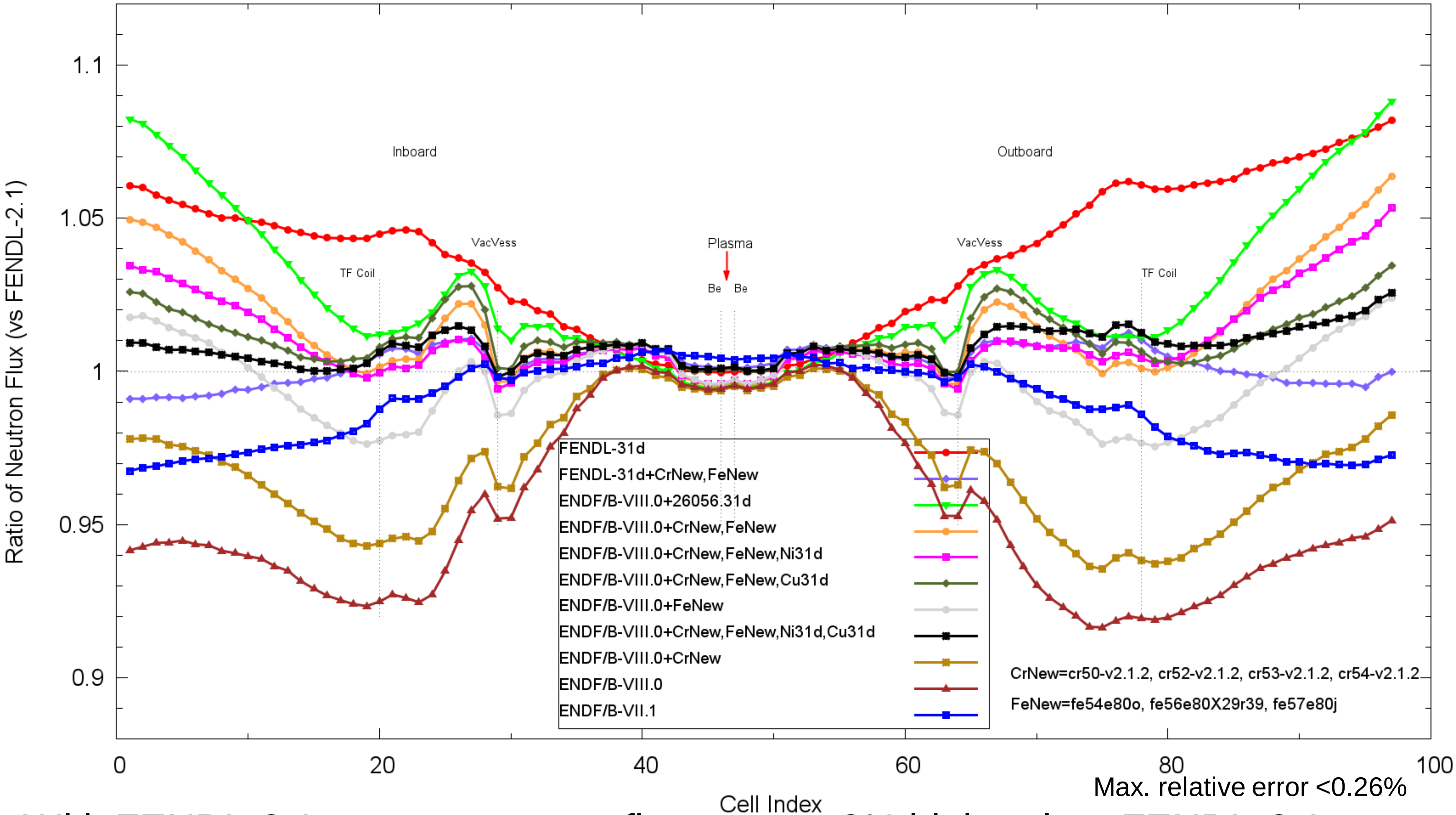
Nuclear heating mapped to ANSYS mesh for thermal analysis







ITER-1D Neutron Flux (isotopic substitution study)



- With FENDL-3.1, we see neutron fluxes up to 8% higher than FENDL-2.1
- With ENDF/B-VIII.0 we see neutron fluxes up to 8% lower than FENDL-2.1
- ENDF/B-VIII.0+CrNew,FeNew closer to FENDL-2.1 but see structure at VV, TFC
- FENDL-3.1+CrNew,FeNew quite close to FENDL-2.1 but structure at VV

