Impact of latest INDEN Cross sections in Fusion Applications and Update of the Fusion Evaluated Nuclear Data Library (FENDL)

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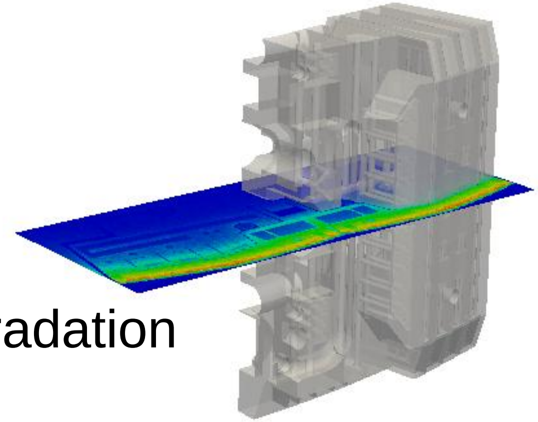
National Nuclear Data Week 2023
CSEWG Validation Session, 16 November, 2023

Outline

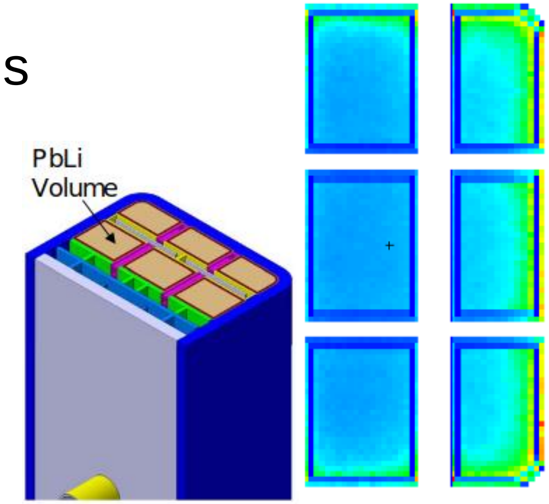
1) Introduction
   - Neutron libraries examined
   - Computational models used
2) Impact of latest INDEN Fe-56 XS
   - ITER 1-D
   - FNSF 1-D
3) Impact of latest INDEN Cu-63,65
   - ITER 1-D
4) Impact of latest INDEN F-19 XS
   - FNSF FLIBE 1-D
5) FENDL Updates

Important Fusion Neutronics Responses

- Neutron flux/fluence (**neutron**)
  - structure, magnets
- Radiation damage/dpa & transmutation products (**neutron**)
  - structural material degradation, magnet degradation
- Hydrogen/Helium production (**neutron**)
  - structural material degradation, re-weldability
- Tritium production (**neutron**)
  - breeding for D-T reactors, 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 (avoid "high" level waste)



ITER Shield Block



ITER DCLL TBM

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:*
    1. FENDL-2.1 (21c)
    2. FENDL-3.1d (31c)
    3. FENDL-3.2b (32c)
    4. ENDF/B-VIII.0 (00c)
    5. New INDEN evaluations for Fe-56, F-19, Cu-63,65
  - *Photon:*
    1. mcplib84 (84p)**

standard MCNP id

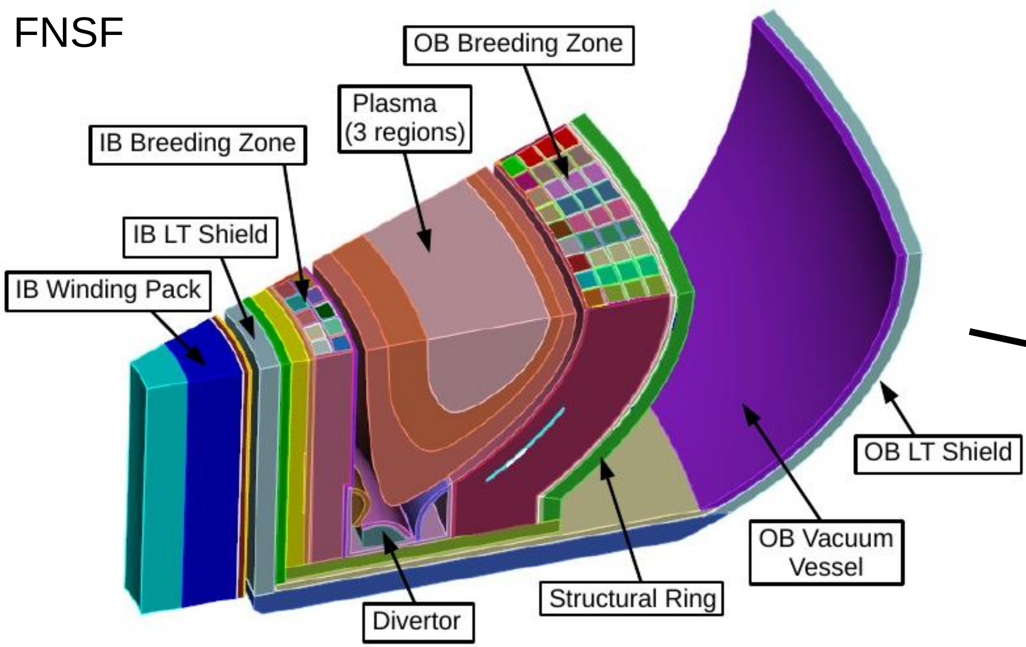
New work

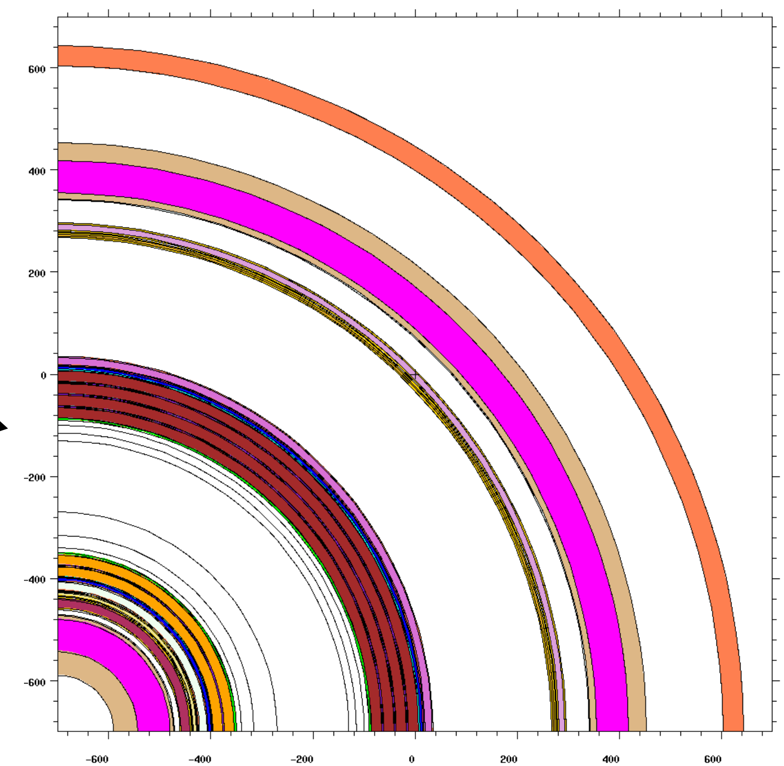
> *Previous work has shown that mcplib84 produces results similar to the newer MCNP eprdata12 library, the latest MCNP photon library (eprdata14) has not been tested yet*

** Bohm T.D, Sawan M.E. "Neutronics calculations to support the Fusion Evaluated Nuclear Data Library (FENDL)", Fusion Science and Technology, Vol 77, p. 813-828, 2021.*
***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.*

1-D Cylindrical Computational Benchmark Models

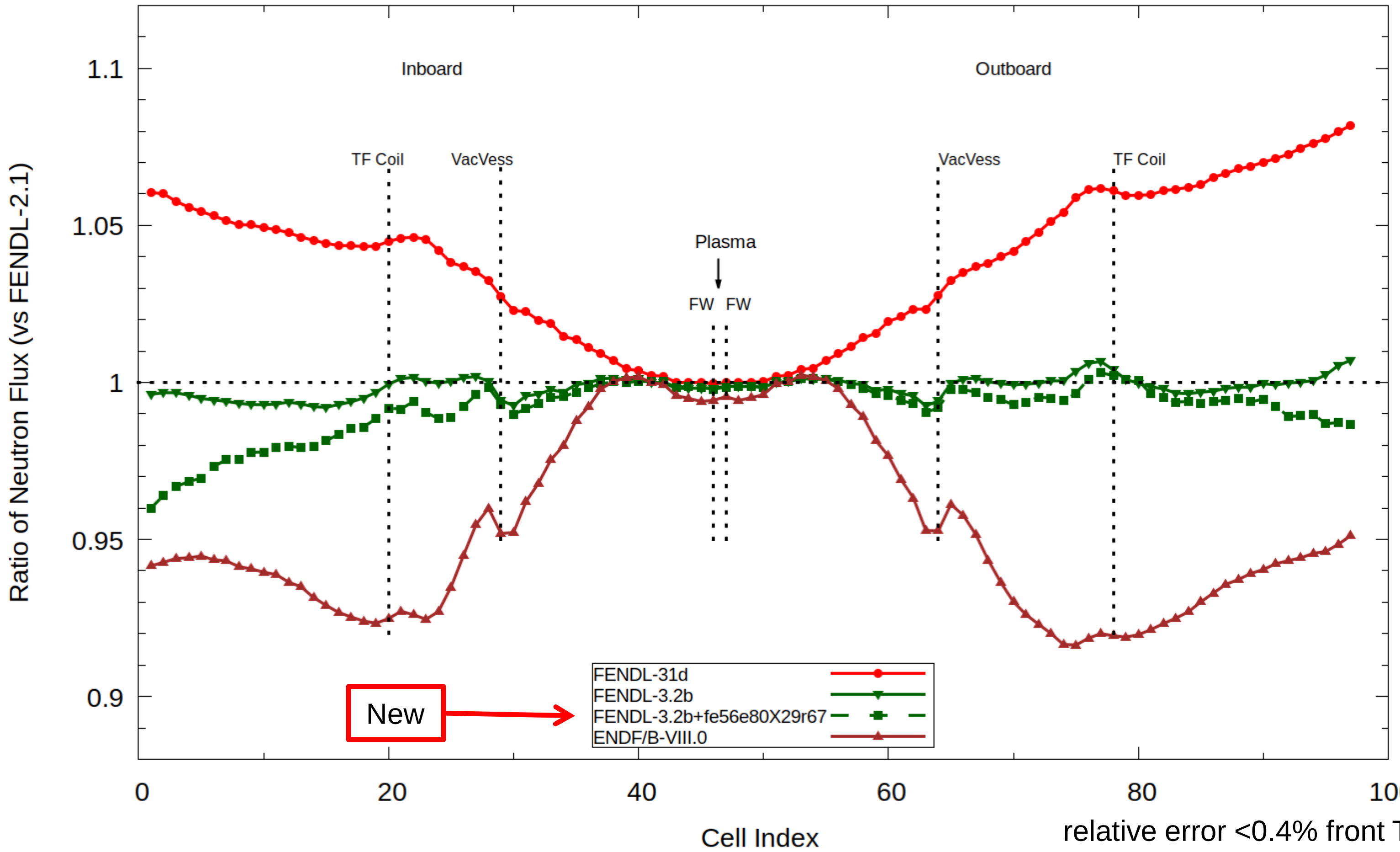
1. FNSF- *Fusion Energy Systems Studies Fusion Nuclear Science Facility*
   - **Coolant:** He gas, **structure:** RAFM steel, **blanket:** PbLi, **shielding filler:** WC, borated steel
2. FNSF FLIBE- *FNSF with a 2(LiF)-1(BeF$_2$) blanket*
   - **Coolant:** He gas, **structure:** RAFM steel, **blanket:** flibe, **shielding filler:** WC, borated steel
3. ITER- *Early ITER design*
   - **Coolant:** water, **structure: SS-316**, **blanket:** none, **shielding filler:** borated steel





