Impact of INDEN F-19 XS in Fusion and Overview of the Fusion Evaluated Nuclear Data Library (FENDL)

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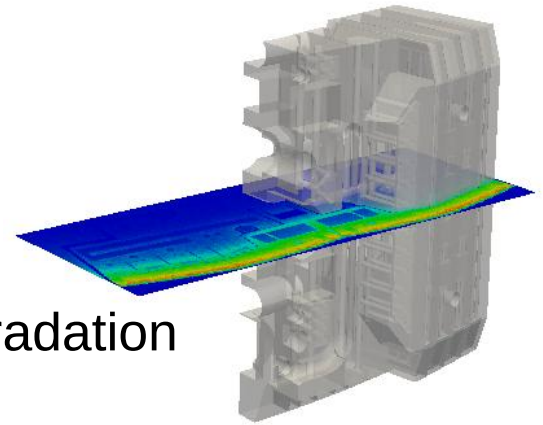
Outline

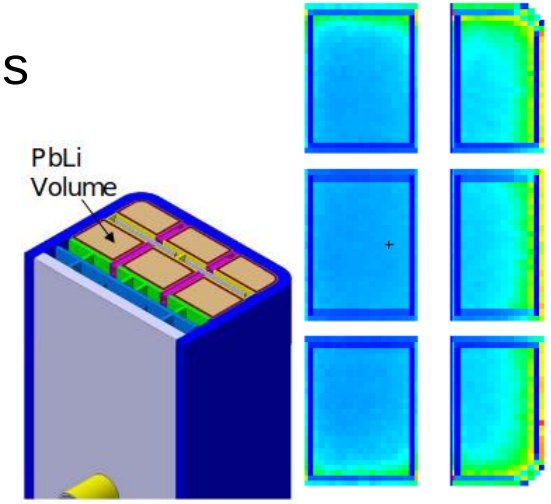
1) Impact of INDEN F-19 XS in Fusion
2) FENDL Introduction
   - Web page
   - Brief History of FENDL
   - Distribution: IAEA webpage or Github
   - Overview of FENDL content (sub-libraries)
   - Preparation of NDS paper
3) FENDL Neutron sub-library validation benchmarks
   - Computational benchmarks
   - Experimental benchmarks
   - JADE V&V automation tool
4) FENDL Future Work

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

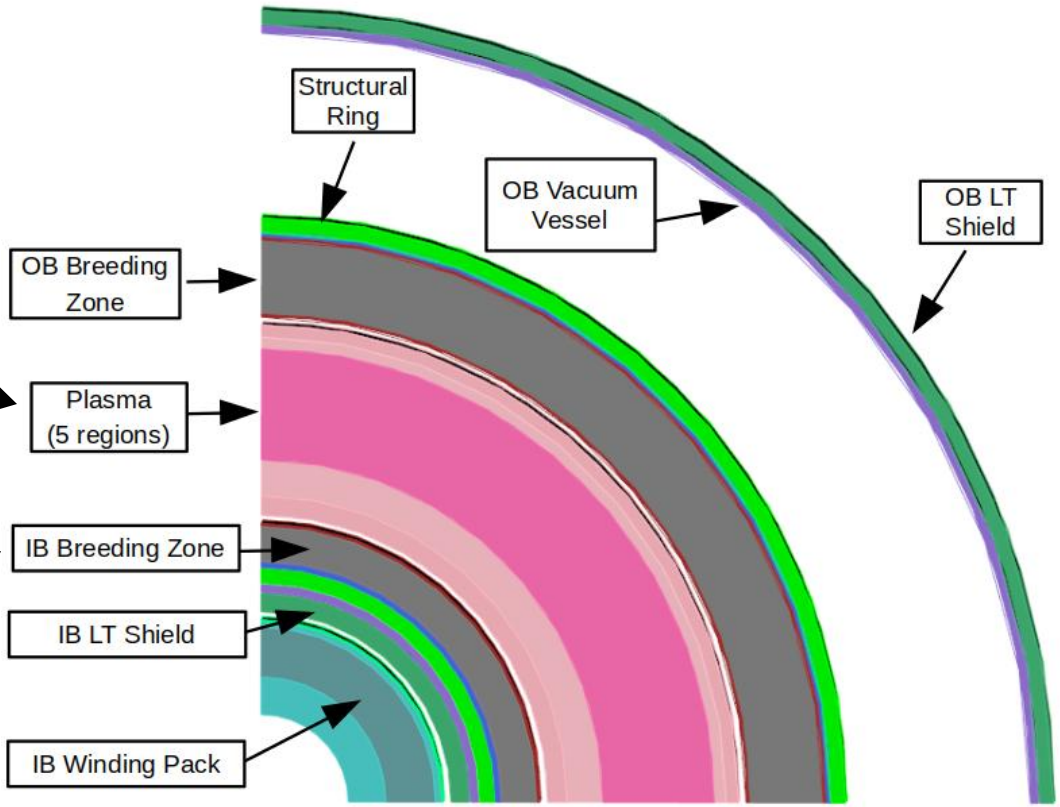
1-D Cylindrical Computational Benchmark (flibe blanket)

