Development of Integrated Neutronics and Thermal Analysis Capabilities to Support Analysis and Optimization of Fusion Systems and Blanket Design

Summary of Capabilities

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Our Team 2020-2021

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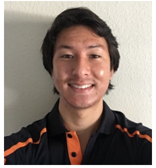

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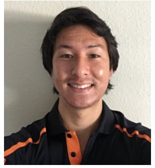


Primary Objectives

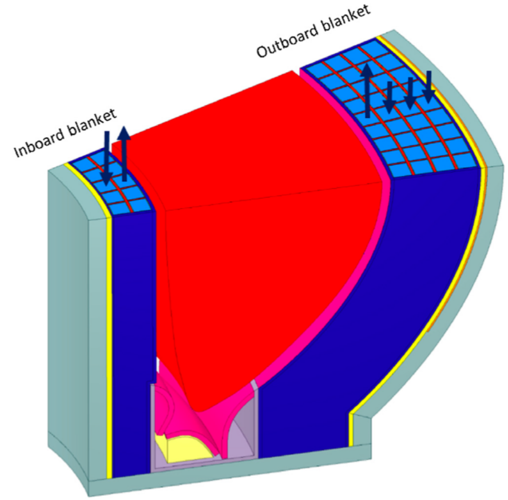
- The ***primary objective*** of this project is to develop and demonstrate an integrated capability between neutronics and thermal analysis tools in support of systems studies for the Fusion Nuclear Science Facility (FNSF) and future facilities.
- This capability will be built from high-fidelity models but will evolve into the creation of reduced-order-models (ROMs) for the rapid evaluation of various design options from a holistic and design optimization perspective.
- The neutronics information will be useful to generate isotopic and transmutation information to determine breeding blanket design effectiveness, waste characteristics and fuel cycle, and heat generation terms for the steady state thermal, anticipated transient, and accident analysis.

Direct Needs

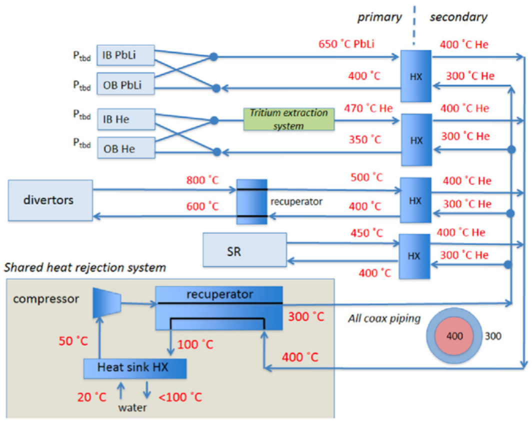
- **Heat generation** terms, including both neutron and gamma heating, throughout fusion core components and the rest of the system
- **Tritium production** in fusion core components, including breeding materials (e.g. lithium) and also in neutron multipliers (e.g. beryllium)
- **Material damage and transmutation**, including gas production from fusion core components to magnets
- Material radial build and **shielding choices** to inform iteration between design and nuclear analysis
- **Shutdown dose** of fusion core components, maintenance, transport and hot cell impacts and impact on specified acceptable material performance limits
- **Afterheat/decay heat** to support safety assessments (e.g. loss-of-flow accident) in accident scenarios and develop source terms for accident progression analysis
- Fusion system **transient analysis**, including startup, shutdown, and anticipated transients and associated impact on specified acceptable material performance limits
- **Waste generation** per unit energy generated, short-term and long-term behavior, classification, and other fuel cycle performance metrics

Multiphysics Simulation Needs

- End Goal: multiphysics analysis capabilities for the Fusion Nuclear Science Facility (FNSF) and beyond.
  - Reduced order, mid- and high-fidelity all have a role
- Important interactions between physics
  1) Design optimization of fusion system with DCLL to meet thermal safety margins.
  2) Prediction of tritium transport inside the blanket.
  3) For the steady state, and specifically operational or anticipated transient modes.
  4) Coupled technique between high-fidelity or mid-fidelity tools for steady state and system tools for steady state and transient.
- Integrated with neutronics analysis for:
  - Heat generation terms
    - Steady state and after heat
  - Performance of breeding blanket including tritium production, material selection, and coolant/moderator



S. Smolentsev, et al., (2018). MHD thermohydraulics analysis and supporting R&D for DCLL blanketin the FNSF. *Fusion Engineering and Design, 135*, 314-323 (2018)



P.W. Humrickhouse et al., (2018) Tritium aspects of the fusion nuclear science facility. *Fusion Engineering and Design, 135*, 302-313

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R&D Vision – Multi-physics analysis

- Development of integrated between neutronics and thermal analysis
  - Neutronics → thermal analysis → tritium transport
    - Plasma power output to first wall
    - Nuclear heating of structures
    - Tritium production
    - Temperature of structures
- External or tight integration as necessary (ROMs as needed)

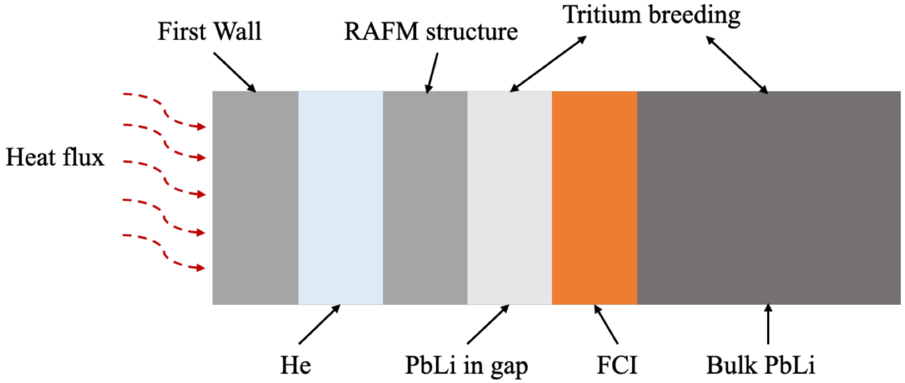


Fig. Scheme of DCLL blanket representing coupled modeling between thermal hydraulics and tritium transport

