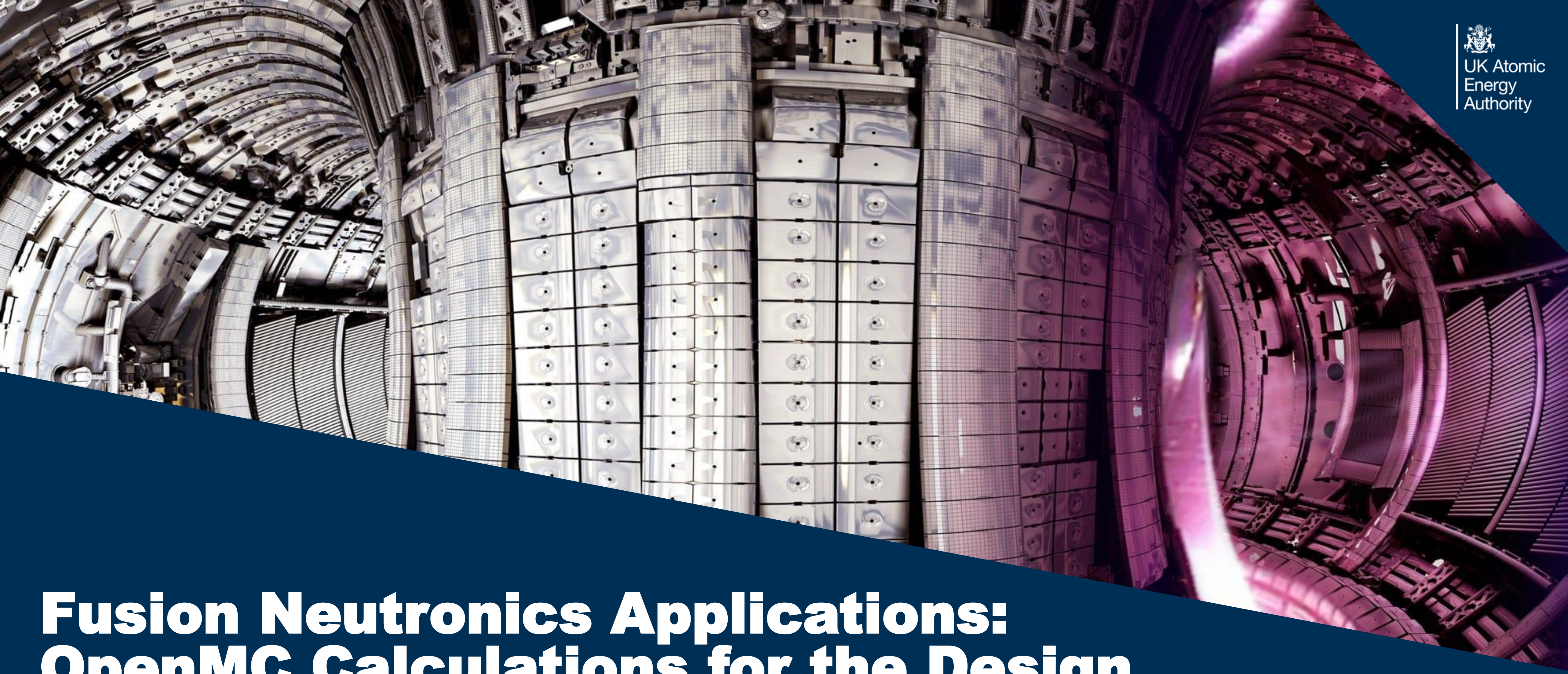

UK Atomic Energy Authority

Fusion Neutronics Applications: OpenMC Calculations for the Design of Fusion Reactors

James Hagues, Lee Packer

Contents

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Background and Basic OpenMC Fusion Calculations

James Hagues

Current Fusion Status Around the World

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Experimental fusion reactor being built in France that will be the largest experimental tokamak. First Plasma scheduled circa 2025. International collaboration with €22 billion construction budget.

Chinese reactor design intended to follow ITER and demonstrate net electricity and fuel self-sufficiency. Projected to be built in 2030s.

JET: Experimental fusion device in UK operating since 1984. Originally DD fusion but modified for DT fusion.

DEMO: Planned successor to ITER. Will produce 300 MW net electricity and incorporate tritium breeding.

UK spherical tokamak design programme to demonstrate net electricity generation. Currently in concept design phase. Completion targeted in 2040.