ITER-1D Results: dpa (% difference vs. FENDL-2.1)

	FENDL-2.1	FENDL-3.1d	ENDF/B-VII.1	ENDF/B-VIII.0	FENDL-3.1d +CrNew,FeNew	ENDF/B-VIII.0 +CrNew,FeNew
IB						
FW Cu (Cu)	0	-0.32	0.22	-1.16	-0.26	-1.03
FW SS (Fe)	0	-0.07	5.58	0.15	-0.47	-0.37
VV Inc. (Ni)	0	3.03	0.09	-7.96	0.22	-2.24
VV SS (Fe)	0	2.74	3.25	-3.69	1.52	1.66
Mag. (Cu)	0	4.52	-1.01	-8.96	1.04	-1.47
OB						
FW Cu (Cu)	0	-0.28	0.14	-1.04	-0.23	-0.94
FW SS (Fe)	0	-0.03	5.66	0.10	-0.49	-0.40
VV Inc. (Ni)	0	3.07	0.04	-7.95	0.19	-2.33
VV SS (Fe)	0	2.82	3.28	-3.44	1.57	1.76
Mag. (Cu)	0	6.30	-1.17	-9.27	1.60	-1.14

Max. relative error <0.15%

- different neutron flux and spectrum at FWSS, VV, magnet
- dpa values higher for FENDL-3.1d than FENDL-2.1 (up to 6%)
- dpa values lower for ENDF/B-VIII.0 than FENDL-2.1 (up to 9%)

➢ With the new evaluations for Cr and Fe, dpa values within 2.4%

ITER-1D Results: He production (% diff. vs. FENDL-2.1)

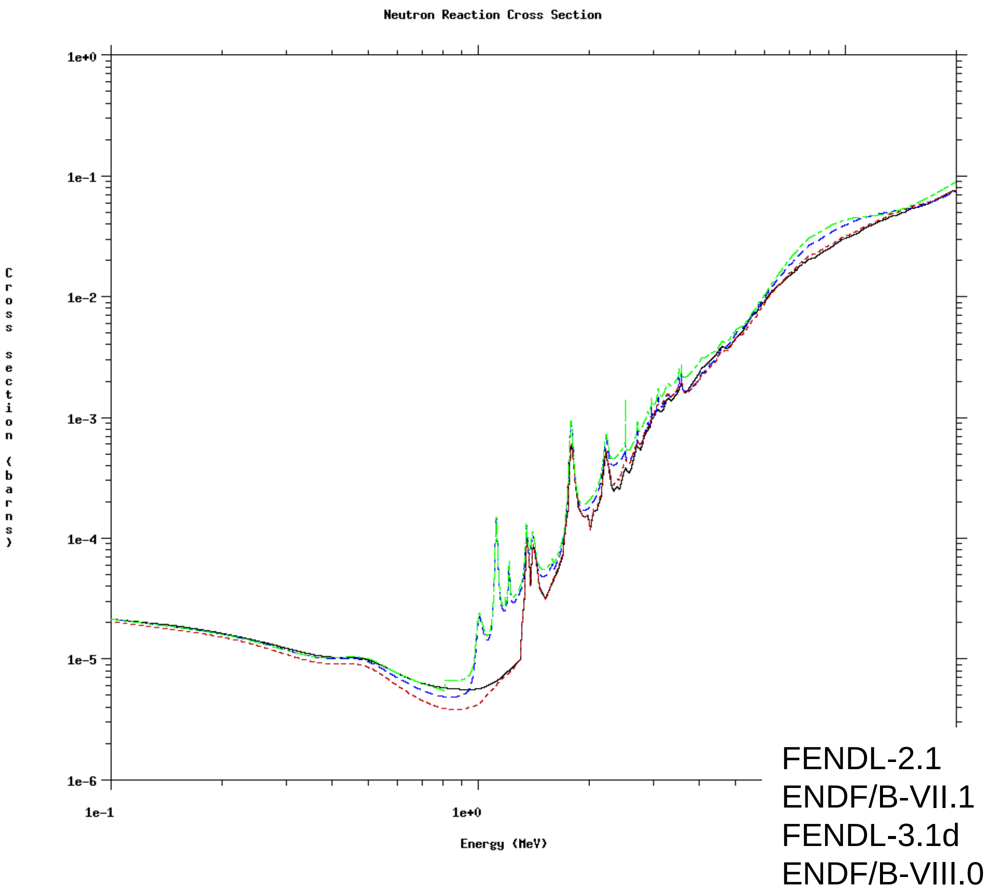
	FENDL-2.1	FENDL-3.1d	ENDF/B-VII.1	ENDF/B-VIII.0	FENDL-3.1d +CrNew,FeNew	ENDF/B-VIII.0 +CrNew,FeNew
IB						
FW Be	0	0.04	0.60	0.80	0.08	0.92
FW CuBeNi	0	0.39	0.91	3.70	0.49	3.84
FW SS316	0	4.24	6.37	6.16	13.00	10.30
VV Inconel	0	17.96	13.58	6.84	19.41	15.28
VV SS316	0	8.06	4.52	1.26	11.28	8.75
Mag. (Cu)	0	5.02	-0.20	-1.17	1.91	4.95
OB						
FW Be	0	0.07	0.50	0.90	0.12	0.99
FW CuBeNi	0	0.47	0.87	3.75	0.54	3.85
FW SS316	0	4.41	7.09	6.98	14.16	11.62
VV Inconel	0	17.98	13.51	6.96	19.33	15.33
VV SS316	0	8.07	4.61	1.49	11.29	8.71
Mag. (Cu)	0	6.86	-0.62	-1.52	2.55	5.72