Current Status

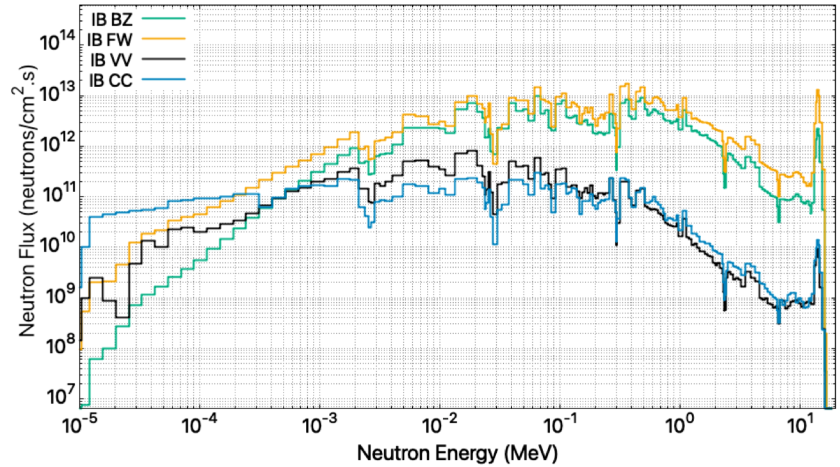
- Neutronics-related efforts with FNSF as basis
  - Automated conversion of CAD model from SolidWorks into MCNP using McCad (Karlsruhe Institute of Technology)
  - Consistent Comparison against Prior Works (TBR, Nuclear Heating, DPA, H and He production)
  - Manual conversion of CAD into MCNP (as backup, for validation, and input flexibility)
  - Preliminary evaluation of OpenMC for related calculations
  - Creation of Serpent-based Model for Activation Analysis and Waste Characterization

- Coupled Neutronics/Thermal-Hydraulic blanket(*) simulation and experimental validation using RELAP5-3D
- Tritium transport models using BISON(*)

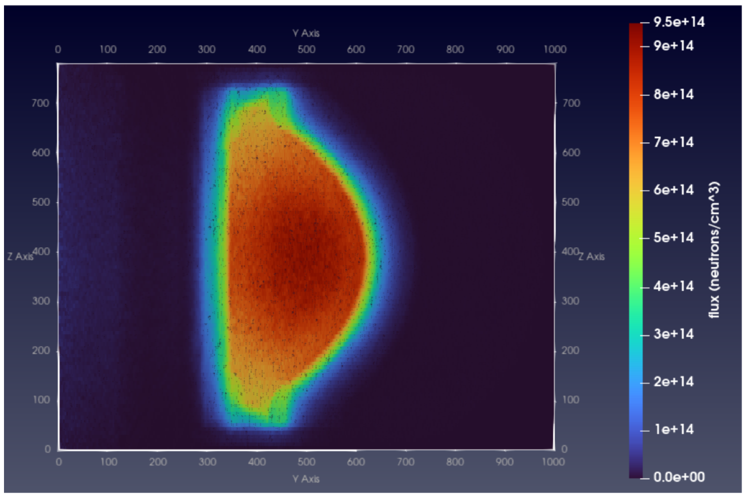
(*) Not presented within the scope of this presentation but materials available upon request

Latest 3D FNSF model

- 22.5-degree FNSF sector
- Model based on the most recent FNSF design [1]
- Neutron flux, neutron spectrum, TBR and tritium spatial distribution



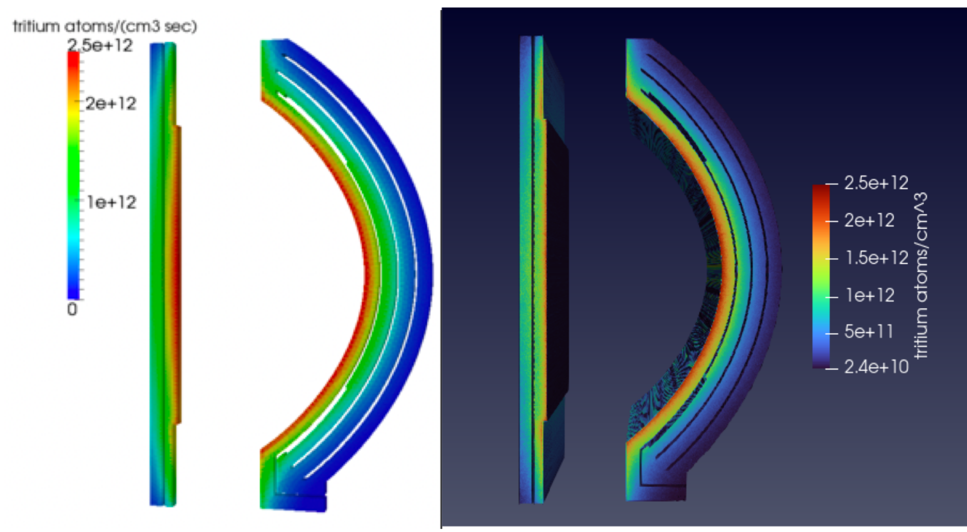
IB neutron spectrum



FNSF 3D neutron flux

	TBR
IB	0.2702
OB	0.8392
TOTAL	1.1094

FNSF DCLL TBR

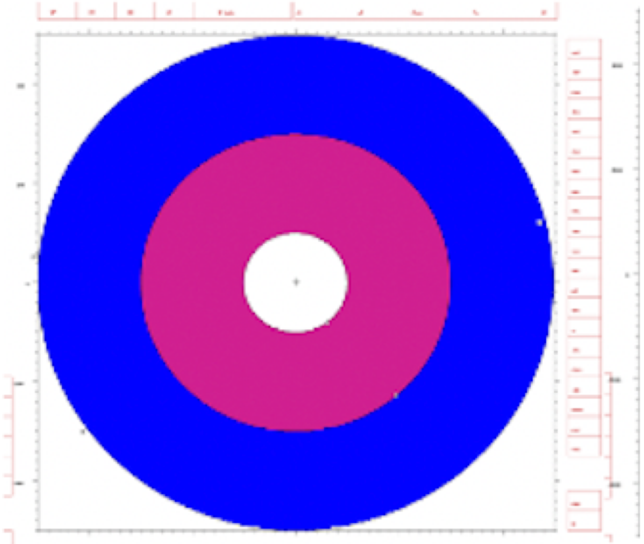


IB and OB tritium production (left [2], right UTK)

[1] Davis, A et al. "Neutronics Aspects of the FESS-FNSF." Fusion engineering and design 135 (2018): 271–278. Web.
[2] T.D. Bohm, et al. (2019) Initial Neutronics Investigation of a Liquid-Metal Plasma-Facing Fusion Nuclear Science Facility, Fusion Science and Technology, 75:6, 429-437, DOI: 10.1080/15361055.2019.1600930