T. Bohm et al. "Initial Neutronics Investigation of a Liquid Metal Plasma Facing Fusion Nuclear Science Facility, *Fusion Science and Technology*, 2019.

Fe-56 Preliminary Results: Neutron Flux ITER

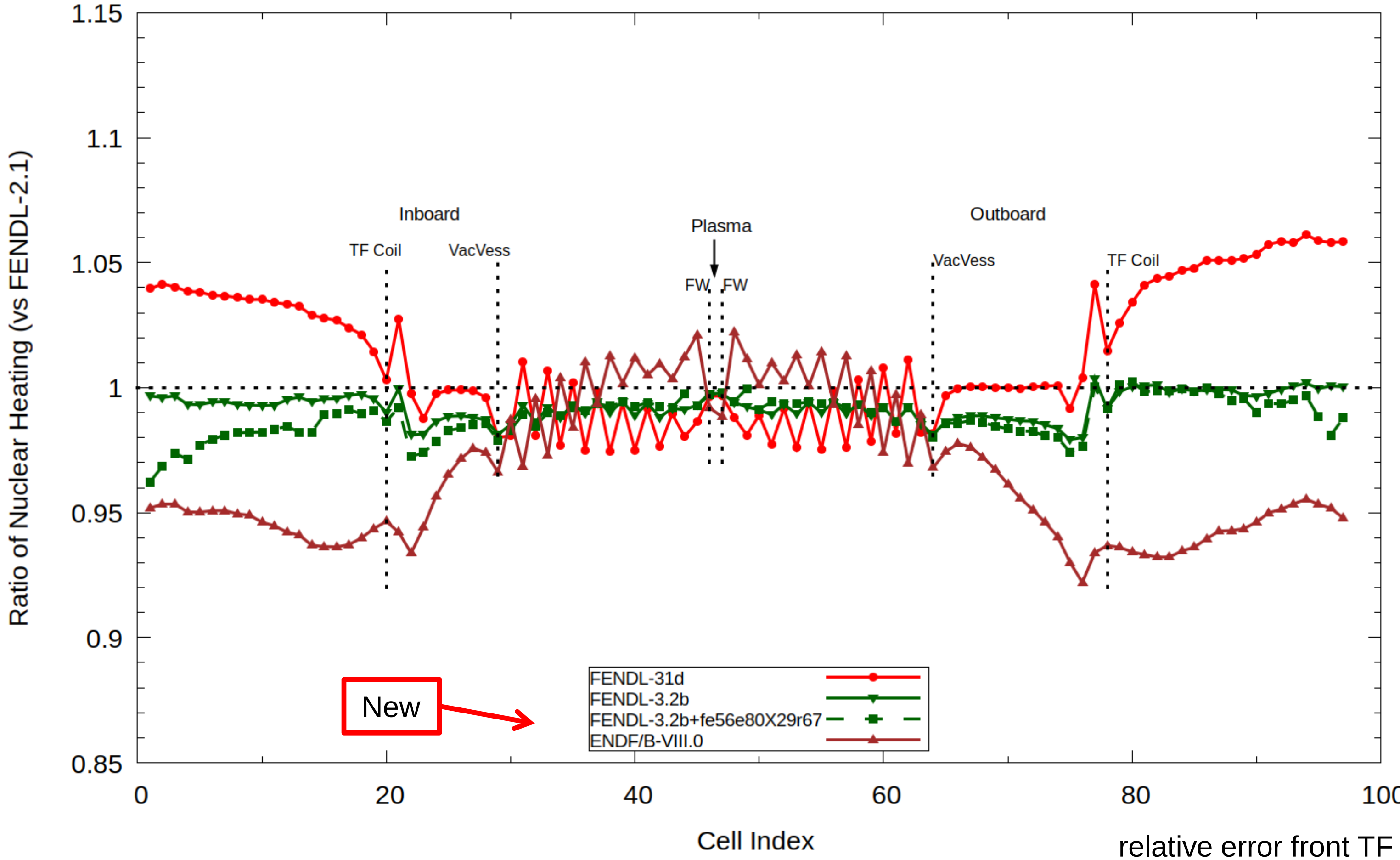


relative error <0.4% front TF coil

- FENDL-3.2b and FENDL-3.2b+fe56e80X29r67 are quite close to each other

note: FENDL-3.2b uses fe56e80X29r48

Fe-56 Preliminary Results: Total Nuclear Heating ITER

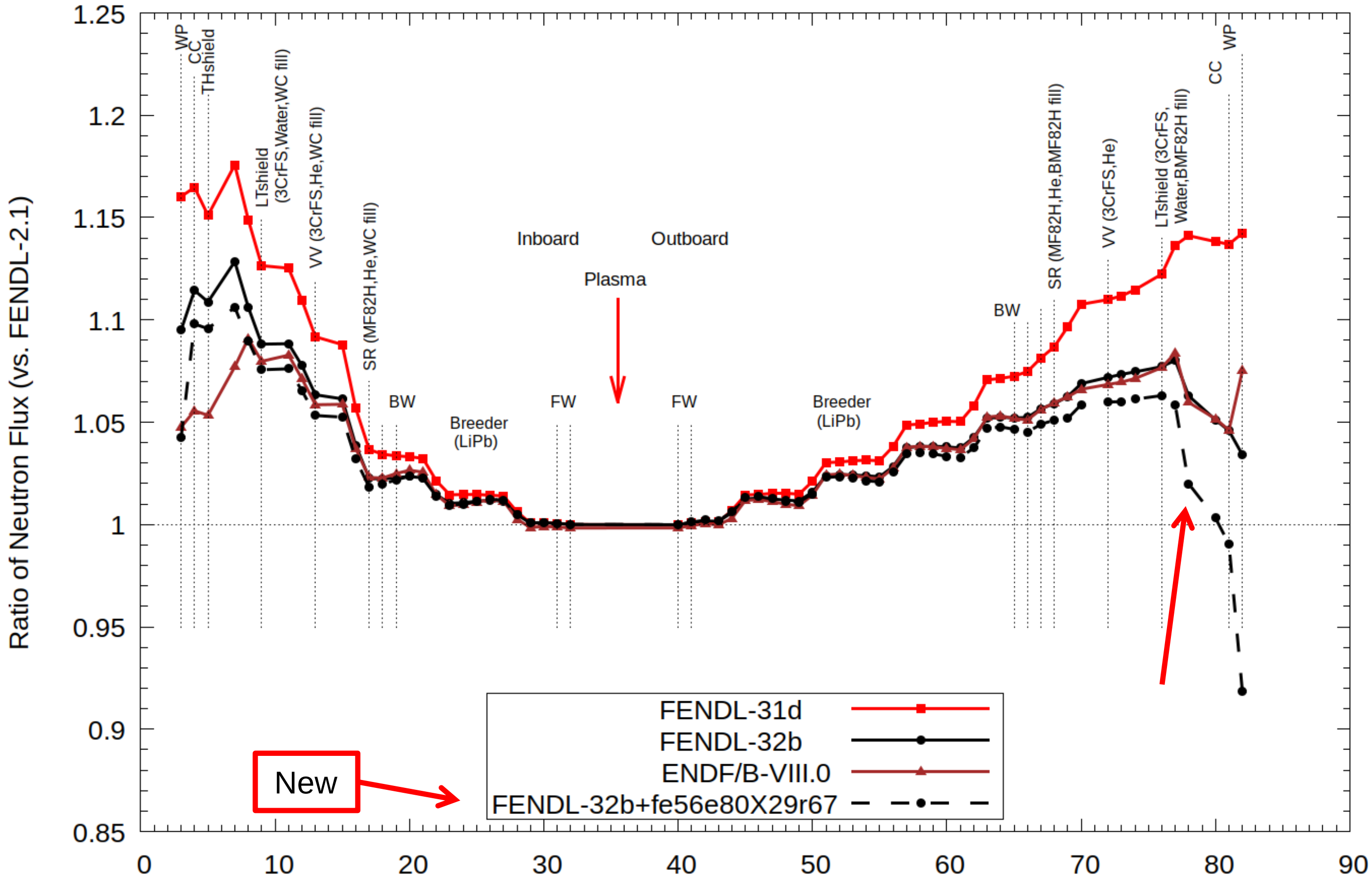


relative error front TF coil <0.4%

➢FENDL-3.2b and FENDL-3.2b+f56e80X29r67 are quite close to each other

note: FENDL-3.2b uses fe56e80X29r48

Fe-56 Preliminary Results: Neutron Flux FNSF



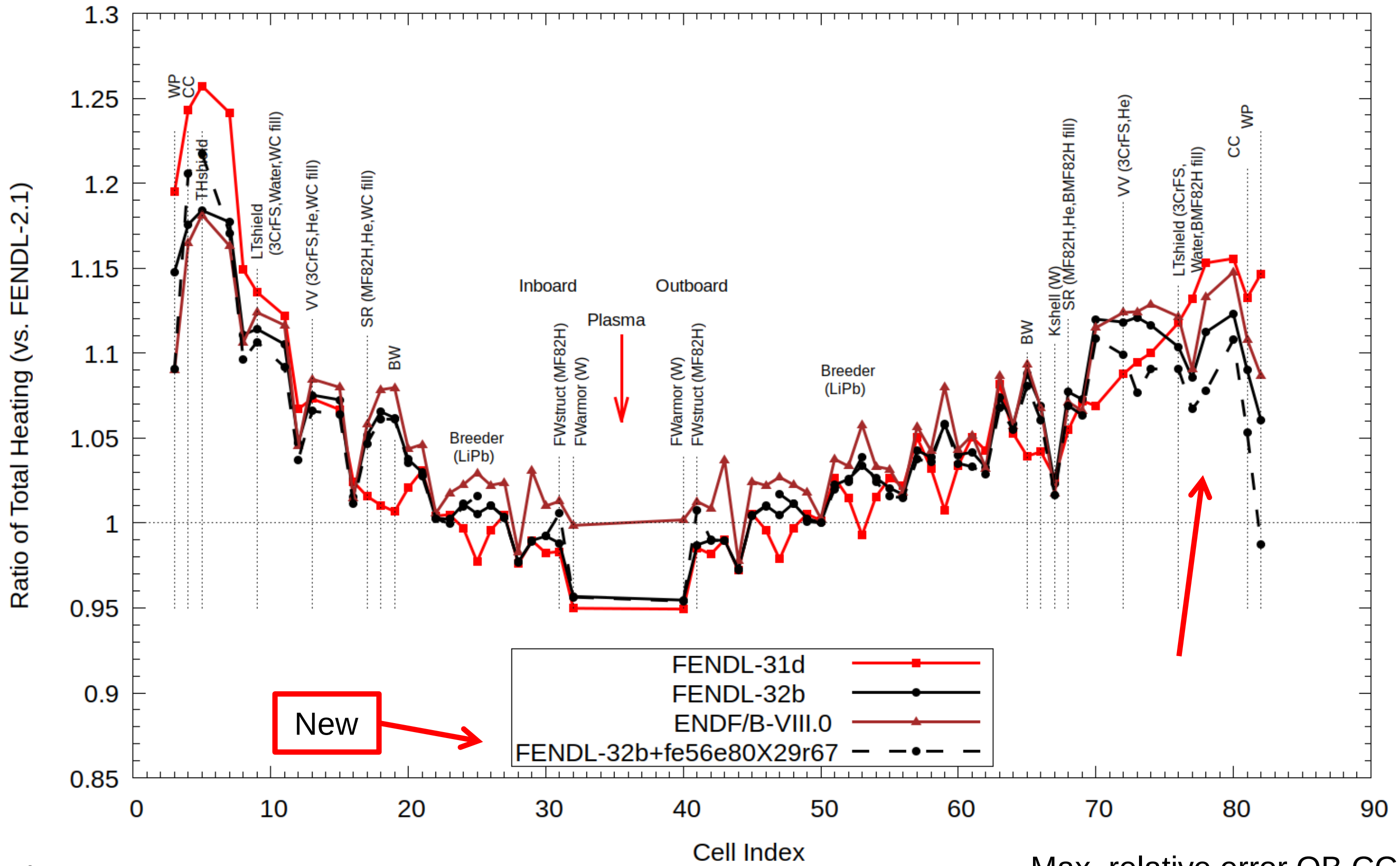
Max. relative error IB CC, WP 3-5%

Max. relative error OB CC, WP 1-2%