- Molten salt 2(LiF)-1(BeF_2) sometimes proposed as a liquid blanket
  - Commonwealth Fusion Systems reactor design
  - *note: Li enriched in Li-6 for fusion*
- INDEN provides a new XS for F-19: *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

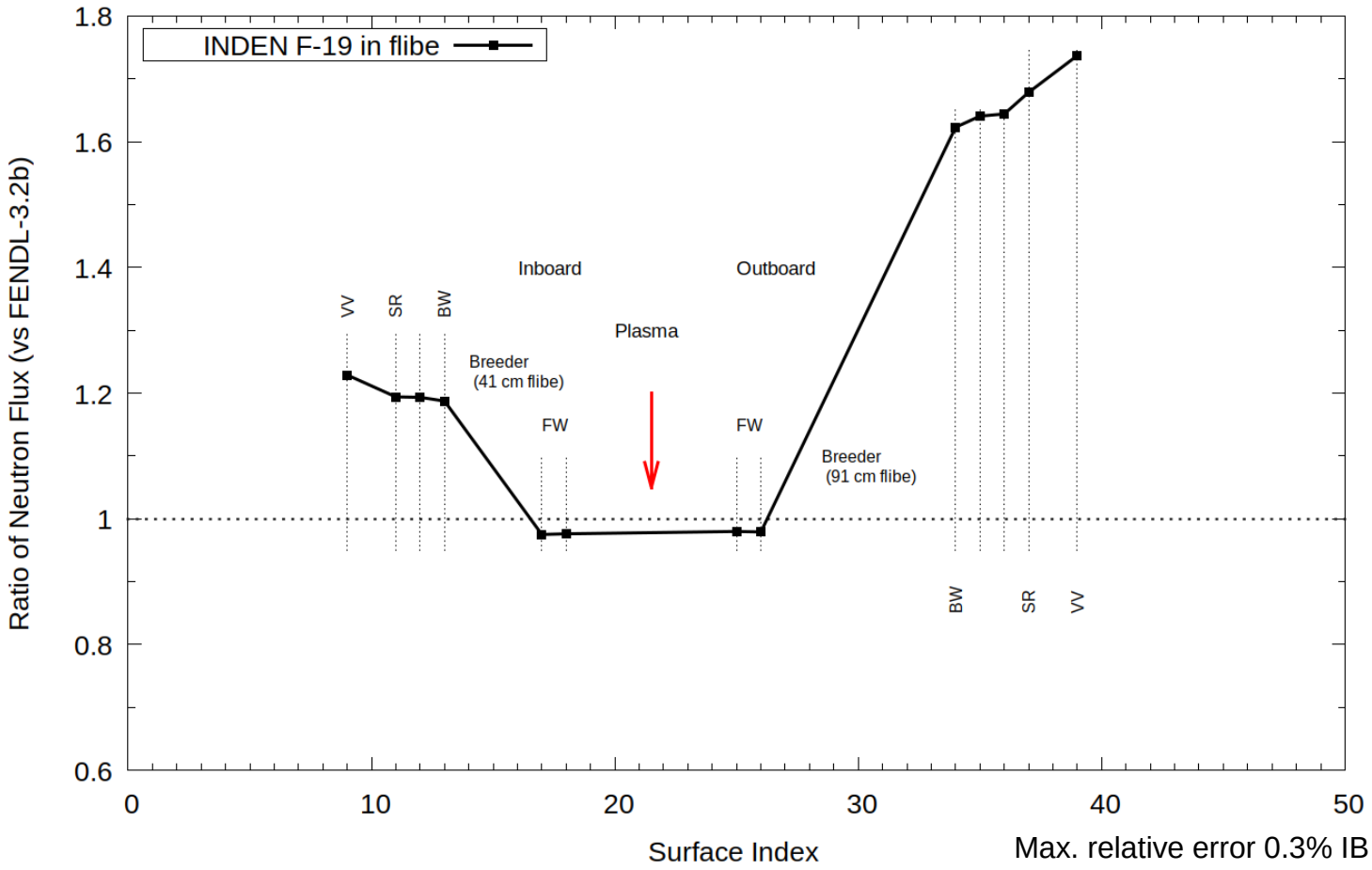
OB flibe thickness 91 cm

D-T plasma (14.1 MeV n)

IB flibe thickness 41 cm



Results: Neutron Flux, TBR (impact of INDEN F-19 XS)

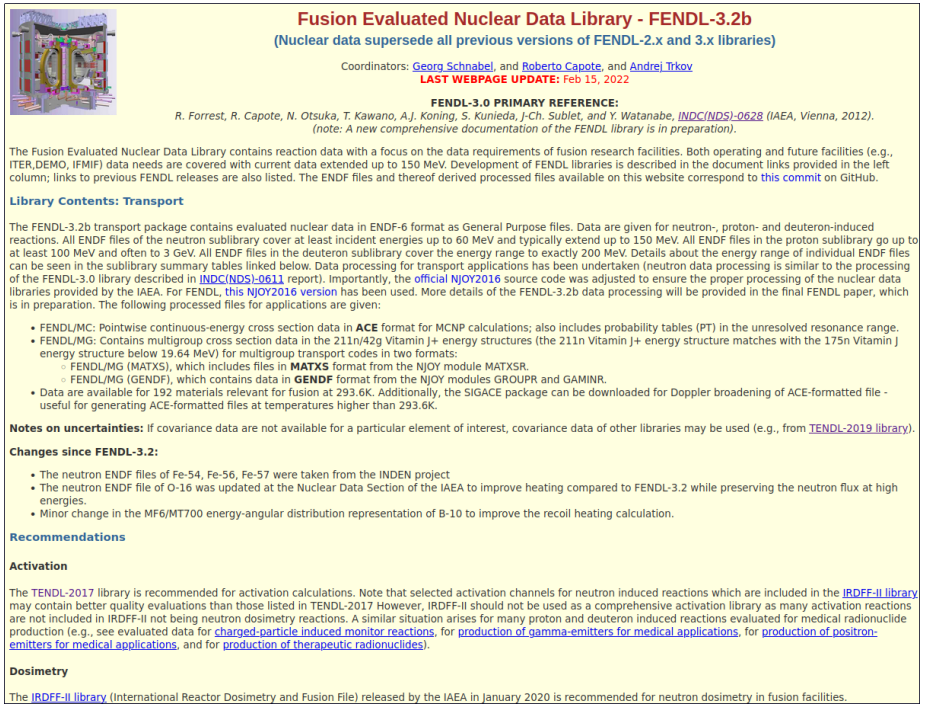


Max. relative error 0.3% IB VV, 2% OB VV

- **Neutron flux:** 20%-70% higher neutron fluxes behind the flibe breeder regions
  - ➢ may need more shielding for components behind blanket
- **TBR:** increases by 1.4%
  - ➢ good since flibe designs tend to need more margin to be tritium self-sufficient

FENDL Library

- 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 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:



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.