Solid Breeder Study

- Introduction of Reduced-Order-Models (ROMs) 1-D study of the TBR capability of different solid breeder compounds
  - infinite cylinder
  - axial 14.1 MeV neutron source
  - one thick breeder region ~2m (maximum achievable TBR) with additional homogenized materials
- Neutron multiplier materials
  - Be12Ti, Be and Be12V
  - parametric study varying volume fraction of solid breeder and neutron multiplier
- RAFM structure ($MF82H$)
- SiC-SiC
- Coolant ($H_2O\ and\ He$)
- Tungsten
- WC

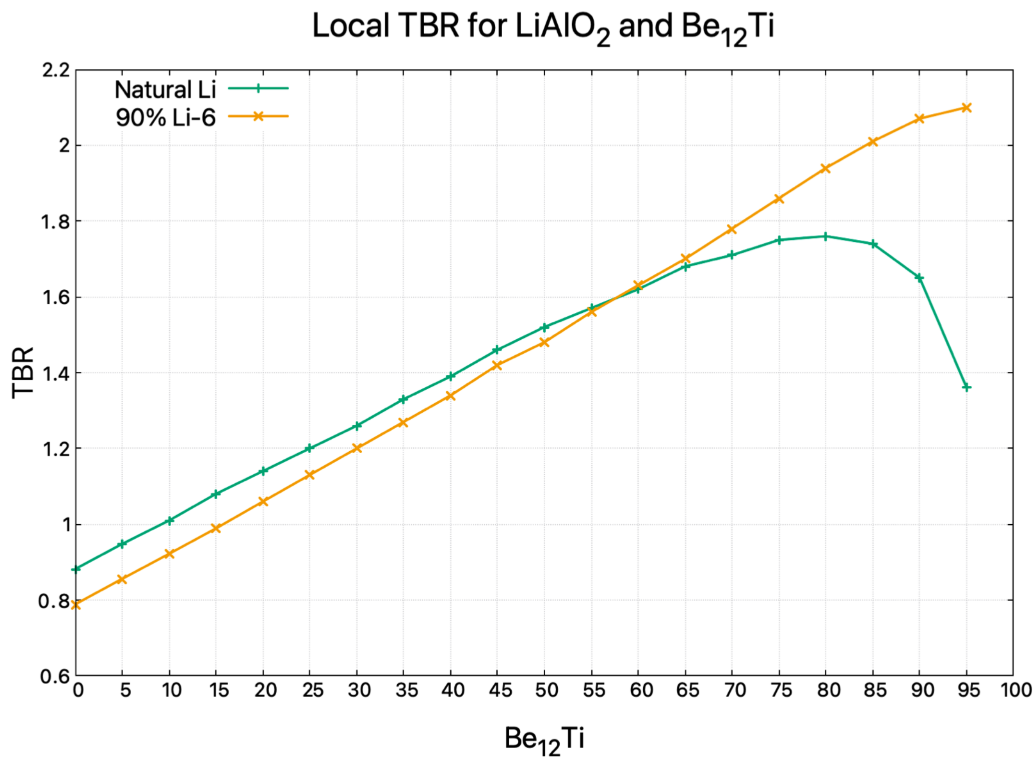


1-D model – Source, breeder and reflector

Optimizing breeder/multiplier ratio

Breeder	Multiplier	% Breeder	% Multiplier	TBR
LiAlO2	Be12Ti	5	95	**2.101**
Li2tiO3	Be12Ti	5	95	**2.127**
LiO2	Be12Ti	5	95	**2.166**
Li2ZrO3	Be12Ti	5	95	**2.116**
Li4SiO4	Be12Ti	5	95	**2.146**
Li4TiO4	Be12Ti	5	95	**2.149**
Li4GeO4	Be12Ti	5	95	**2.132**
Li8ZrO6	Be12Ti	5	95	**2.149**
LiAlO2	Be	5	95	**2.448**
Li2tiO3	Be	5	95	**2.421**
LiO2	Be	5	95	**2.447**
Li2ZrO3	Be	5	95	**2.434**
Li4SiO4	Be	5	95	**2.446**
Li4TiO4	Be	5	95	**2.452**
Li4GeO4	Be	5	95	**2.431**
Li8ZrO6	Be	5	95	**2.444**
LiAlO2	Be12V	5	95	**2.110**
Li2tiO3	Be12V	5	95	**2.128**
LiO2	Be12V	5	95	**2.161**
Li2ZrO3	Be12V	5	95	**2.122**
Li4SiO4	Be12V	5	95	**2.088**
Li4TiO4	Be12V	5	95	**2.151**
Li4GeO4	Be12V	5	95	**2.130**
Li8ZrO6	Be12V	5	95	**2.160**

TBR for solid breeder and 90% Li-6



Optimum ratio for solid breeder and neutron multiplier

Additional blanket materials

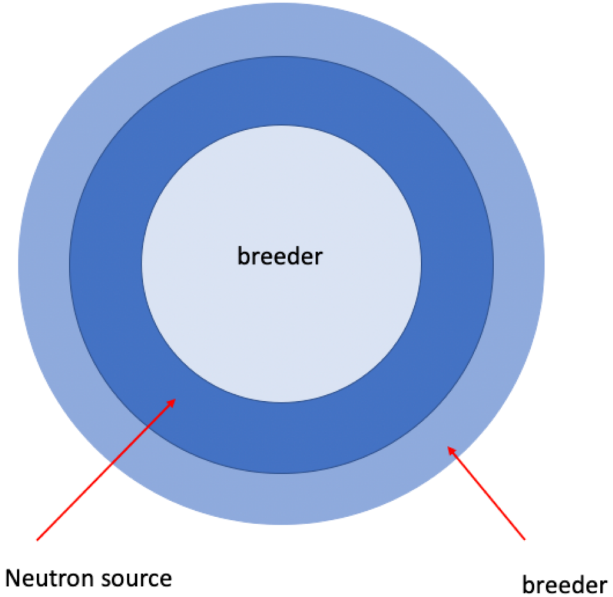
- Volume fractions based on CAD model (FW, BW, SW, DIV, He - manifold, BZ)
  - 16% RAMF, 2% SiC-SiC, 16.4% He, 0.45% Water and 0.5% W