- FENDL-3.2b vs. FENDL-3.2b+fe56e80X29r67 in generally good agreement with each other *except deviation at OB LTshield*
    - OB LTshield uses a thick water cooled borated steel filler

note: FENDL-3.2b uses fe56e80X29r48

Fe-56 Preliminary Results: Total Nuclear Heating FNSF



Max. relative error IB CC, WP 3-5%

Max. relative error OB CC, WP 1-2%

- FENDL-3.2b vs. FENDL-3.2b+fe56e80X29r67 in generally good agreement
- Not seeing deviation at OB LTshield as observed with neutron flux
    - need to refine statistics at deep locations

➢ **Also:** generally **good agreement** observed for **TBR, dpa, helium production**

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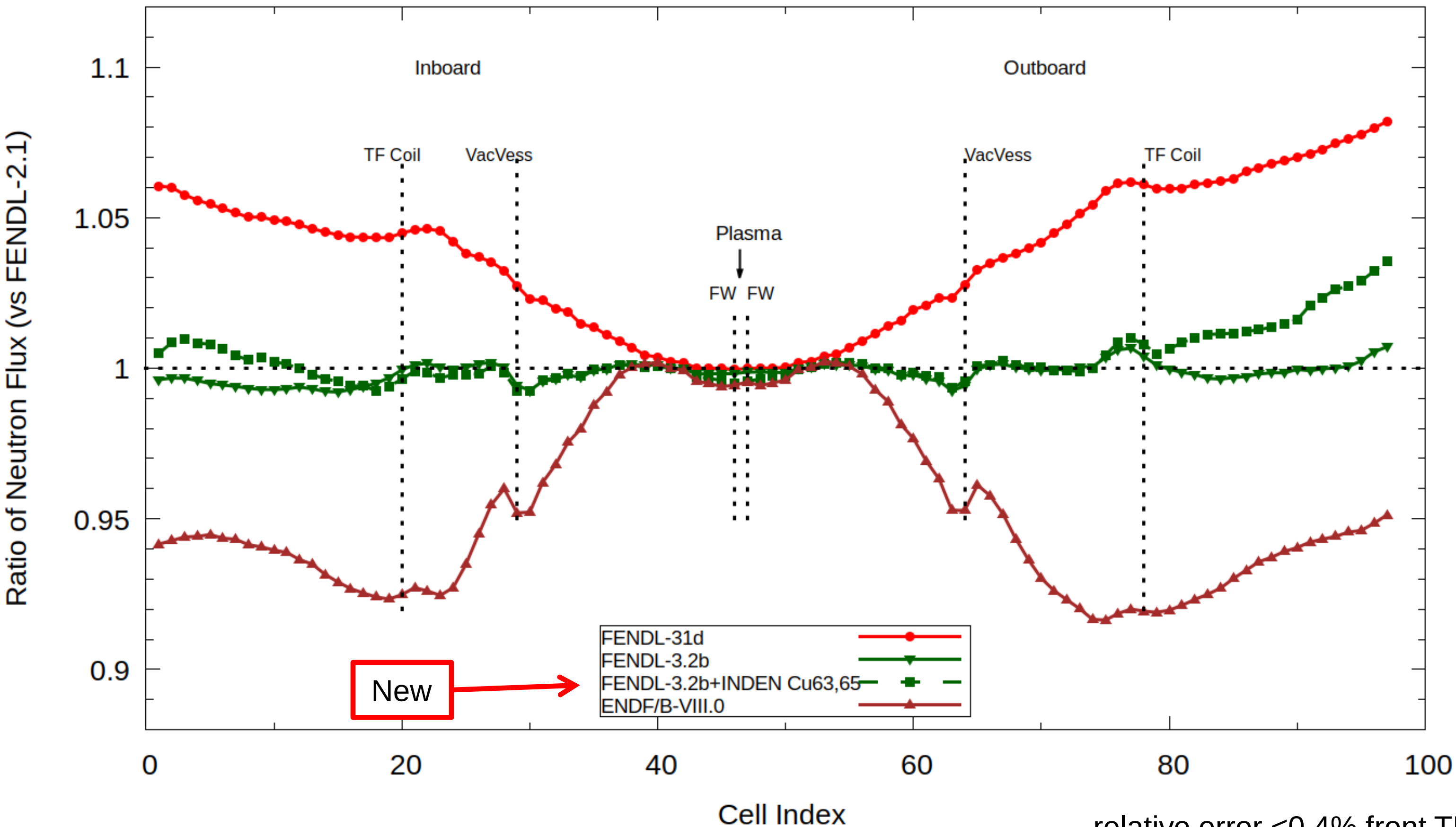
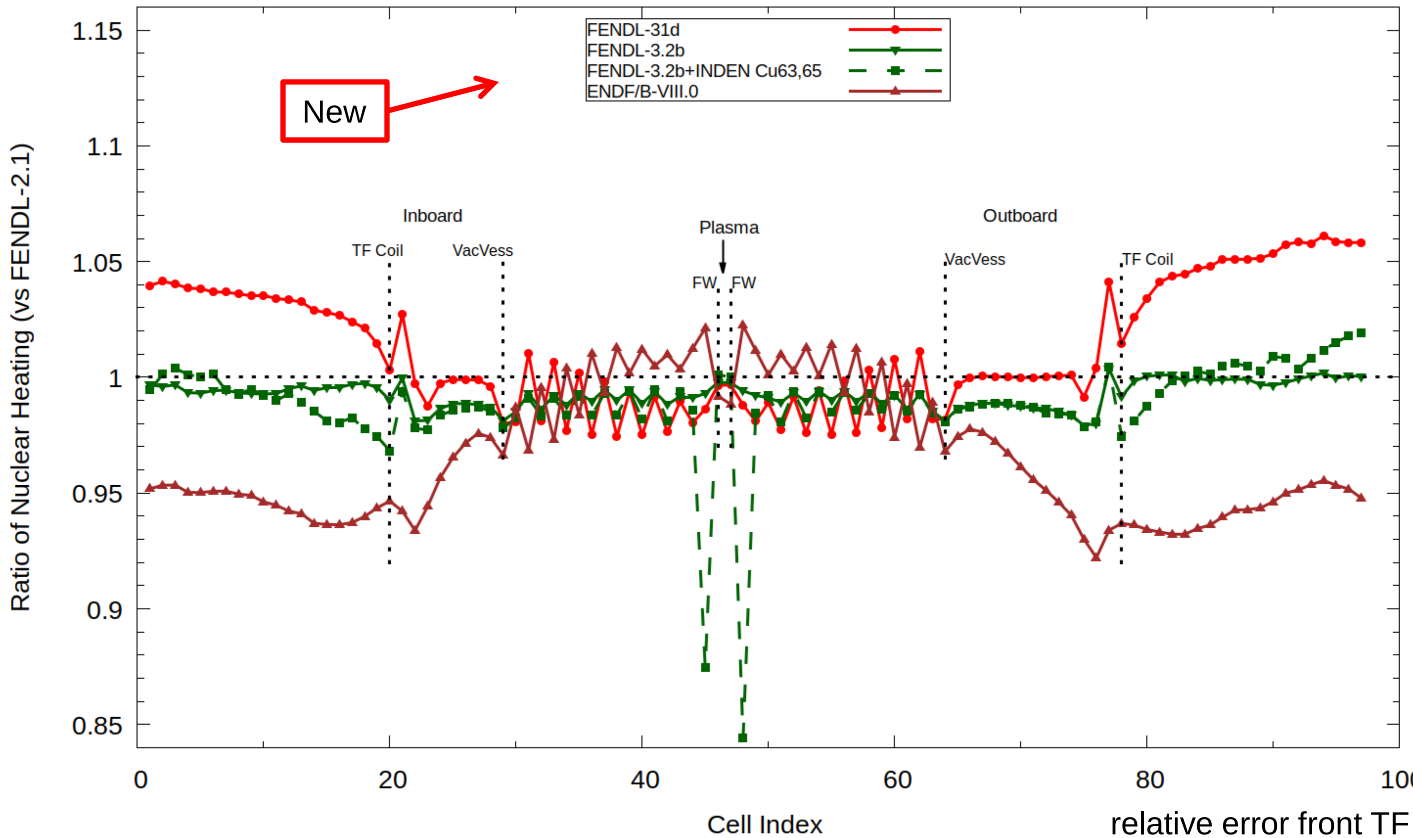
Cu-63,65 Preliminary Results: Neutron Flux ITER