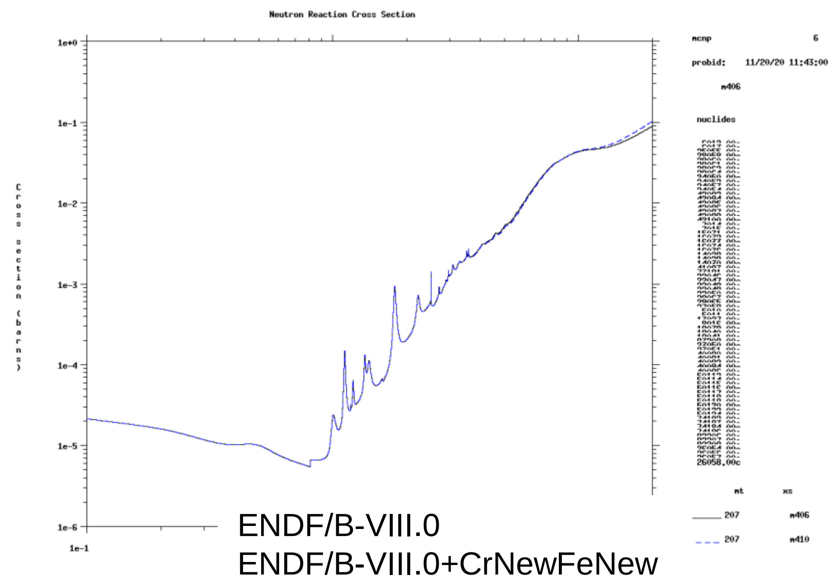
Max. relative error <0.19%

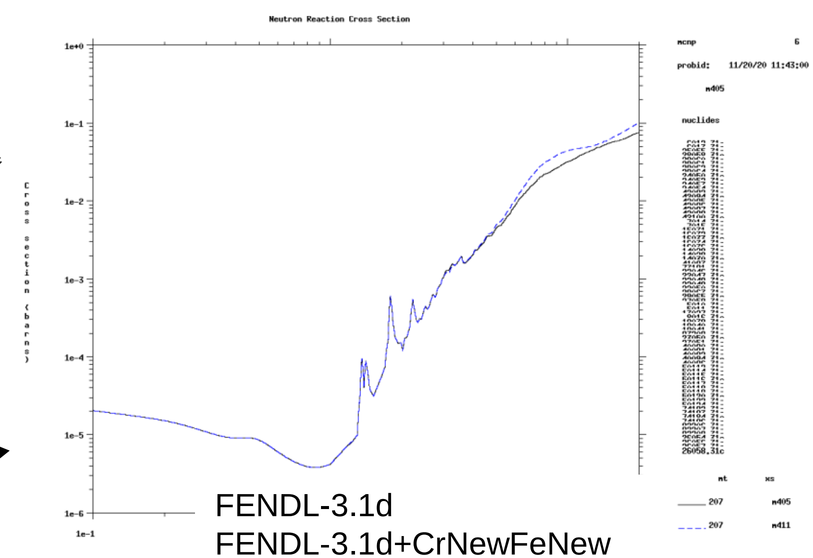
- He production values higher for FENDL-3.1d than FENDL-2.1 (up to 18%)
- He production values higher for ENDF/B-VIII.0 than FENDL-2.1 (up to 7%) except magnet (lower)