		Mutiplier		RAFM (MF82H)		SiC-SiC		He		Water		W	
Breeder	Multiplier	TBR	Diff	TBR	Diff	TBR	Diff	TBR	Diff	TBR	Diff	TBR	Diff
LiAlO2	Be12Ti	2.1013	0%	1.5884	-27.8%	1.5665	-1.4%	1.4704	-1.6%	1.4630	-0.5%	1.2312	-17.2%
Li2tiO3	Be12Ti	2.1271	0%	1.6676	-24.2%	1.6449	-1.4%	1.5596	-1.3%	1.5514	-0.5%	1.3695	-12.5%
LiO2	Be12Ti	2.1656	0%	1.7903	-19.0%	1.7646	-1.4%	1.6870	-1.1%	1.6822	-0.3%	1.5833	-6.1%
Li2ZrO3	Be12Ti	2.1164	0%	1.6476	-24.9%	1.6216	-1.6%	1.5315	-1.4%	1.5322	0.0%	1.3268	-14.4%
Li4SiO4	Be12Ti	2.1459	0%	1.7143	-22.4%	1.6929	-1.3%	1.6018	-1.4%	1.5970	-0.3%	1.4381	-10.5%
Li4TiO4	Be12Ti	2.1494	0%	1.7041	-23.1%	1.6815	-1.3%	1.5931	-1.3%	1.5873	-0.4%	1.4174	-11.3%
Li4GeO4	Be12Ti	2.1320	0%	1.6838	-23.5%	1.6735	-0.6%	1.5836	-1.4%	1.5777	-0.4%	1.4132	-11.0%
Li8ZrO6	Be12Ti	2.1486	0%	1.7507	-20.4%	1.7249	-1.5%	1.6369	-1.3%	1.6388	0.1%	1.4996	-8.9%
LiAlO2	Be	2.4481	0%	1.8103	-30.0%	1.7868	-1.3%	1.6630	-1.8%	1.6622	0.0%	1.3826	-18.4%
Li2tiO3	Be	2.4211	0%	1.8685	-25.8%	1.8403	-1.5%	1.7304	-1.5%	1.7307	0.0%	1.5051	-13.9%
LiO2	Be	2.4472	0%	1.9750	-21.4%	1.9475	-1.4%	1.8565	-1.2%	1.8482	-0.4%	1.7292	-6.7%
Li2ZrO3	Be	2.4339	0%	1.8561	-26.9%	1.8280	-1.5%	1.7135	-1.6%	1.7070	-0.4%	1.4760	-14.5%
Li4SiO4	Be	2.4460	0%	1.9169	-24.3%	1.8871	-1.6%	1.7725	-1.6%	1.7705	-0.1%	1.5773	-11.5%
Li4TiO4	Be	2.4519	0%	1.9015	-25.3%	1.8774	-1.3%	1.7655	-1.5%	1.7569	-0.5%	1.5605	-11.8%
Li4GeO4	Be	2.4313	0%	1.8796	-25.6%	1.8594	-1.1%	1.7538	-1.5%	1.7454	-0.5%	1.5539	-11.6%
Li8ZrO6	Be	2.4438	0%	1.9464	-22.7%	1.9096	-1.9%	1.8104	-1.3%	1.8019	-0.5%	1.6372	-9.6%
LiAlO2	Be12V	2.1104	0%	1.5854	-28.4%	1.5531	-2.1%	1.4666	-1.4%	1.4609	-0.4%	1.2269	-17.4%
Li2tiO3	Be12V	2.1276	0%	1.6606	-24.7%	1.6366	-1.5%	1.5475	-1.4%	1.5408	-0.4%	1.3581	-12.6%
LiO2	Be12V	2.1610	0%	1.7809	-19.3%	1.7532	-1.6%	1.6808	-1.1%	1.6746	-0.4%	1.5742	-6.2%
Li2ZrO3	Be12V	2.1225	0%	1.6347	-26.0%	1.6118	-1.4%	1.5250	-1.4%	1.5261	0.1%	1.3194	-14.5%
Li4SiO4	Be12V	2.0875	0%	1.7065	-20.1%	1.6791	-1.6%	1.5947	-1.3%	1.5844	-0.6%	1.4381	-9.7%
Li4TiO4	Be12V	2.1507	0%	1.6943	-23.7%	1.6683	-1.5%	1.5851	-1.3%	1.5761	-0.6%	1.4036	-11.6%
Li4GeO4	Be12V	2.1299	0%	1.6763	-23.8%	1.6587	-1.1%	1.5703	-1.4%	1.5788	0.5%	1.4012	-11.9%
Li8ZrO6	Be12V	2.1603	0%	1.7398	-21.6%	1.7104	-1.7%	1.6328	-1.2%	1.6190	-0.9%	1.4891	-8.4%
Average Relative Difference			0.0%		-23.9%		-1.4%		-1.4%		-0.3%		-11.8%

Impact upon TBR due to blanket materials

Double breeding zone analysis

- Two breeding zones instead of one to represent inboard and outboard regions
  - IB and OB
- Neutron source placed between two regions
- Similar to the one-zone case, studies were performed with all additional materials



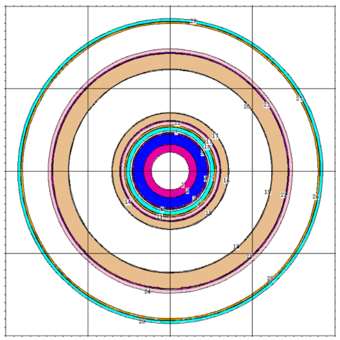
Representation of the two-breeder zone model

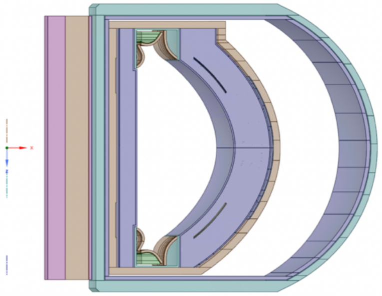
Breeder	Multiplier	TBR 1Z	TBR 2Z
LiAlO2	Be12Ti	**1.231**	**1.231**
Li2tiO3	Be12Ti	**1.369**	**1.369**
LiO2	Be12Ti	**1.583**	**1.583**
Li2ZrO3	Be12Ti	**1.327**	**1.328**
Li4SiO4	Be12Ti	**1.438**	**1.438**
Li4TiO4	Be12Ti	**1.417**	**1.417**
Li4GeO4	Be12Ti	**1.413**	**1.413**
Li8ZrO6	Be12Ti	**1.500**	**1.500**
LiAlO2	Be	**1.383**	**1.380**
Li2tiO3	Be	**1.505**	**1.511**
LiO2	Be	**1.729**	**1.728**
Li2ZrO3	Be	**1.476**	**1.467**
Li4SiO4	Be	**1.577**	**1.586**
Li4TiO4	Be	**1.560**	**1.562**
Li4GeO4	Be	**1.554**	**1.552**
Li8ZrO6	Be	**1.637**	**1.638**
LiAlO2	Be12V	**1.227**	**1.224**
Li2tiO3	Be12V	**1.358**	**1.357**
LiO2	Be12V	**1.574**	**1.575**
Li2ZrO3	Be12V	**1.319**	**1.323**
Li4SiO4	Be12V	**1.438**	**1.432**
Li4TiO4	Be12V	**1.404**	**1.402**
Li4GeO4	Be12V	**1.401**	**1.402**
Li8ZrO6	Be12V	**1.489**	**1.491**