relative error <0.4% front TF coil

- FENDL-3.2b and FENDL-3.2b +cu63ane6k09aRR +cu65ane5k05 are quite close to each other
- see some deviation deep in TF coil (contains substantial copper)

Cu-63,65 Preliminary Results: Total Nuclear Heating ITER



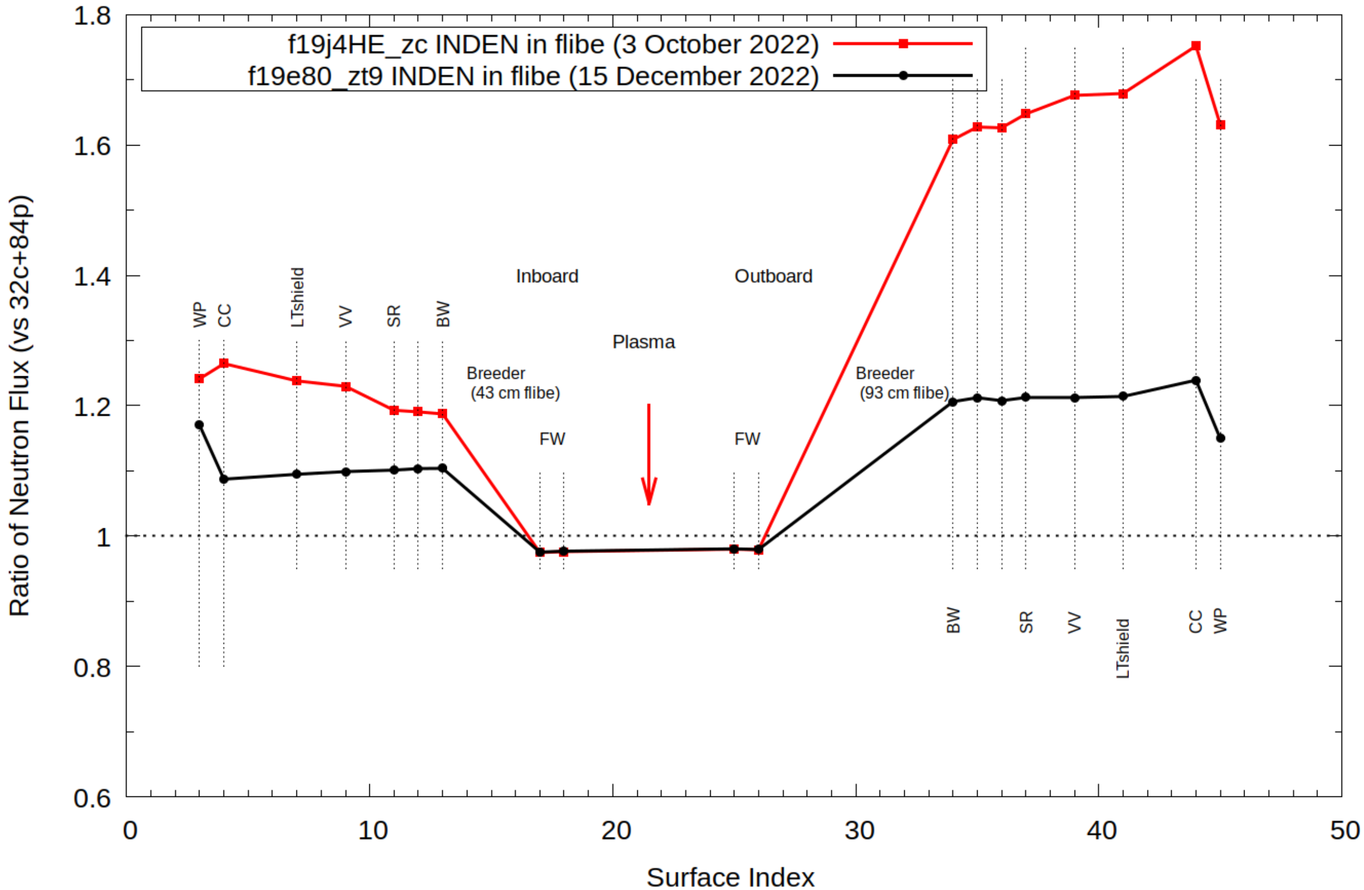
relative error front TF coil <0.4%

➢FENDL-3.2b vs. FENDL-3.2b +cu63ane6k09aRR +cu65ane5k05 we see up to 15% difference in Cu layer (near cell 45 and 48)

- **Due to neutron heating numbers being 0**

- **Other issues: missing mt 444 (dpa), missing mt 203-207 (total h, d, t, He production)**

F-19 Results: Neutron Flux FNSF FLIBE

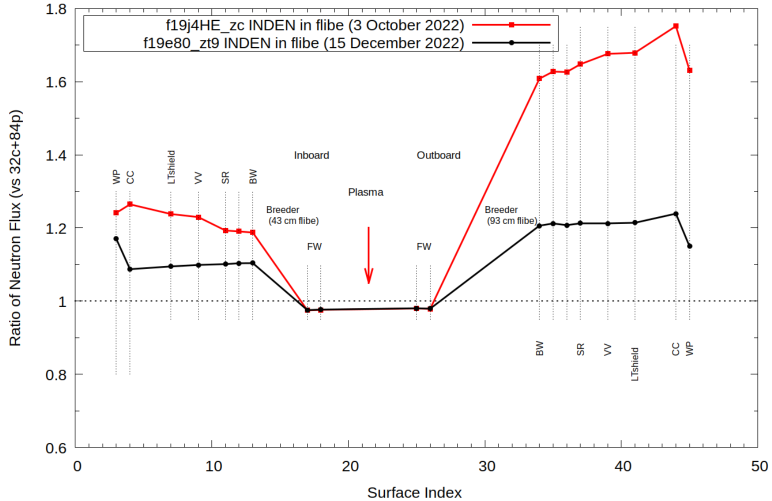


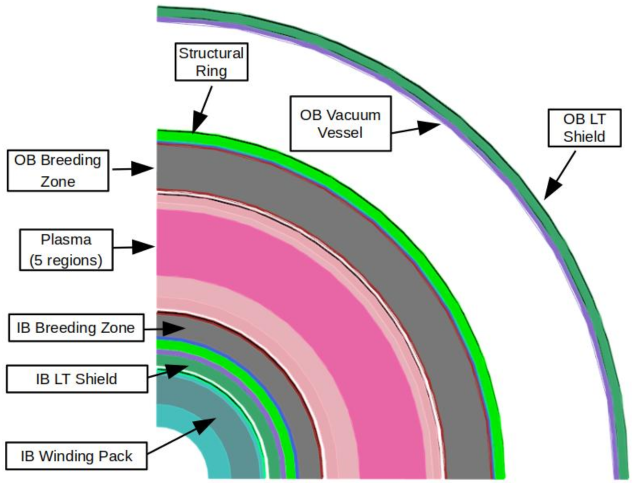
Max. relative error <0.6% except CC <2.5% and WP 3.6%

- **Neutron flux:** higher neutron fluxes behind the flibe breeder vs. FENDL-3.2b
    - ➢ 10-20% higher flux behind the IB flibe breeder zone
    - ➢ 20-70% higher flux behind the OB flibe breeder zone