➢ Libraries with the new Cr and Fe evaluations:
  - He production up to 19% higher in VV Inconel than FENDL-2.1
  - He production 9-14% higher in SS316

He production XS (mt 207) SS-316 L(N)-IG (17.5 w/o Cr)

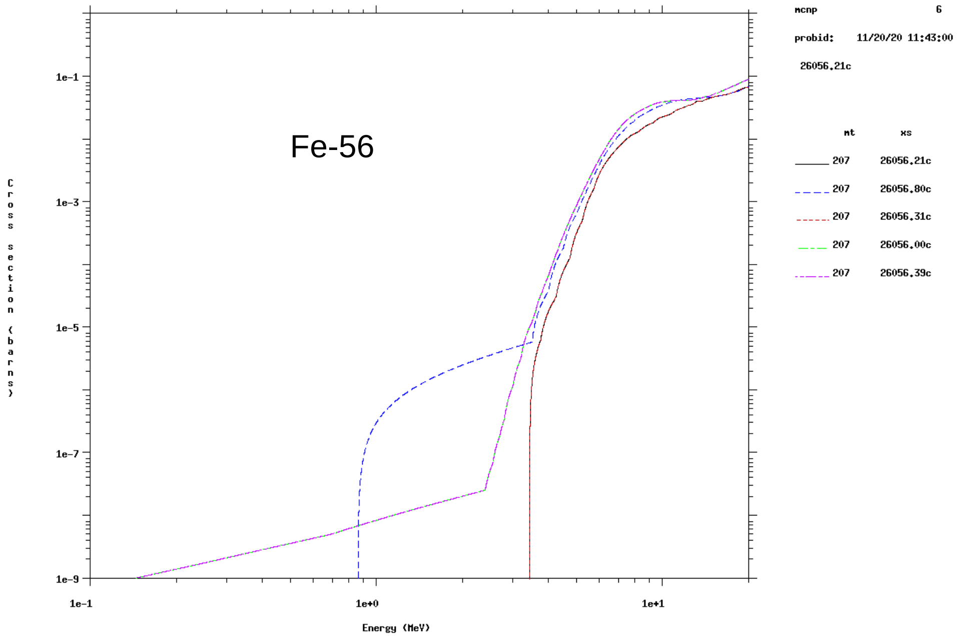


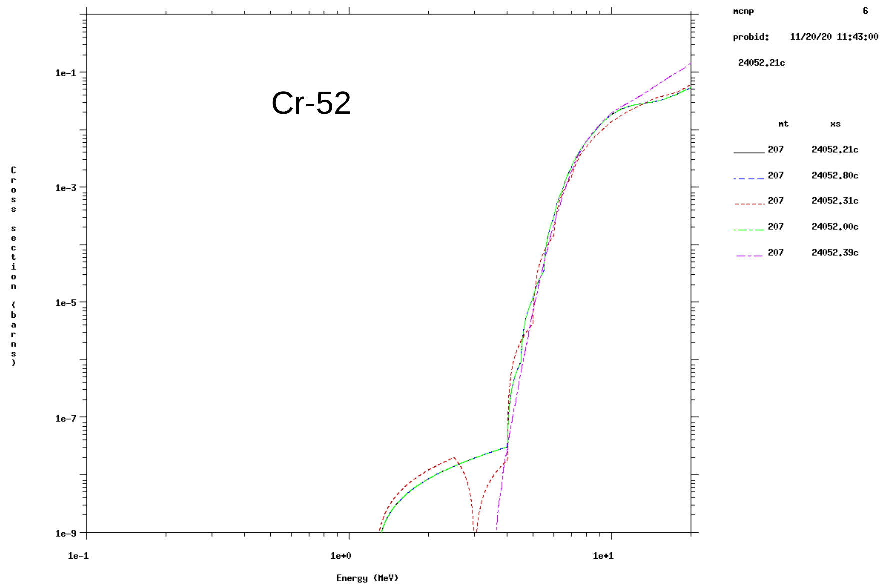


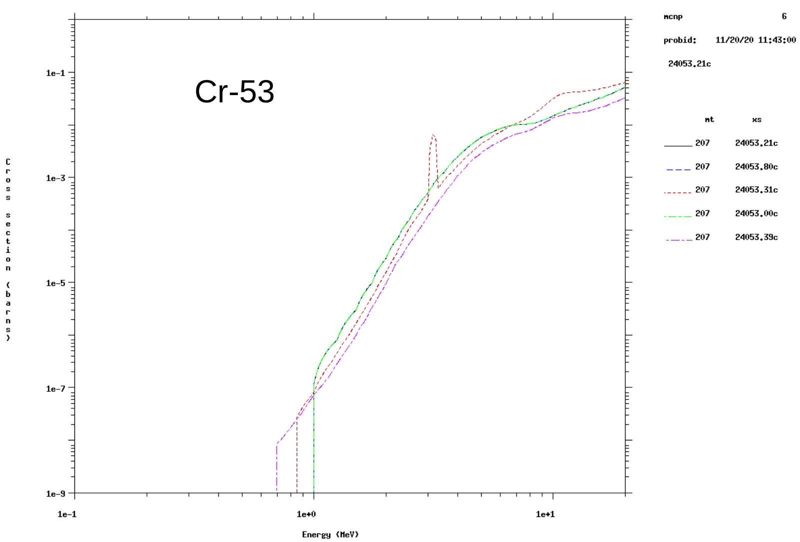