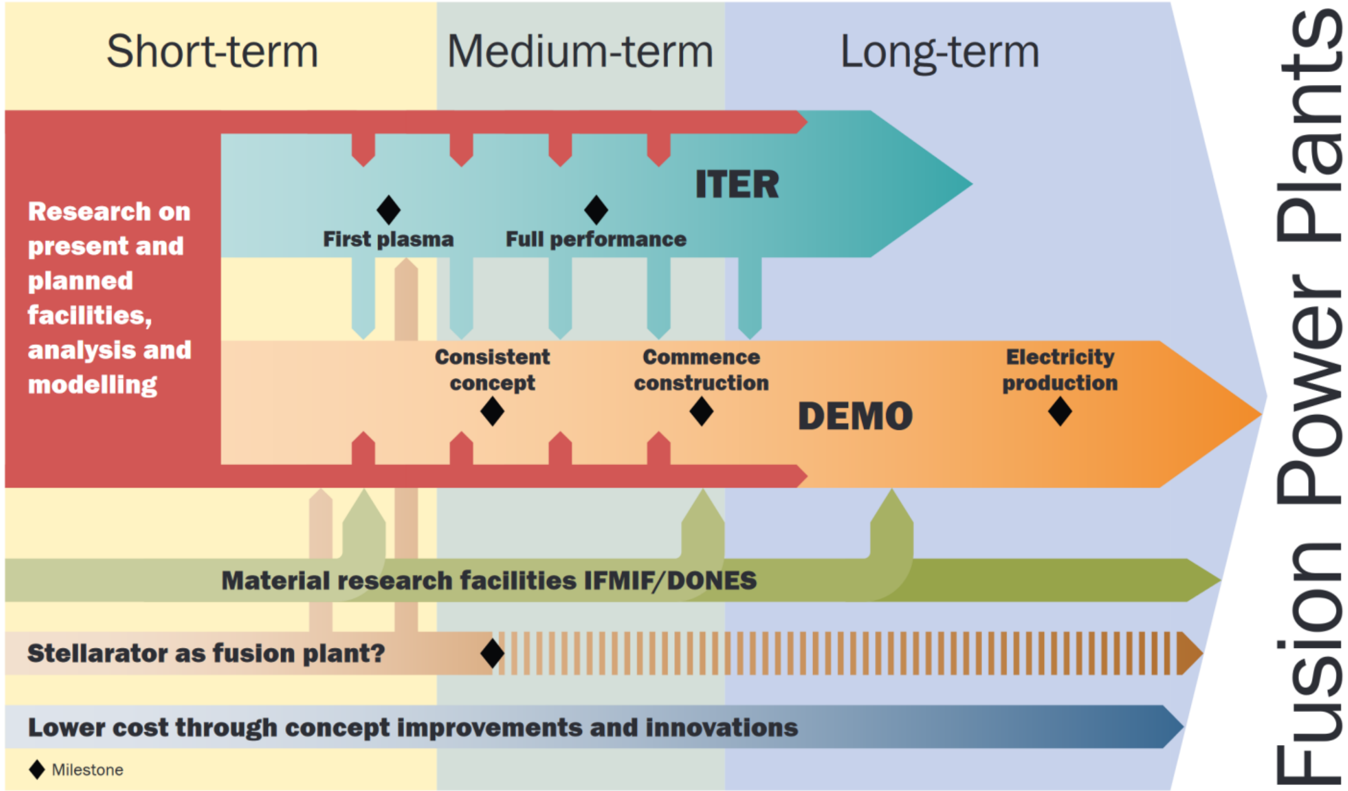
Over 40 private fusion companies. Most based in the USA and offer a wide range of approaches from stellarators to laser inertial confinement to liquid liner compressor. Over $6bn investment in private fusion.

EU fusion strategy

UK Atomic Energy Authority

The first comprehensive roadmap to powerplants

An ‘evidence-driven’ approach



UK fusion strategy

Department for Business, Energy & Industrial Strategy

UK Atomic Energy Authority

"Overarching goals of the fusion strategy

1. For the UK to demonstrate the commercial viability of fusion by building a prototype fusion power plant in the UK that puts energy on the grid.

2. For the UK to build a world-leading fusion industry which can export fusion technology around the world in subsequent decades."

Towards Fusion Energy

The UK Government's Fusion Strategy

October 2021

US fusion strategy

The White House published a decadal plan to deliver fusion which cites "the UK doubled its 24-year-old record" and "countries such as the UK and China are making major investments" in fusion amongst reasons for their raised ambitions.

The total US budget for fusion is currently $720M p.a., but the new plan is considering a budget considerably larger than this.

Already announced a new public-private partnerships programme now open.

China fusion strategy

Joined ITER to pursue ITER-like designs and aim to drive down cost through repetition. Have been designing a prototype powerplant called CFETR for 5+ years. In parallel, well progressed with building CRAFT – technology development facilities and now planning a JET-scale intermediate device called BEST by 2030 too

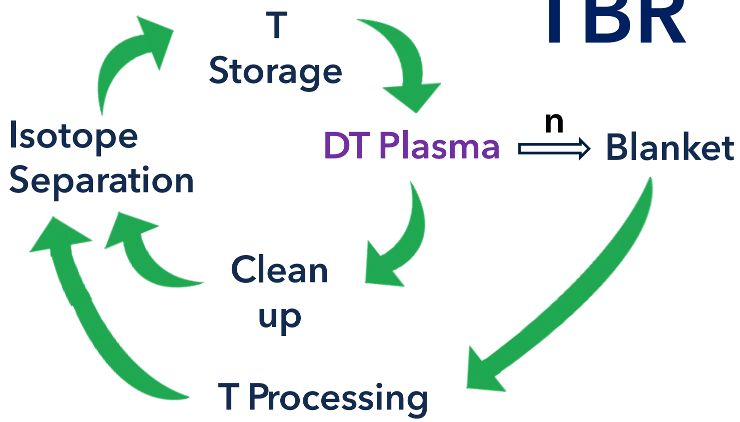
CFETR aiming for 2040 completion

What is OpenMC used for in Fusion Reactor Design?