F-19 Possible Impact on Reactor Design: FNSF FLIBE Model

- For this 1-D model, the e-fold attenuation distance for neutron flux in the SR shield (MF82H face plates + He cooled WC filler) was 14 cm
  - ➢ **Added shielding required to compensate for f19j4HE_zc:**
    - **IB: 3 cm**
    - **OB: 17 cm**





Note: a candidate Commonwealth Fusion Systems flibe immersion blanket design has ~25 cm thick IB blanket and 110 cm thick OB blanket

F-19 Results: TBR FNSF FLIBE Model

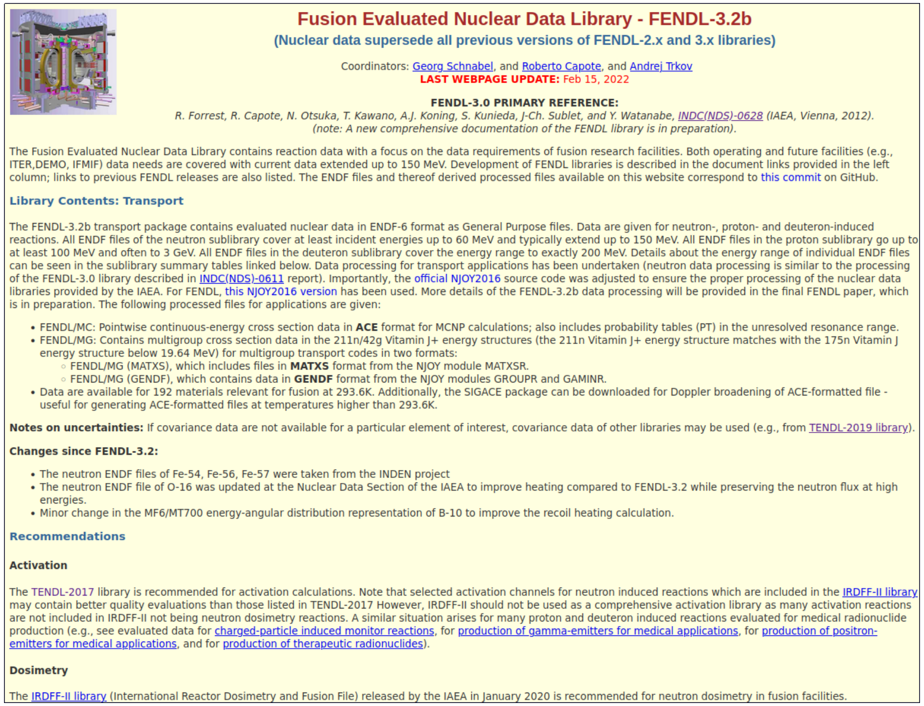
Region	FENDL-3.2b	FENDL-3.2b +INDEN f19j4HE_zc	Ratio	FENDL-3.2b +INDEN f19e80_zt9	Ratio
IB	0.39594	0.39861	1.007	0.39769	1.004
OB	0.90622	0.92137	1.017	0.91543	1.010
Total	1.3022	1.3200	1.014	1.31312	1.008

- **Total TBR:**
  - increases by 1.4% for f19j4HE_zc in flibe blanket
  - increases by 0.8% for f19e80_zt9 in flibe blanket

➢ while small, this is good for reactor design since flibe designs tend to need more margin to be tritium self-sufficient

FENDL Library (latest Feb. 2022)

- The Fusion Evaluated Nuclear Data Library (FENDL) is the result of an international effort coordinated by the IAEA Nuclear Data Section
- Assembles a collection of the best nuclear data selected 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:
    - ❑ web page or github



Fusion Evaluated Nuclear Data Library - FENDL-3.2b

(Nuclear data supersede all previous versions of FENDL-2.x and 3.x libraries)

Coordinators: Georg Schnabel, and Roberto Capote, and Andrej Trkov
LAST WEBPAGE UPDATE: Feb 15, 2022

FENDL-3.0 PRIMARY REFERENCE:
R. Forrest, R. Capote, N. Otsuka, T. Kawano, A.J. Koning, S. Kunieda, J-Ch. Sublet, and Y. Watanabe, INDC(NDS)-0628 (IAEA, Vienna, 2012).
(note: A new comprehensive documentation of the FENDL library is in preparation).

The Fusion Evaluated Nuclear Data Library contains reaction data with a focus on the data requirements of fusion research facilities. Both operating and future facilities (e.g., ITER,DEMO, IFMIF) data needs are covered with current data extended up to 150 MeV. Development of FENDL libraries is described in the document links provided in the left column; links to previous FENDL releases are also listed. The ENDF files and thereof derived processed files available on this website correspond to this commit on GitHub.

Library Contents: Transport

The FENDL-3.2b transport package contains evaluated nuclear data in ENDF-6 format as General Purpose files. Data are given for neutron-, proton- and deuteron-induced reactions. All ENDF files of the neutron sublibrary cover at least incident energies up to 60 MeV and typically extend up to 150 MeV. All ENDF files in the proton sublibrary go up to at least 100 MeV and often to 3 GeV. All ENDF files in the deuteron sublibrary cover the energy range to exactly 200 MeV. Details about the energy range of individual ENDF files can be seen in the sublibrary summary tables linked below. Data processing for transport applications has been undertaken (neutron data processing is similar to the processing of the FENDL-3.0 library described in INDC(NDS)-0611 report). Importantly, the official NJOY2016 source code was adjusted to ensure the proper processing of the nuclear data libraries provided by the IAEA. For FENDL, this NJOY2016 version has been used. More details of the FENDL-3.2b data processing will be provided in the final FENDL paper, which is in preparation. The following processed files for applications are given:

- FENDL/MC: Pointwise continuous-energy cross section data in **ACE** format for MCNP calculations; also includes probability tables (PT) in the unresolved resonance range.
- FENDL/MG: Contains multigroup cross section data in the 211n/42g Vitamin J+ energy structures (the 211n Vitamin J+ energy structure matches with the 175n Vitamin J energy structure below 19.64 MeV) for multigroup transport codes in two formats:
    - FENDL/MG (MATXS), which includes files in **MATXS** format from the NJOY module MATXSR.
    - FENDL/MG (GENDF), which contains data in **GENDF** format from the NJOY modules GROUPR and GAMINR.
- Data are available for 192 materials relevant for fusion at 293.6K. Additionally, the SIGACE package can be downloaded for Doppler broadening of ACE-formatted file - useful for generating ACE-formatted files at temperatures higher than 293.6K.

Notes on uncertainties: If covariance data are not available for a particular element of interest, covariance data of other libraries may be used (e.g., from TENDL-2019 library).

Changes since FENDL-3.2:

- The neutron ENDF files of Fe-54, Fe-56, Fe-57 were taken from the INDEN project
- The neutron ENDF file of O-16 was updated at the Nuclear Data Section of the IAEA to improve heating compared to FENDL-3.2 while preserving the neutron flux at high energies.
- Minor change in the MF6/MT700 energy-angular distribution representation of B-10 to improve the recoil heating calculation.

Recommendations

Activation

The TENDL-2017 library is recommended for activation calculations. Note that selected activation channels for neutron induced reactions which are included in the IRDFF-II library may contain better quality evaluations than those listed in TENDL-2017 However, IRDFF-II should not be used as a comprehensive activation library as many activation reactions are not included in IRDFF-II not being neutron dosimetry reactions. A similar situation arises for many proton and deuteron induced reactions evaluated for medical radionuclide production (e.g., see evaluated data for charged-particle induced monitor reactions, for production of gamma-emitters for medical applications, for production of positron-emitters for medical applications, and for production of therapeutic radionuclides).

Dosimetry

The IRDFF-II library (International Reactor Dosimetry and Fusion File) released by the IAEA in January 2020 is recommended for neutron dosimetry in fusion facilities.

FENDL-3.2 Sub-libraries:

- **Activation** – TENDL-2017 is the recommended library
  https://tendl.web.psi.ch/tendl_2017/tendl2017.html
- **Dosimetry** – IRDFF-II is the recommended library
  https://nds.iaea.org/IRDFF/
- **Proton transport** (179 evaluations ENDF and ACE format)
- **Deuteron transport** (179 ENDF, 169 ACE evaluations)
- **Photo-atomic transport** (61 evaluations ENDF, no ACE)
- **Neutron transport** (192 evaluations in ENDF, ACE, MATXS (deterministic), GENDF (sensitivity)

Status of "Big Paper"

- Documents FENDL-3.2
- To appear in *Nuclear Data Sheets* December issue

Sections:

- Evaluations selected
- Processing of data
- Validation for the neutron sub-library
  1. computational
  2. experimental
- Activation library
- to be submitted to *Nuclear Data Sheets*

FENDL: A library for fusion research and applications

G. Schnabel,[1,*] D.L. Aldama,[2] T. Bohm,[3] U. Fischer,[4] S. Kunieda,[5] A. Trkov,[6] R. Capote,[1] and To.Be. Completed[7]

[1] *NAPC–Nuclear Data Section, International Atomic Energy Agency, Vienna, Austria*
[2] *Agencia de Energía Nuclear y Tecnologías, La Habana, Cuba*
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[4] *Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany*
[5] *Nuclear Science and Engineering Center, Japan Atomic Energy Agency, Tokai, Ibaraki, Japan*
[6] *Josef Stefan Institute, Ljubljana, Slovenia*
[7] *Many more institutions*

This is the abstract of the Fusion Evaluated Nuclear Data Library, abbreviated FENDL. This is not yet a meaningful abstract but only a placeholder that needs to be replaced. Here is an example of a reference [1] to the FENDL-3 report. For useful information and guidelines for collaborators, please consult section I.