Brief History

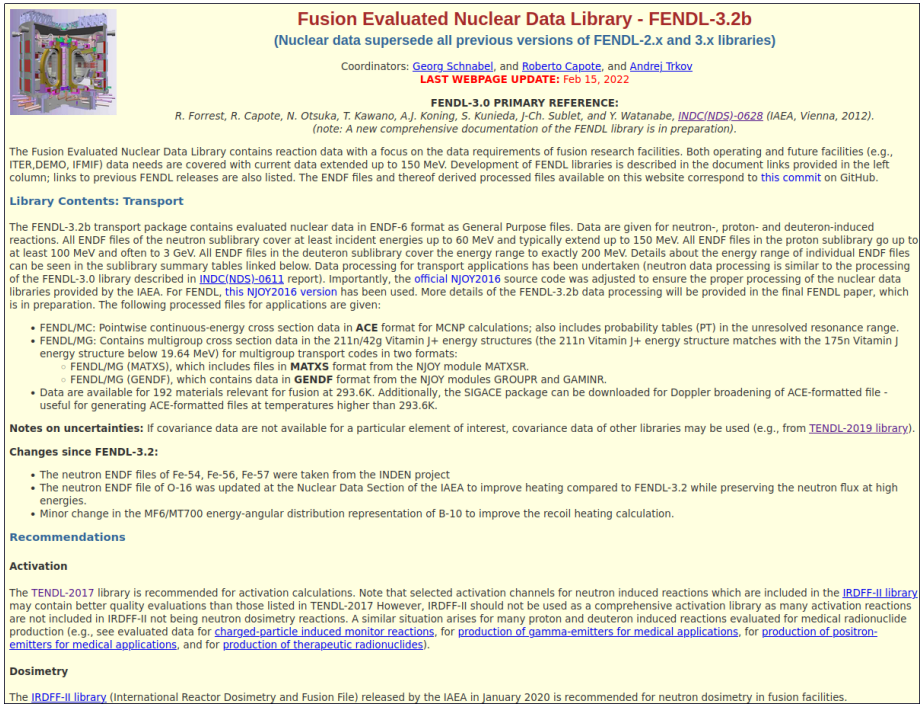
- **FENDL-1.0** MC, 1.0 MG -work started 1987, released 1994, (see indc-nds-0352, indc-ger-041)
- **FENDL-2.0** MC, 2.0 MG-released 1997, 57 materials
- **FENDL-2.1** MC, 2.1 MG-released 2004, 71 materials, Emax=20 MeV, ITER reference/design library
- **FENDL-3.0**, result of CRP 2008-2011, introduced charged particle libraries (proton and deuteron) and extended energy range to at least 60 MeV in transport library, IFMIF was a major application driver, 180 materials
- **FENDL-3.2b**, Feb. 15, 2022 current version, 192 materials, updates described in following slides

Distribution: IAEA Webpage or Github

- All data available including: processed formats, IAEA-NDS NJOY patches, NJOY input files
- Files can be downloaded directly:

Webpage in various formats:

➢ *https://www-nds.iaea.org/fendl/*



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Download

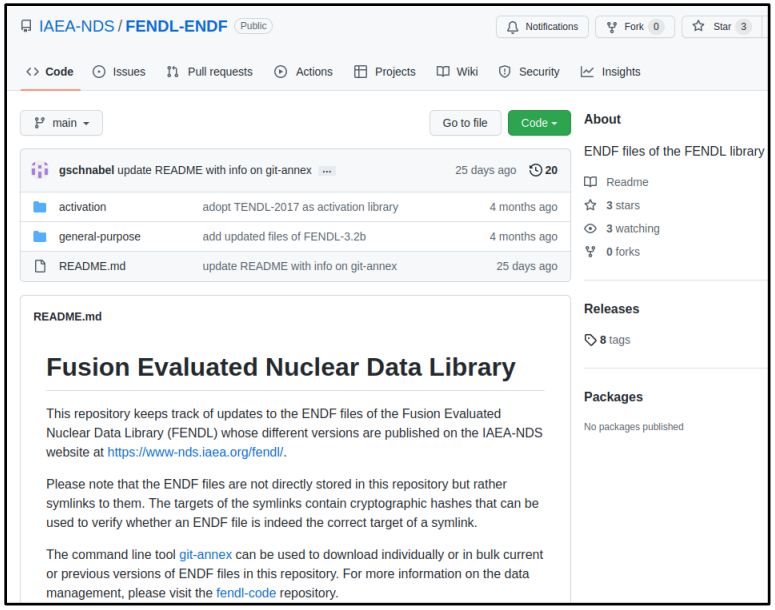
The zipped files contain the entire library of a certain type.