TBR for 1 Zone and 2 Zone model with all materials homogenized (RAMF, W, He, H2O and SiC)

3-D and Reduced-Order Analysis

- 22.5-degree FNSF sector and its Reduced Order Model (ROM)
- Material composition from the most recent design
- Swapped PbLi for solid breeder and neutron multiplier in the 3D model
- The differences between the simplified and 3D versions are consistent for each solid breeder





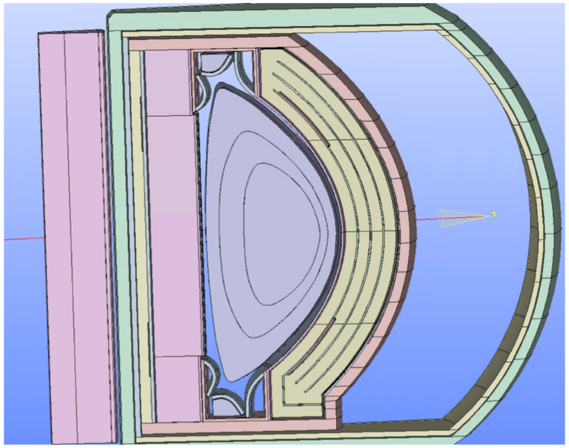
Reduced order model (left), FNSF sector (right)

Breeder	Multiplier	3D FNSF sector	1D Model	Difference 1D-3D	ROM	Difference ROM - 3D
LiAlO2	Be12Ti	1.251	1.231	1.6%	1.111	11.8%
Li2tiO3	Be12Ti	1.315	1.369	-4.1%	1.250	5.1%
LiO2	Be12Ti	1.434	1.583	-9.9%	1.487	-3.6%
Li2ZrO3	Be12Ti	1.297	1.327	-2.3%	1.209	7.0%
Li4SiO4	Be12Ti	1.355	1.438	-6.0%	1.331	1.8%
Li4TiO4	Be12Ti	1.344	1.417	-5.3%	1.298	3.5%
Li4GeO4	Be12Ti	1.307	1.413	-7.8%	1.307	0.0%
Li8ZrO6	Be12Ti	1.383	1.500	-8.1%	1.400	-1.2%
LiAlO2	Be	1.422	1.383	2.8%	1.239	13.7%
Li2tiO3	Be	1.470	1.505	-2.3%	1.373	6.8%
LiO2	Be	1.567	1.729	-9.8%	1.609	-2.6%
Li2ZrO3	Be	1.456	1.476	-1.4%	1.334	8.7%
Li4SiO4	Be	1.503	1.577	-4.8%	1.454	3.3%
Li4TiO4	Be	1.496	1.560	-4.2%	1.423	5.0%
Li4GeO4	Be	1.484	1.554	-4.6%	1.423	4.2%
Li8ZrO6	Be	1.528	1.637	-6.9%	1.516	0.8%
LiAlO2	Be12V	1.243	1.227	1.3%	1.100	12.2%
Li2tiO3	Be12V	1.309	1.358	-3.6%	1.244	5.1%
LiO2	Be12V	1.420	1.574	-10.3%	1.479	-4.1%
Li2ZrO3	Be12V	1.290	1.319	-2.2%	1.201	7.2%
Li4SiO4	Be12V	1.348	1.438	-6.4%	1.323	1.9%
Li4TiO4	Be12V	1.336	1.404	-4.9%	1.299	2.8%
Li4GeO4	Be12V	1.325	1.401	-5.6%	1.294	2.4%
Li8ZrO6	Be12V	1.375	1.489	-8.0%	1.388	-0.9%

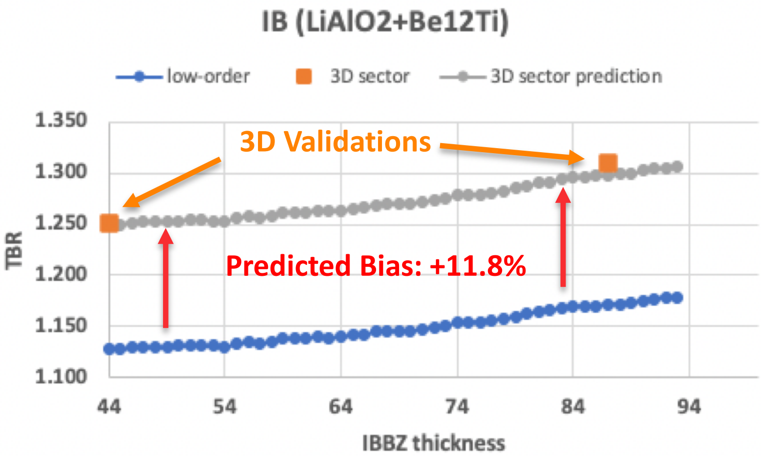
TBR comparison between 1D, ROM, and 3D sector models

IBBZ optimization

- Python script for automated generation of several **reduced-order-models** (ROMs) with homogenized materials (defined by user input) for quick automated execution
- Increase the thickness of In-Board Breeding Zone (IBBS) by ~50cm in 1cm increments
- Predicted the TBR for the 3D sector using the Predicted Bias
- Created a new FNSF sector with an 87cm thick IBBZ (Inboard Breeding Zone) to confirm bias
- Validated the results with 3D sector (base and modified)