CONTENTS

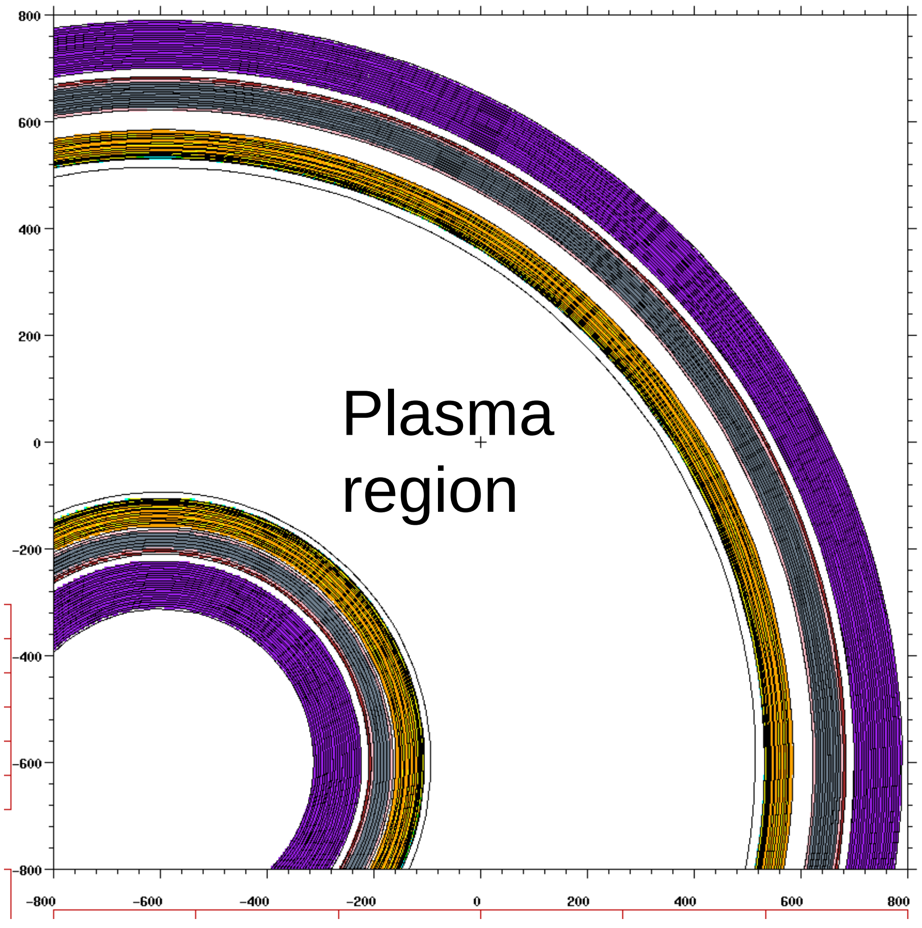
Future Work for FENDL

- Follow up on issues from current validation efforts
- Develop more computational benchmarks for existing and emerging reactor designs
    - ❑ e.g., variety of blanket designs: Li ceramics, flibe, and chloride salt
- Incorporate more experimental and computational benchmarks into JADE (automation/continuous integration package)
- Extend JADE V&V to Linux platform, open source spreadsheet, and add OpenMC inputs for transport calculations
- Validation of proton and deuteron transport libraries
- Prepare consistent covariance matrices for uncertainty analysis
    - ❑ It is important to determine the uncertainty due to nuclear data for key neutronics responses in reactor design (e.g. TBR)
- Other user requests?

Backup slides

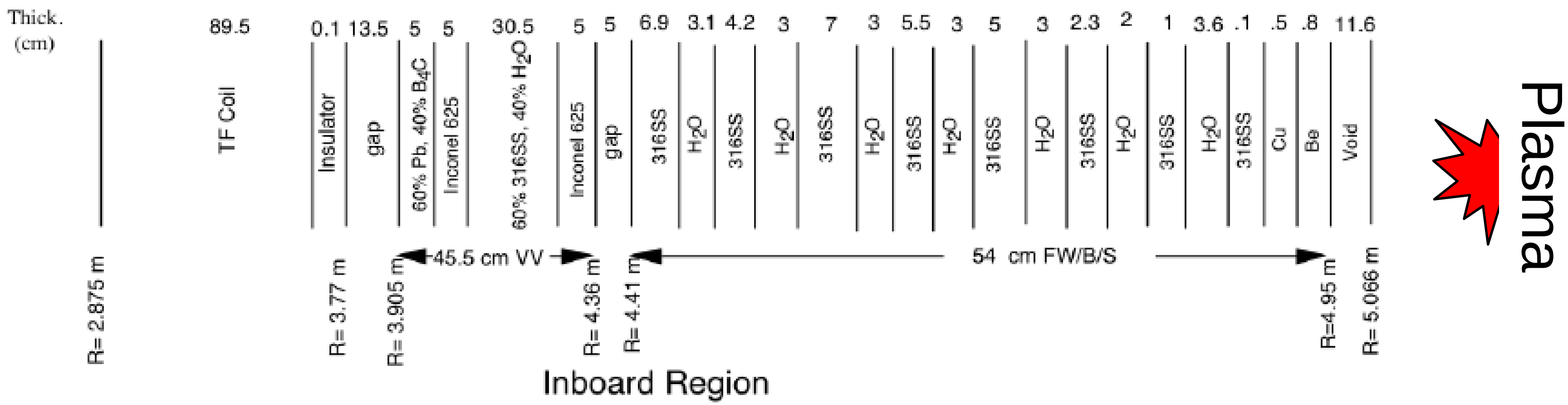
ITER 1-D Cylindrical Calculation Benchmark

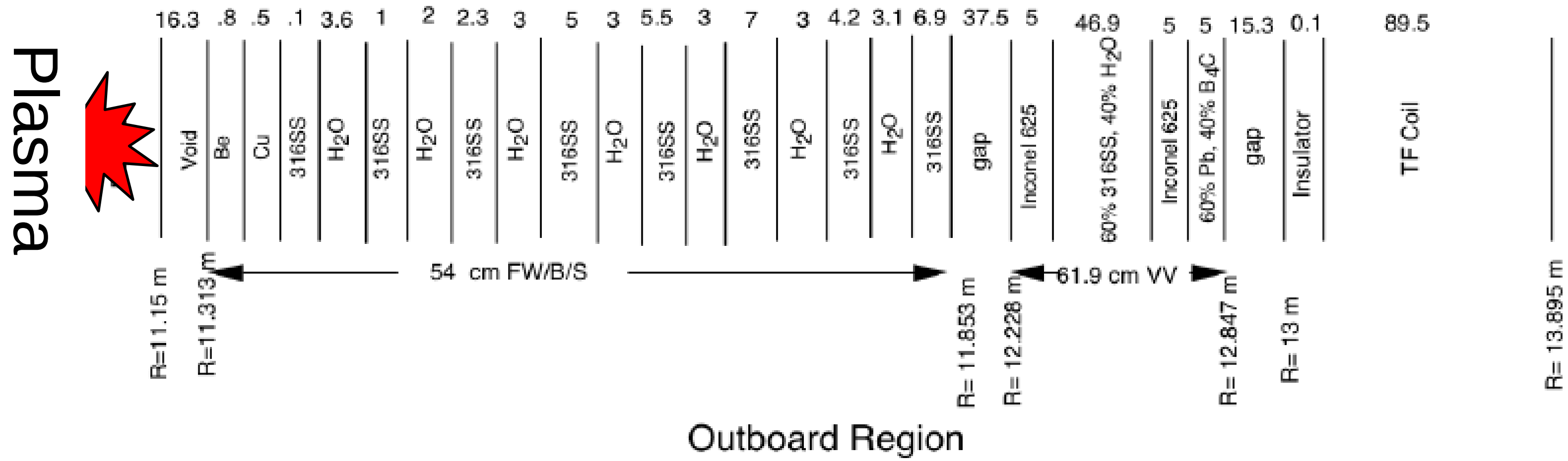
- Based on an **early** ITER design
- Developed for the FENDL evaluation process
- Simple but realistic model of ITER with the Inboard and Outboard portions modeled with the plasma in between
- D-T fusion (14.1 MeV neutrons)
- Flux (neutron and photon), heating, dpa, and gas production calculated



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

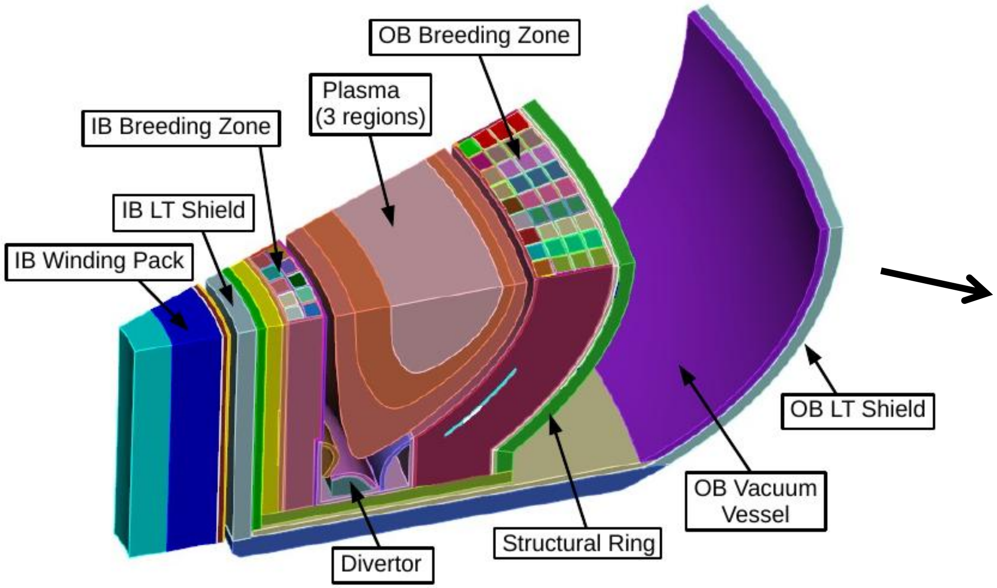
ITER 1-D Cylindrical Benchmark continued