- He production XS for new evaluations higher near 10 MeV

He production XS (mt 207) Cr and Fe





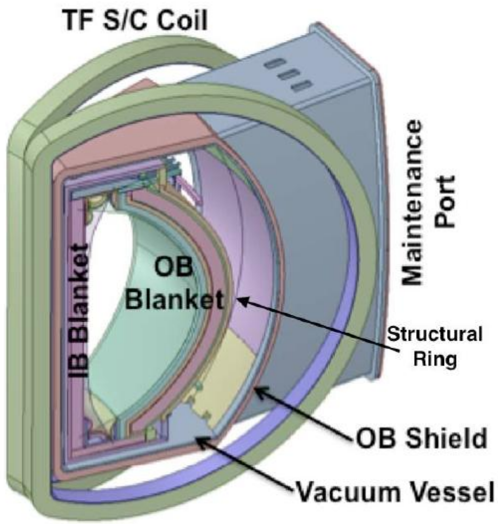


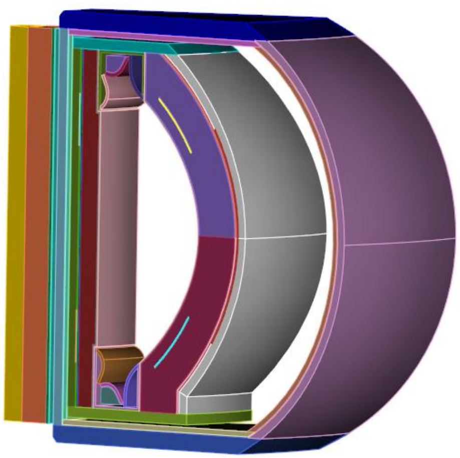
21c=FENDL-2.1
31c=FENDL-3.1d
80c=ENDF/B-VII.1
00c=ENDF/B-VIII.0
39c=New Evaluation

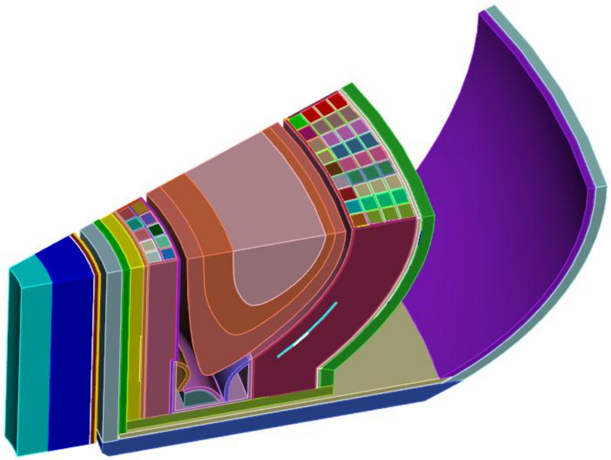
- ➢He production XS for FENDL-2.1 and ENDF/B-VII.1 are overlapping