Modified FNSF sector



IBBZ optimization study with ROMs

He & H Production, DPA, Heating

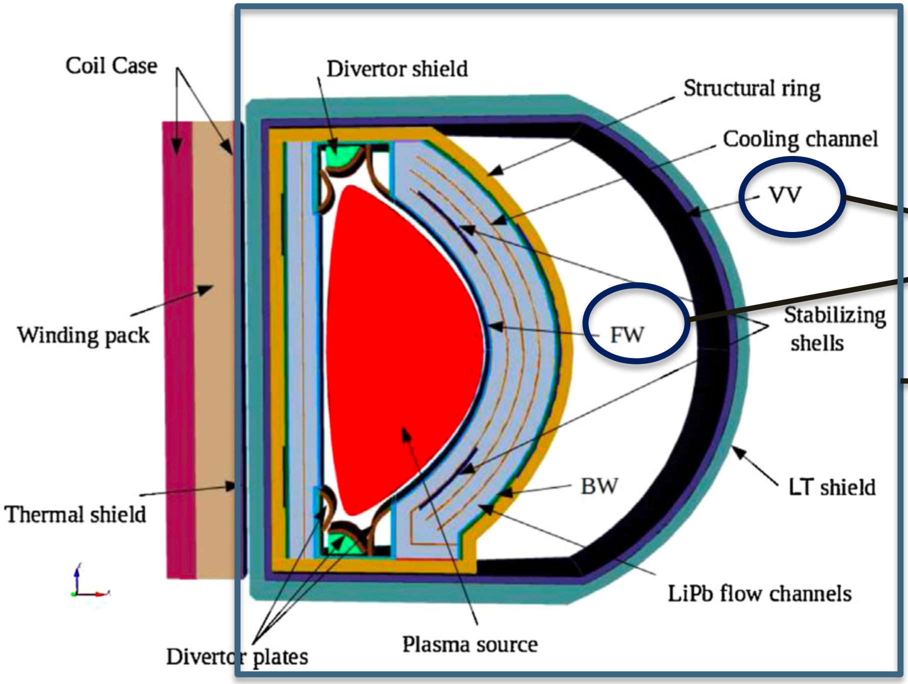


Figure 1. 3D CAD model of a single FESS-FNSF sector.[1]

DPA, helium & hydrogen production calculations

Nuclear heating regions

- F5 tally (point flux) for helium & hydrogen production in addition to dpa
  - MT=207 total helium production, MT=203 total hydrogen production
  - MT=444 (dpa) $\mathrm{DPA}_{\mathrm{NRT}} = \frac{0.8 \int \sigma_d dt\phi}{2E_d}$
- F6 tally was used: calculated energy deposition in MeV/g then multiplied by source term (S= $\frac{0.8 \times 518 \text{ MW}}{14.1 \text{ MeV}}$)

[1] Davis, A et al. "Neutronics Aspects of the FESS-FNSF." Fusion engineering and design 135 (2018): 271–278. Web.

Helium & Hydrogen Production & DPA in VV

IB VV He[appm/fpy]

UTK (2021)	DAVIS (2018)[1]	BOHM (2019)[2]	UTK (2022)*
0.3599 ± 29.51%	0.3109 ± 8.83%	0.09621 ± 1.6%	0.4123± 4.38%

IB VV H[appm/fpy]

UTK (2021)	DAVIS (2018)[1]	BOHM (2019)[2]	UTK (2022)*
0.1339 ± 31.47%	0.2462 ± 8.92%	0.418 ± 1.6%	0.2779 ± 4.01%

OB VV He[appm/fpy]

UTK (2021)	DAVIS (2018)[1]	BOHM (2019)[2]	UTK (2022)*
0.00704 ± 24.55%	0.0029 ± 13.81%	0.00244 ± 4.5%	0.00167 ± 10.47%

OB VV H[appm/fpy]

UTK (2021)	DAVIS (2018)[1]	BOHM (2019)[2]	UTK (2022)*
0.0280 ± 22.99%	0.0025 ± 12.99%	0.0107 ± 4.5%	0.0273 ± 9.78%

IB VV [DPA/fpy]

UTK (2021)	DAVIS (2018)[1]	BOHM (2019)[2]	UTK (2022)*
0.219 ± 2.00%	0.1495 ± 0.64%	0.0816 ± 0.6%	0.18576 ± 0.29%

OB VV [DPA/fpy]

UTK (2021)	DAVIS (2018)[1]	BOHM (2019)[2]	UTK (2022)*
0.001 ± 5.89%	0.0114 ± 0.36%	0.00348 ± 0.6%	0.00821 ± 0.86%

1. Davis, A et al. "Neutronics Aspects of the FESS-FNSF." Fusion engineering and design 135 (2018): 271–278. Web.
2. T.D. Bohm, et al. (2019) Initial Neutronics Investigation of a Liquid-Metal Plasma-Facing Fusion Nuclear Science Facility, Fusion Science and Technology, 75:6, 429-437, DOI: 10.1080/15361055.2019.1600930

Nuclear Heating

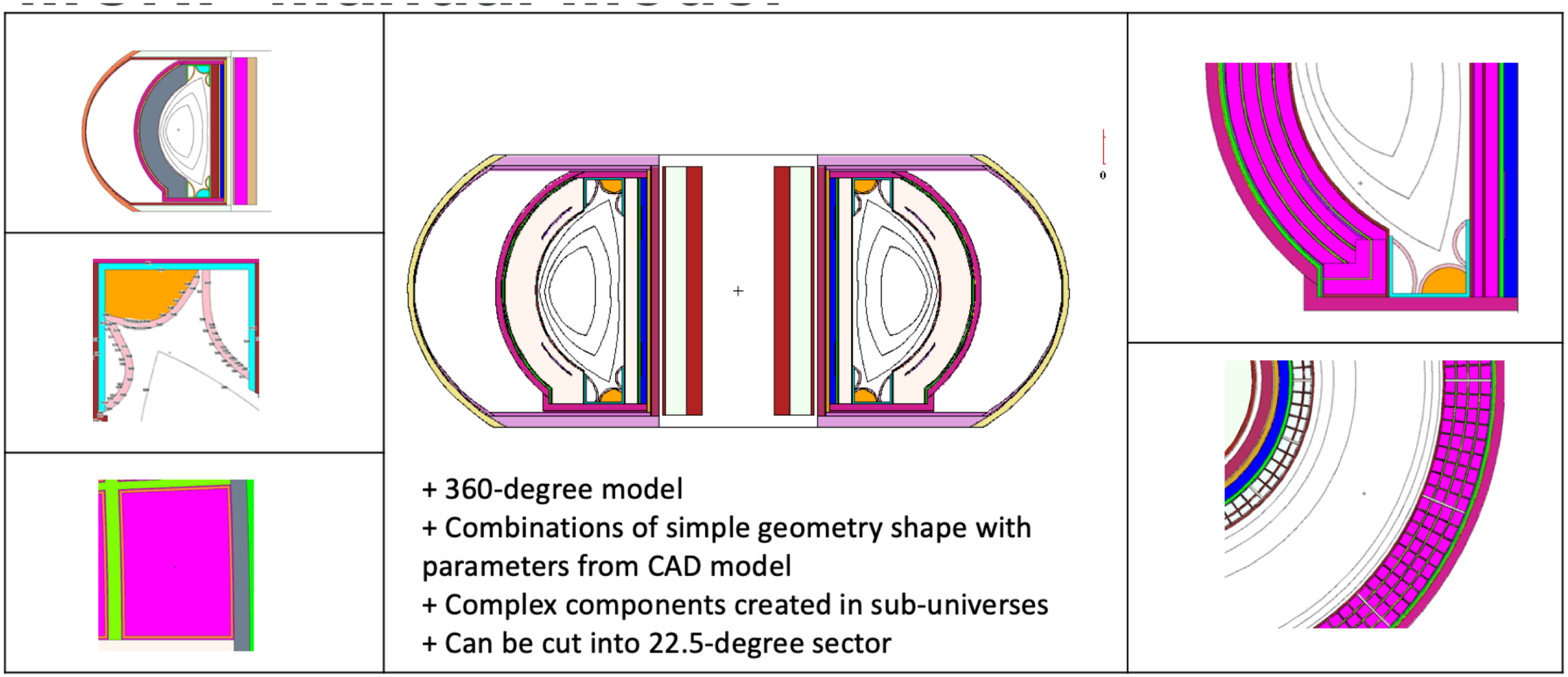
- Used reflective boundaries on boundaries of sector
- Total heating = 477.83±0.80%
- Comparison to Prior Works:
  - +0.45% higher than Davis, et al., (2018)[1] (475.70 MW)
  - -0.93% lower than Bohm, et al., (2019)[2] (482.29 MW)