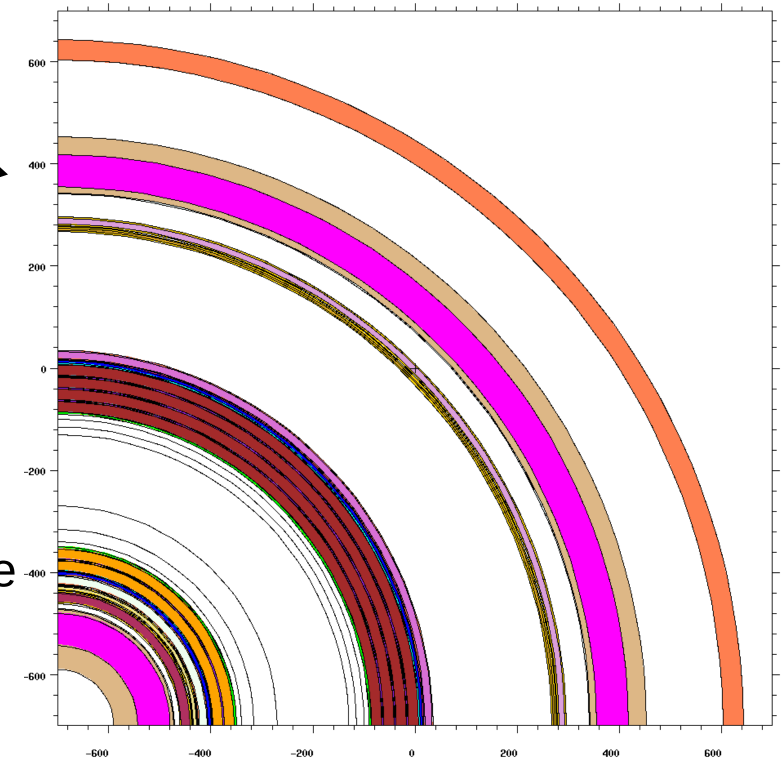




FNSF 1-D Cylindrical Computational Benchmark

- Fusion Energy Systems Studies Fusion Nuclear Science Facility (FESS-FNSF)
- Breeding Zone: He cooled steel structure (90 w/o Fe, 7.5 w/o Cr, 2 w/o W, 0.2 w/o V), PbLi breeder (Dual Coolant Lithium Lead-DCLL)

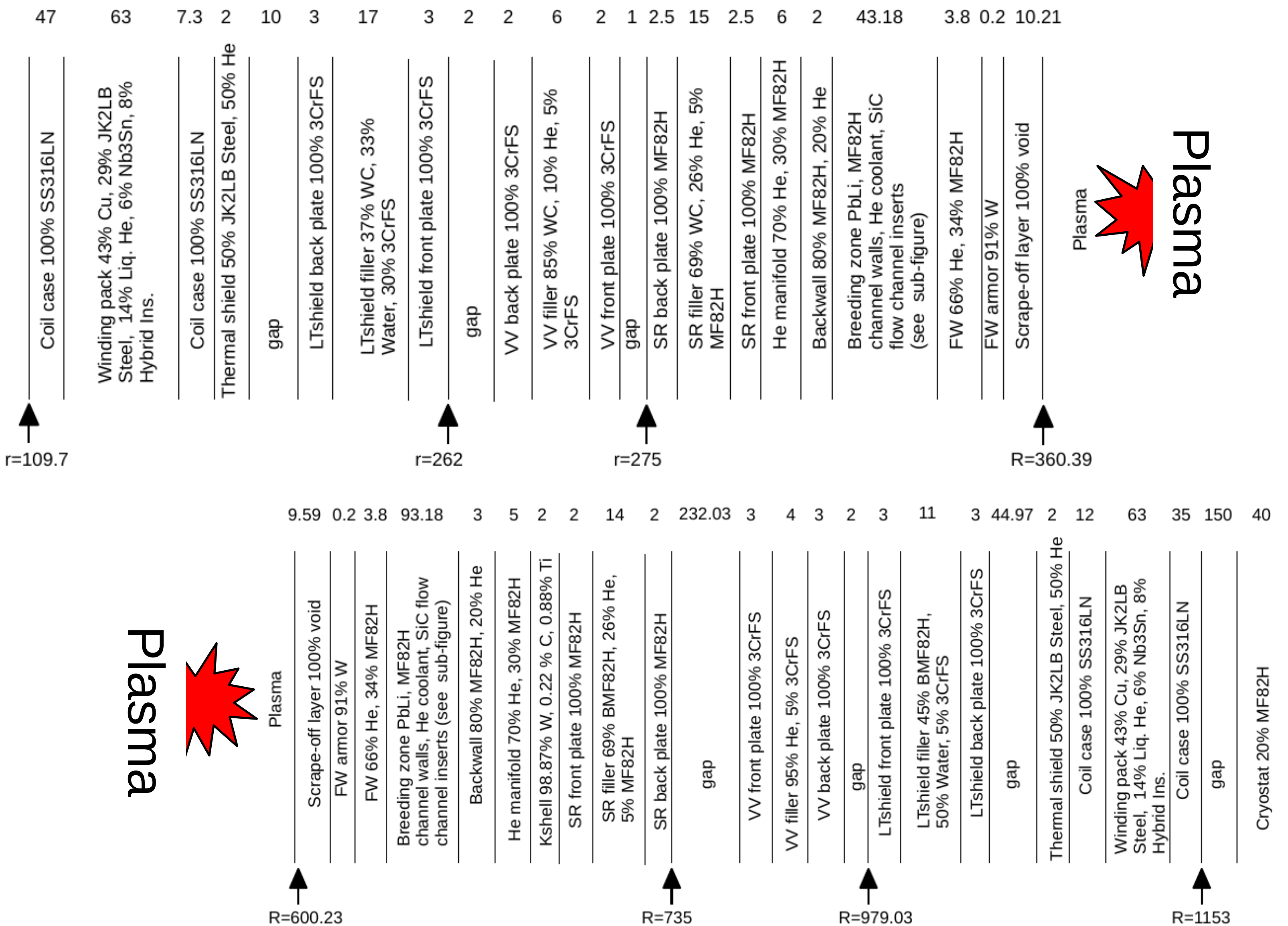




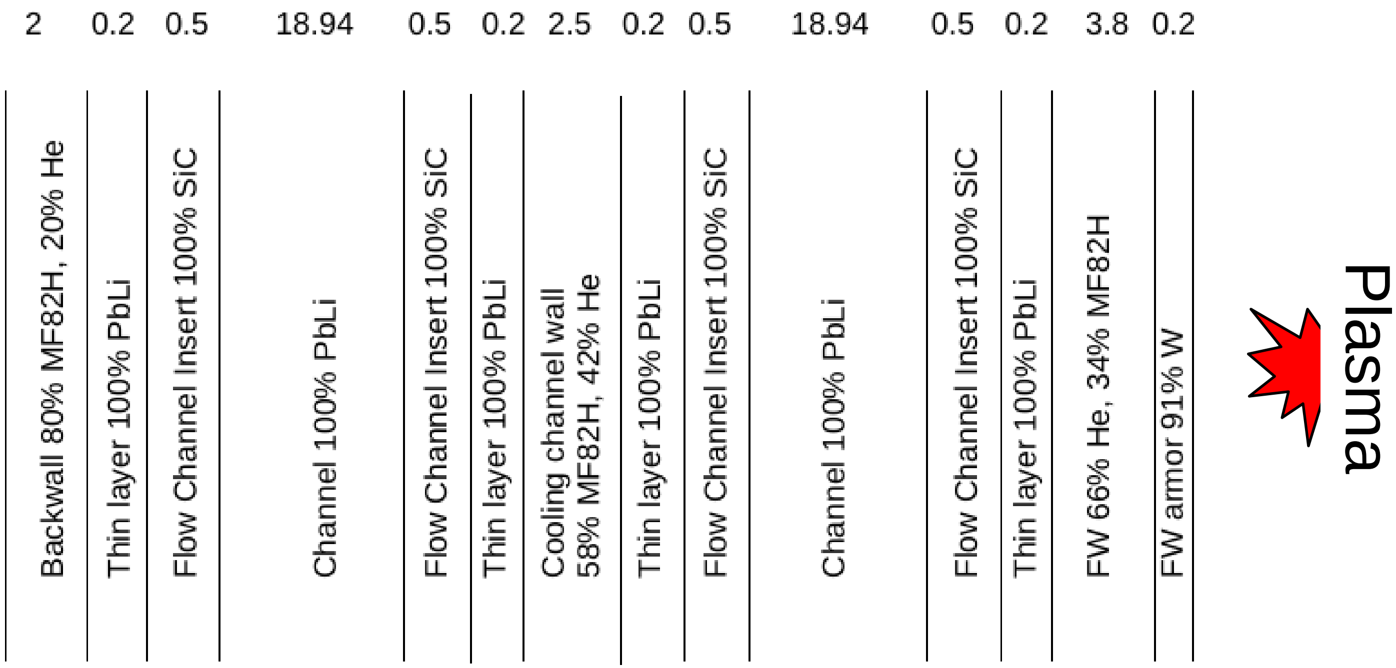
- 85 radial zones
- Includes SiC flow channel inserts in breeding zone
- Includes face plates and filler for SR, VV, LTshield
- Includes IB, OB magnet and cryostat
- MCNP materials created with PyNE

T. Bohm et al. "Initial Neutronics Investigation of a Liquid Metal Plasma Facing Fusion Nuclear Science Facility, *Fusion Science and Technology*, 2019.