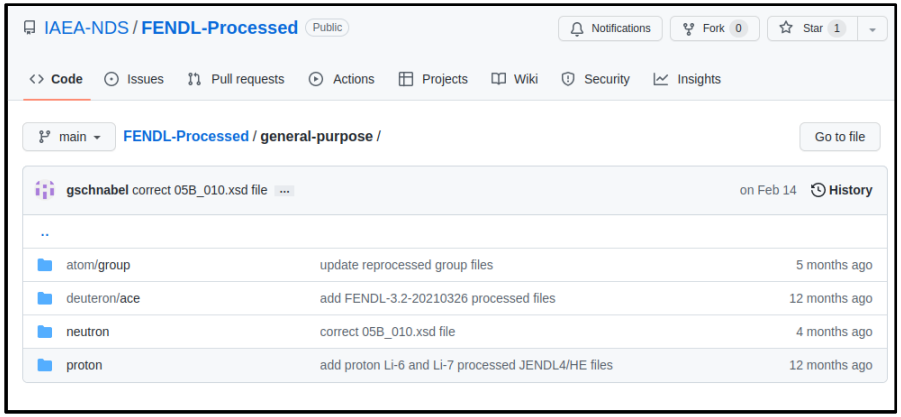
Library	Sublibrary	ENDF	PENDF	ACE	MATXS	GENDF	GND
FENDL-3.2b (transport)	Neutron	[zip]		[zip]	[zip]	[zip]	
	Photo-atomic	[zip]				[zip]	
	Proton	[zip]		[zip]			
	Deuteron	[zip]		[zip]			

Distribution continued: Github

Github based system:

- Evaluations (ENDF):
  - *https://github.com/IAEA-NDS/FENDL-ENDF*
- Processed files (also includes NJOY inputs):
  - *https://github.com/IAEA-NDS/FENDL-Processed*
- IAEA-NDS NJOY patches:
  - *https://github.com/IAEA-NDS/NJOY2016*





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)

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/

Preparing "Big Paper"

- Document FENDL-3.2

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*
[3] *University of Wisconsin, Madison, Wisconsin*
[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.

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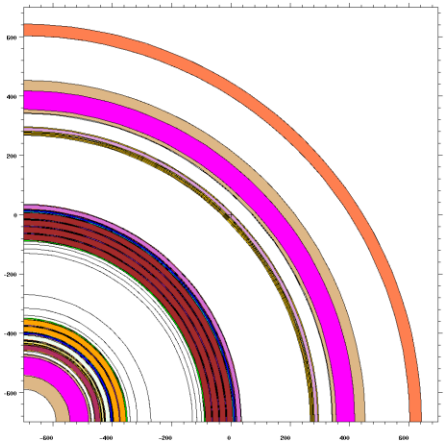
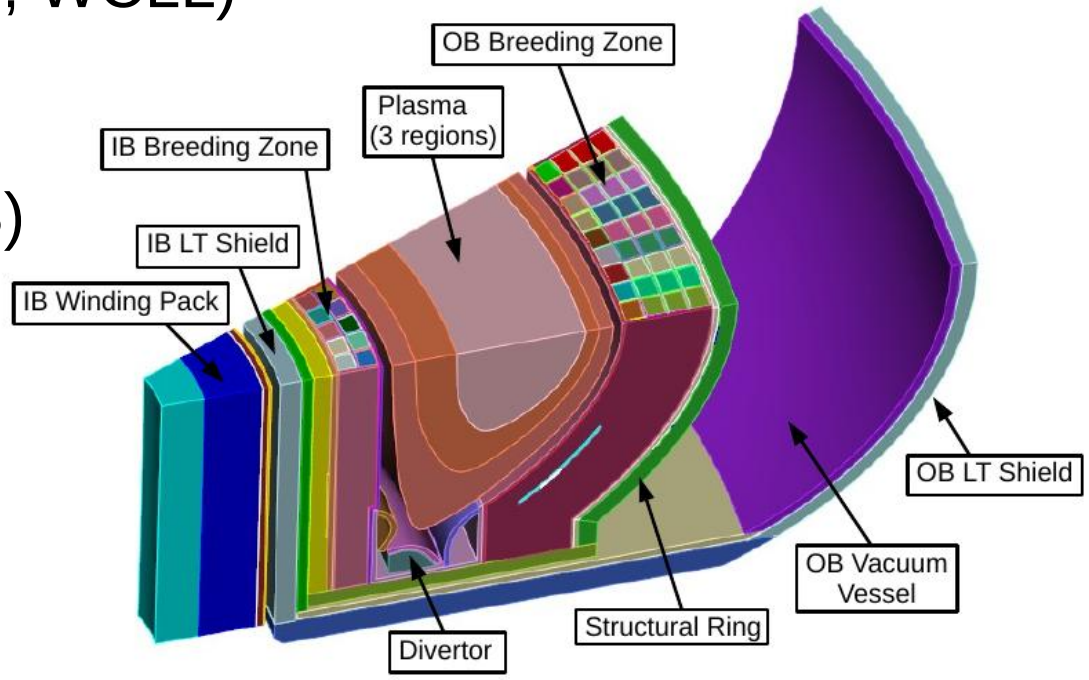
Validation with Computational Benchmarks