	Neutron heating for 16 sectors (MW)	Gamma heating for 16 sectors (MW)	Total heating for 16 sectors (MW)
SR	6.83±4.82%	17.21±0.12%	24.04±2.47%
Divertor box and shield	3.45±0.10%	16.91±0.11%	20.36±0.11%
Divertor plates	1.34±0.07%	28.52±0.08%	29.86±0.08%
Lt shield	4.32±4.55%	5.21±0.20%	9.53±2.38%
VV	0.186±0.23%	4.42±0.21%	4.61±0.22%
OB	153.383±0.13%	138.73±0.26%	292.116±0.20%
IB	52.25±0.13%	45.06±0.22%	97.31±0.17%

1. Davis, A et al. "Neutronics Aspects of the FESS-FNSF." Fusion engineering and design 135 (2018): 271–278. Web.
2. T.D. Bohm, et al. (2019) Initial Neutronics Investigation of a Liquid-Metal Plasma-Facing Fusion Nuclear Science Facility, Fusion Science and Technology, 75:6, 429-437, DOI: 10.1080/15361055.2019.1600930

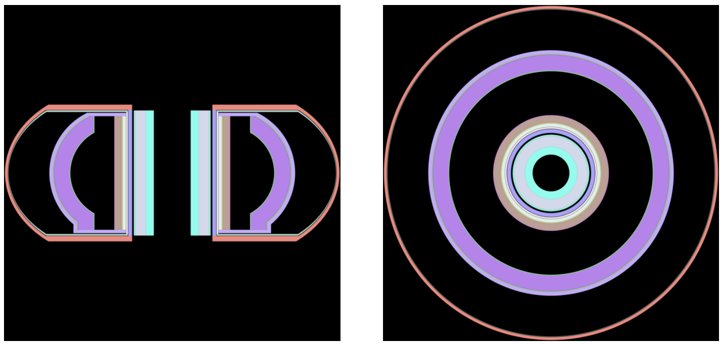
MCNP Manual Model

- Important alternative or backup to automated models which can often end up into a “wall of numbers” and can be very difficult to adjust/modify/optimize especially with regard to naming and labeling of regions.



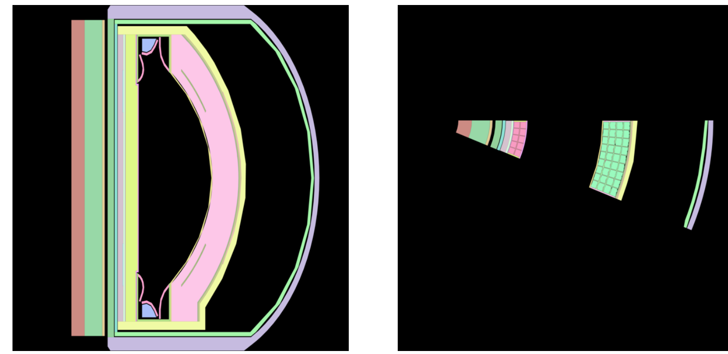
* C.J. Werner, et al., "MCNP6.2 Release Notes", Los Alamos National Laboratory, report LA-UR-18-20808 (2018).

SERPENT-based Models



Manual Model

+ Converted from MCNP manual model
+ 360-degree model
+ Homogenized blanket (using SERPENT’s mix)
+ 14.1 MeV neutron cell source
+ Source rate normalized to neutron flux from MCNP model



CAD-based Model

+ Generated using .stl CAD files
+ 22.5-degree sector model
+ 14.1 MeV neutron cell source
+ Source rate normalized to neutron flux from MCNP model

* Leppänen, J., et al. (2015) "The Serpent Monte Carlo code: Status, development and applications in 2013." Ann. Nucl. Energy, 82 (2015) 142-150.

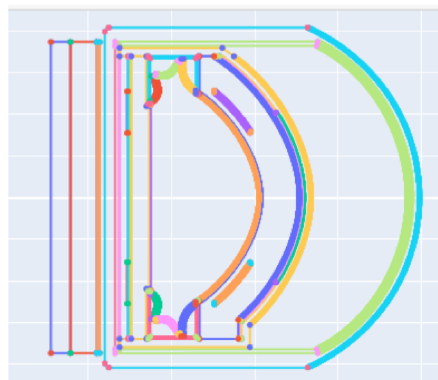
OpenMC model (using PARAMAK)

- **PARAMAK***

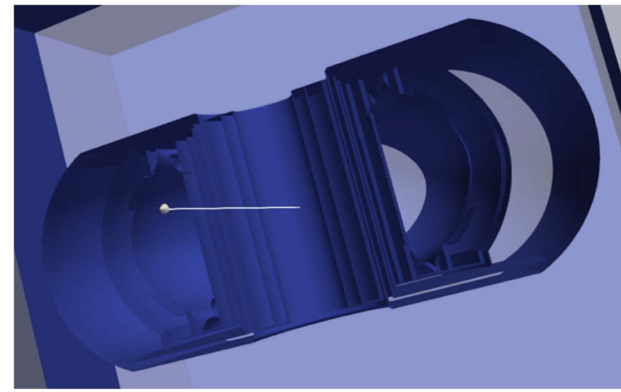
+ 2D plot created using points
+ Rotate 2D plot to create 3D model
+ Export 3D model into neutronics geometry (h5m)