3-D FNSF Model

- U.S. Fusion Nuclear Science Facility (step to DEMO)
- Single sector (22.5 deg.) neutronics model:
  - No ports, 2 cm straight gaps between sectors
  - 518 MW fusion power, 3 region plasma source model
  - PbLi breeding region detailed, other components partially homogenized
- ***Calculations run with DAG-MCNP6.2***

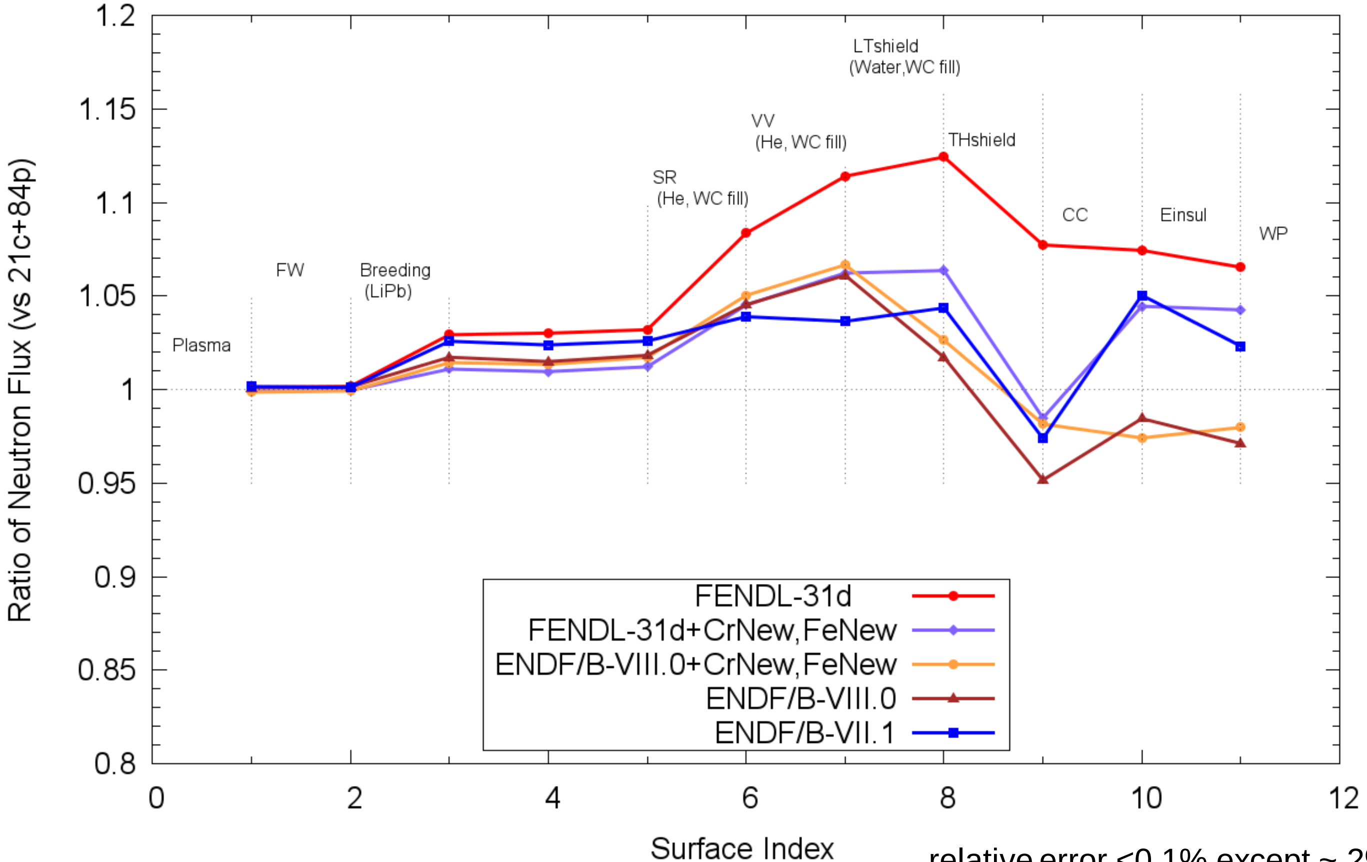






A. Davis et al. "Neutronics aspects of the FESS-FNSF", *Fusion Engineering and Design*, 2017.
T. Bohm et al. "Initial Neutronics Investigation of a Liquid Metal Plasma Facing Fusion Nuclear Science Facility, *Fusion Science and Technology*, 2019.