- **D-T relevant models:**
  - 14 MeV Leakage Sphere
  - ITER 1-D
  - ITER 3-D
  - ITER 1-D TBM (HCPB, WCLL)
  - FNSF 1-D (DCLL)
  - FNSF 3-D (DCLL)
  - EU DEMO 3-D (HCPB)

Tritium breeding blanket concepts:
TBM= Test blanket module
HCPB=He cooled ceramic pebble bed
WCLL=water cooled lead lithium
DCLL=dual coolant (He) lead lithium



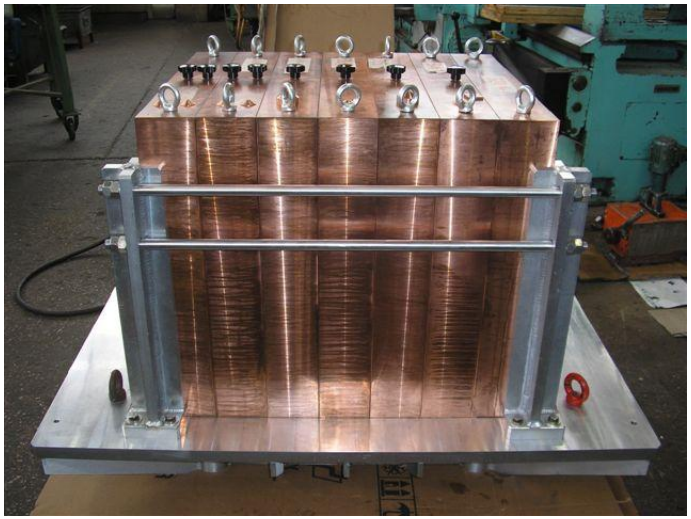
FNSF 1-D



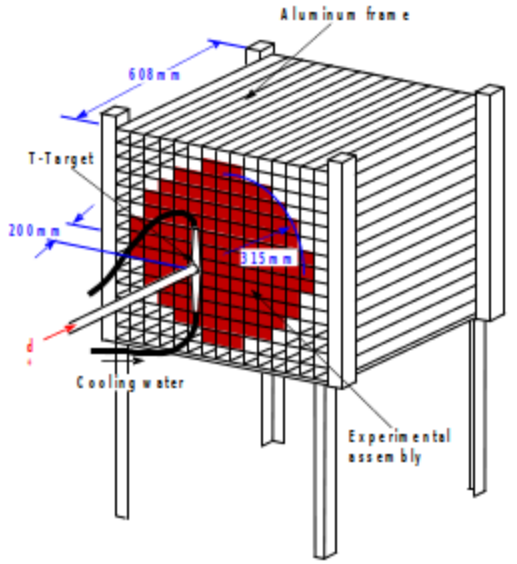
FNSF 3-D (D-T with PbLi blanket)

Validation with Experimental Benchmarks (partial list)

- OKTAVIAN (D-T)
- FNS (D-T)
- TIARA (p+Li-7, 40 MeV or 65 MeV neutrons)
- FNG (D-T)
- LLNL Pulsed sphere (D-T)
- JET (D-D, D-T)
- SINBAD (various)