FNSF 1-D Cylindrical Computational Benchmark



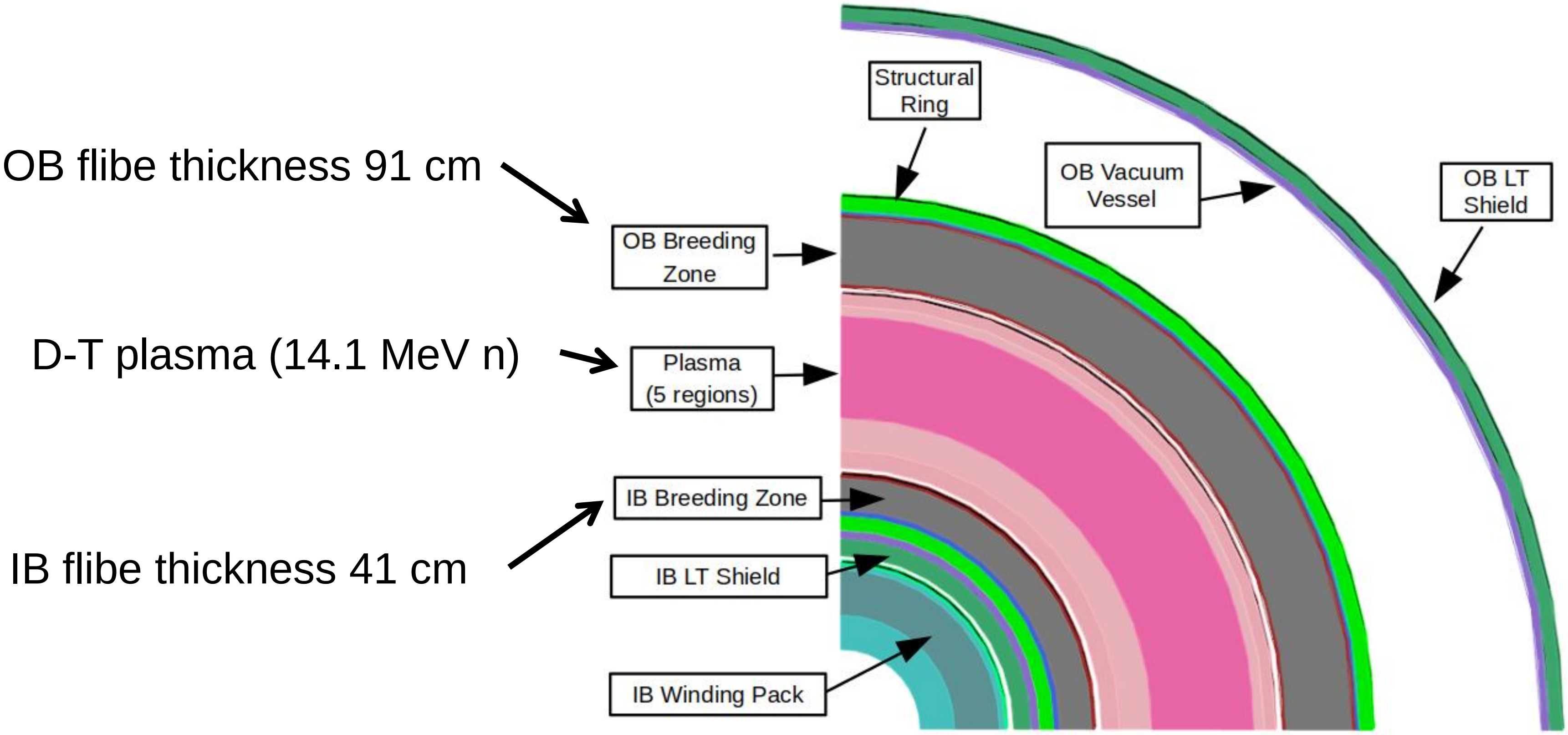
FNSF 1-D Benchmark- Details of IB Breeder Zone



- ➢OB Breeder zone similar but has 4 PbLi channels

1-D Cylindrical Computational Benchmark (flibe blanket)

- Molten salt 2(LiF)-1(BeF_2) sometimes proposed as a liquid blanket
  - Commonwealth Fusion Systems reactor design
- INDEN provides a new XS for ^{19}F: *https://www-nds.iaea.org/INDEN/*
- Created 1-D model based on FESS-FNSF but modified the blanket:
  - Breeding Zone: 2 cm Be multiplier layer, flibe breeder tank



Source of FENDL neutron data

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

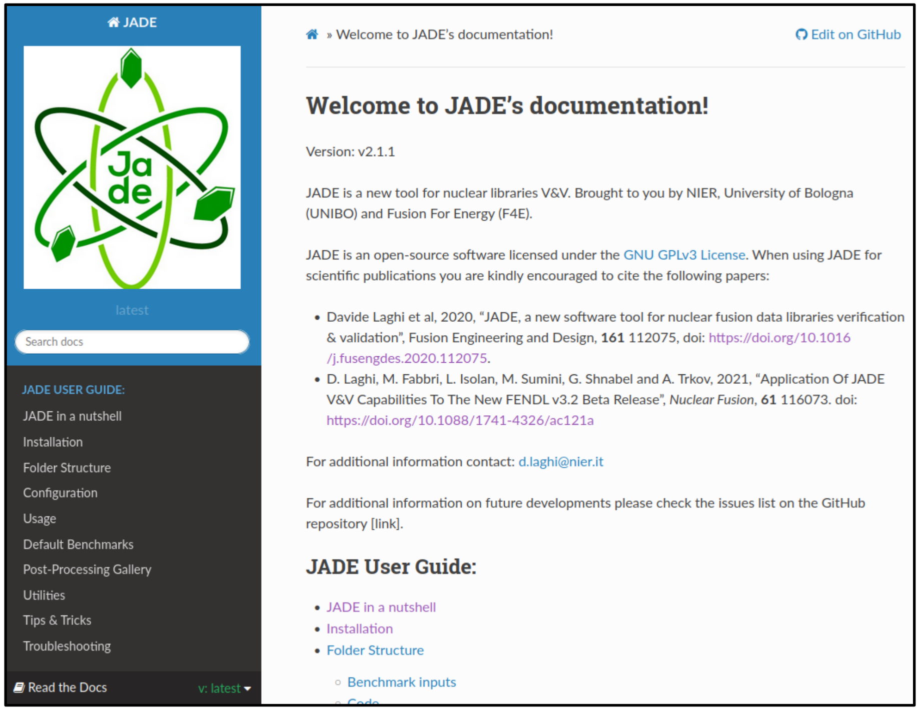
Isotope	FENDL-2.1*	FENDL-3.1	FENDL-3.2b (for E<20 MeV)
H-1	JENDL-3.3	ENDF/B-VII.1	ENDF/B-VII.1
0-16	ENDF/B-VI.8	ENDF/B-VII.1	FENDL/INDEN1.0**
Cr-52	ENDF/B-VI.8	ENDF/B-VII.1	INDEN1.0**
Fe-56	JEFF-3	JEFF-3.1.1	INDEN1.0**
Ni-58	JEFF-3	ENDF/B-VII.0	ENDF/B-VII.1
Cu-63,65	ENDF/B-VI.8	ENDF/B-VII.0	ENDF/B-VII.0

*FENDL-2.1 is the design/reference library for ITER neutronics
**INDEN International Nuclear Data Evaluation Network
https://www.nds.iaea.org/INDEN/

JADE: FENDL V&V automation

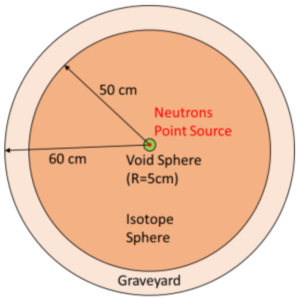
- Tool to automate validation testing of FENDL (and other libs)
- Developed as a collaboration: F4E, NIER, UNIBO, IAEA
- Includes computational and experimental benchmarks
- Uses python, Windows OS, MS Office (tables), MCNP
- Available on github, see full documentation:

https://jade-a-nuclear-data-libraries-vv-tool.readthedocs.io/en/latest/



JADE continued

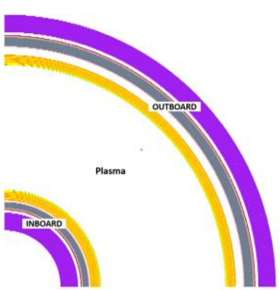
- Generates tables of differences (color coded by percent differences for easy user identification)
- Generates easy to read plots for comparisons of results



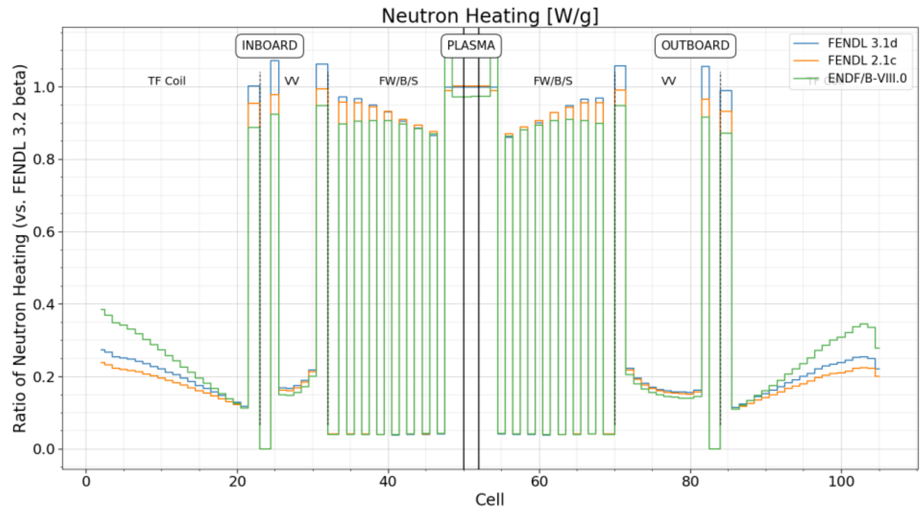
Sphere leakage

SPHERE LEAKAGE COMPARISON RECAP

ZAID		TALLIES				
		T production	He ppm production	DPA production	Neutron heating F6	Gamma heating F6
M901	Polyethylene, Non-borated		-0.01%	0.01%	0.02%	0.02%
M900	Natural silicon		0.00%	0.00%	0.00%	0.00%
M101	SS316L(N)-IG	0.57%	4.18%	79.12%	98.41%	2.38%
M203	Boron carbide (B_4C)	9.68%	0.79%	100.00%	100.00%	-0.01%
M200	Ordinary concrete	1.52%	10.47%	87.15%	97.53%	-8.15%
M400	Water	0.57%	16.37%	-2.82%	6.00%	-3.24%



ITER 1-D



Bohm CSEWG-2023

Courtesy D. Laghi