FNSF Results- IB neutron flux



relative error <0.1% except ~ 2% at TH shield-WP

- With FENDL-3.1 neutron library see neutron fluxes up to 12% higher than FENDL-2.1
- With ENDF/B-VIII.0 we see neutron fluxes 5% lower at coil case
  - ➢ Adding the new Cr and Fe evaluations brings neutron fluxes closer to FENDL-2.1
  - ➢ These trends are similar to what was seen in the ITER-1D model

FNSF Results-total nuclear heating

Library	IB VV (MW)	Ratio	IB Coil Case (MW)	Ratio
FENDL-2.1	1.7573E-01	1	7.1836E-05	1
ENDF/B-VIII.0	1.8418E-01	1.048	7.7464E-05	1.08
FENDL-3.1	1.8521E-01	1.054	8.1532E-05	1.14
ENDF/B-VII.1	1.8038E-01	1.026	7.7310E-05	1.08
E-VIII.0+CrNew,FeNew	1.8439E-01	1.049	7.7924E-05	1.09
F-3.1+CrNew,FeNew	1.8384E-01	1.046	7.8837E-05	1.10

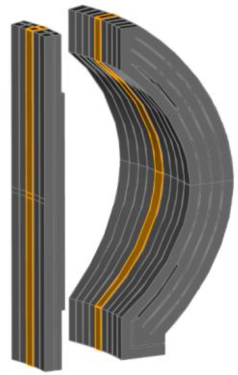
VV is 3CrFS, WC filler, He cooled
Magnet Coil Case is SS316

VV relative error <0.03%
Coil Case relative error <1.3%

- At the VV, heating values are ~5% higher than FENDL-2.1 for all libraries except ENDF/B-VII.1 (~3%)
- At the CC, heating values are 8-14% higher as compared to FENDL-2.1
- This is different than seen with the ITER-1D model (tended to be lower than FENDL-2.1)

Results-Tritium Breeding Ratio

- FNSF uses PbLi for breeding:
  - 84.3 atomic% Pb
  - 15.7 atomic% Li (enriched to 90% Li-6)



Library	IB TBR	Ratio	OB TBR	Ratio
FENDL-2.1	0.2961	1	0.8135	1
ENDF/B-VIII.0	0.3003	1.014	0.8265	1.016
FENDL-3.1	0.3000	1.013	0.8274	1.017
ENDF/B-VII.1	0.2997	1.012	0.8241	1.013
E-VIII.0+CrNew,FeNew	0.2987	1.009	0.8235	1.012
F-3.1+CrNew,FeNew	0.2986	1.008	0.8239	1.013

Max. relative error <0.01%

- We see TBR ~1-1.7% higher than that calculated with FENDL-2.1

FNSF Results-Fe dpa (ratio)

Library	IB FW	IB VV
FENDL-2.1	1	1
ENDF/B-VIII.0	1.010	1.060
FENDL-3.1	1.001	1.092
ENDF/B-VII.1	1.060	1.092
E-VIII.0+CrNew,FeNew	1.008	1.083
F-3.1+CrNew,FeNew	1.003	1.083

FW is MF82H (7.5 w/o Cr), VV is 3CrFS (3 w/o Cr)

VV relative error <0.27%

- At the FW, dpa values are very close except for ENDF/B-VII.1
- At the VV, dpa values are 6-9% higher for all libraries compared to FENDL-2.1

➢ With the new evaluations for Cr and Fe:

  - Fe dpa values are close at the FW
  - Fe dpa values are 8% higher at the VV

FNSF Results-He production (ratio)

Library	IB FW	IB VV
FENDL-2.1	1	1
ENDF/B-VIII.0	1.093	1.120
FENDL-3.1	1.006	1.002
ENDF/B-VII.1	1.075	1.093
E-VIII.0+CrNew,FeNew	1.127	1.137
F-3.1+CrNew,FeNew	1.135	1.151

FW is MF82H (7.5 w/o Cr), VV is 3CrFS (3 w/o Cr)

VV relative error <0.27%

- At the FW, He production values are similar for FENDL-3.1d but the others are 8-14% higher
- At the VV, He production values are similar for FENDL-3.1d but the others are 9-15% higher

➢ With the new evaluations for Cr and Fe, He production is 13-15% higher