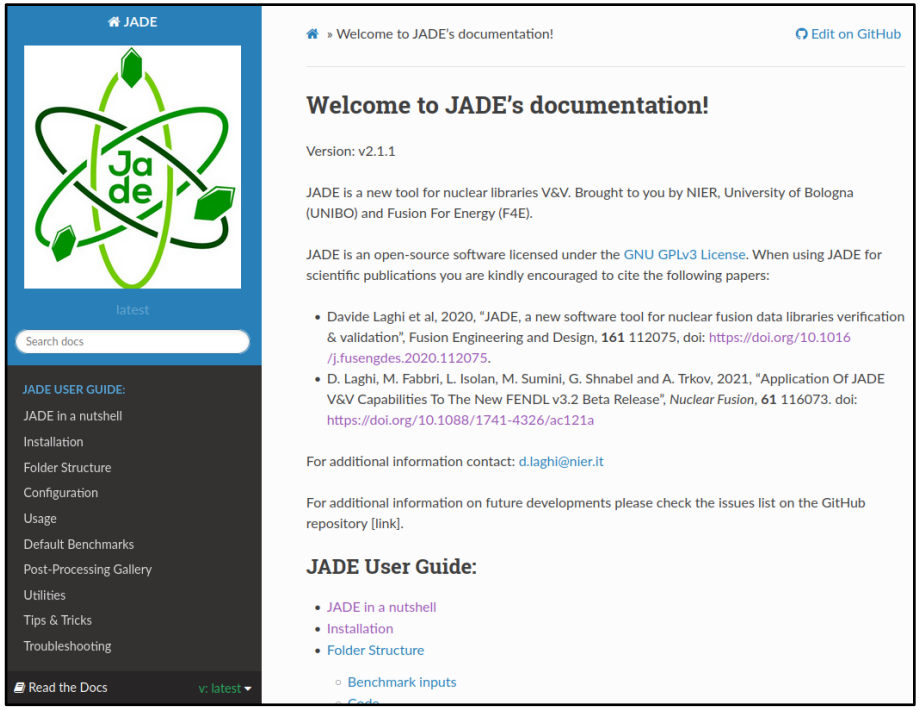
FNG Cu experiment



FNS in-situ experiment

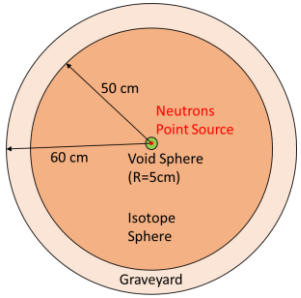
JADE: FENDL V&V automation

- 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

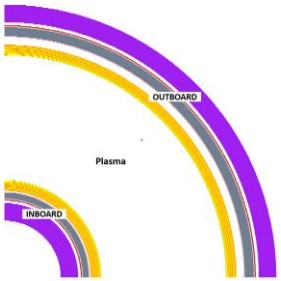
- Generates tables of differences (color coded by percent differences for easy user identification)
- Generates easy to read plots for comparisons of results



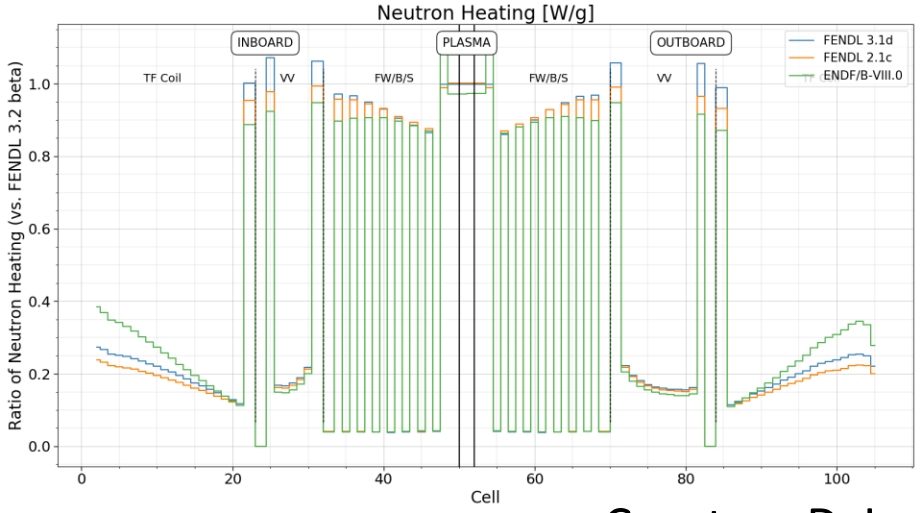
Sphere leakage

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 (B4C)	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-2022

Courtesy D. Laghi

Future Work

- Follow up on issues from current FENDL validation efforts
- Continue following INDEN “work in progress” cross sections
- Develop more computational benchmarks for existing and emerging reactor designs
- Incorporate more experimental and computational benchmarks into JADE
- 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

Questions?