- **OpenMC****

+ Neutronic simulation



x-z 2D plot



3D model

PARAMAK

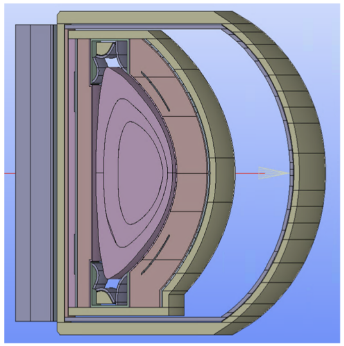
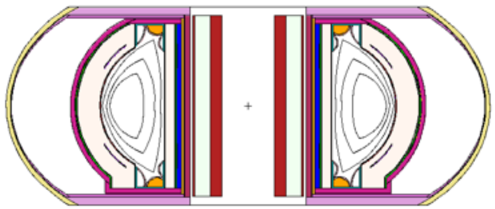
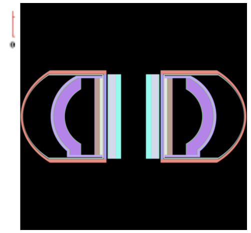
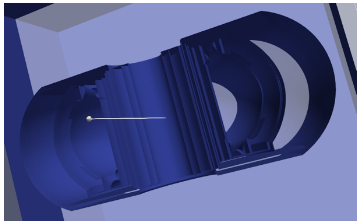
- Geometry
- Material
- Source

.h5m → OpenMC

*Shimwell J, Billingsley J, Delaporte-Mathurin R *et al.* The Paramak: automated parametric geometry construction for fusion reactor designs. [version 1; peer review: 2 approved]. *F1000Research* 2021, **10**:27 (https://doi.org/10.12688/f1000research.28224.1)

** Paul K. Romano, Nicholas E. Horelik, Bryan R. Herman, Adam G. Nelson, Benoit Forget, and Kord Smith, “OpenMC: A State-of-the-Art Monte Carlo Code for Research and Development,” Ann. Nucl. Energy, 82, 90–97 (2015).

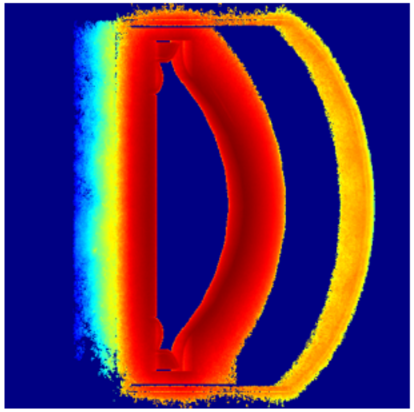
TBR comparison

Model	Davis, et al. (2018) *	MCNP w McCad	MCNP (manual model)		SERPENT		OpenMC
		22.5 sector Auto.	360-degree Manual	22.5 sector manual	Manual	CAD-based	
TBR	1.119	1.109	1.13	1.15	1.15	1.09	1.21
Diff	n/a	-0.9%	+1%	+2.8%	+2.8%	-2.6%	+8.1%

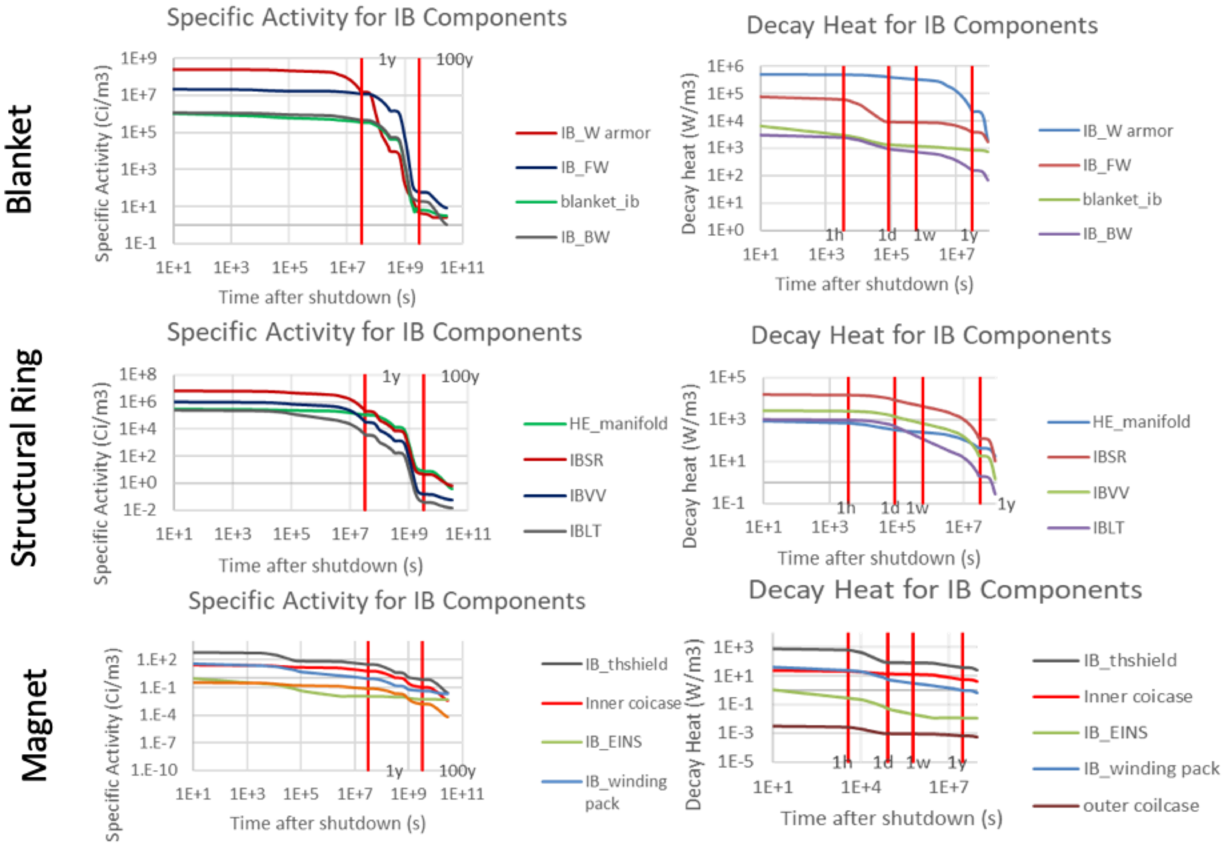
* Davis, A et al. “Neutronics Aspects of the FESS-FNSF.” Fusion engineering and design 135 (2018): 271–278. Web.

Activation Analysis for IB components (using SERPENT)



Relative flux at shutdown

- Plant lifetime ~24 years (~8.5 FPY)
- Assumed all tritium is extracted from blanket components
- FENDL3.1d



Thank you!

Questions?