OpenMC used for neutronics

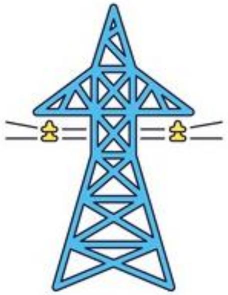
D + T $\longrightarrow$ α (3.5 MeV) + **n** (14.1 MeV)

TBR

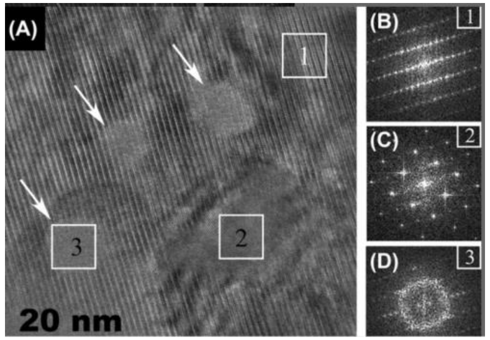


Nuclear Waste

Nuclear Heating



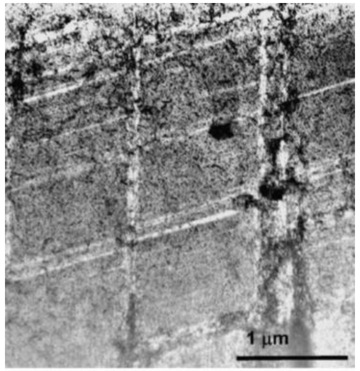
Inboard Shielding



YBCO: https://onlinelibrary.wiley.com/doi/10.1111/jmi.13078

Shutdown Dose Rates

Outboard Shielding

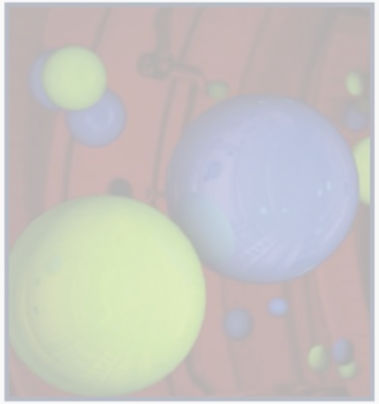


Steel: https://www.mdpi.com/1996-1944/14/10/2622/htm

Challenges of Fusion

Challenge 1

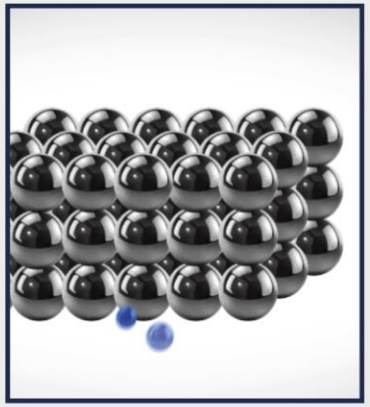
Confining the fuel at temperatures 10x hotter than the centre of the sun



Challenge 2

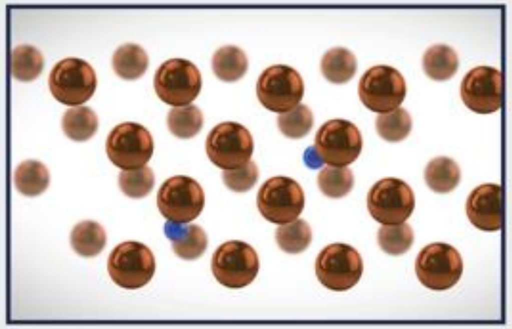
Neutrons damaging the walls atomic structure

OpenMC



Challenge 3

Exhausting extreme heat fluxes



Challenge 4

Breeding tritium and handling it

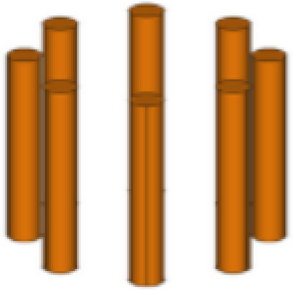
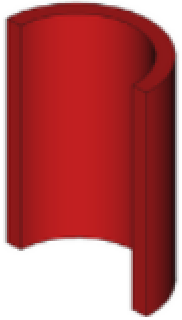
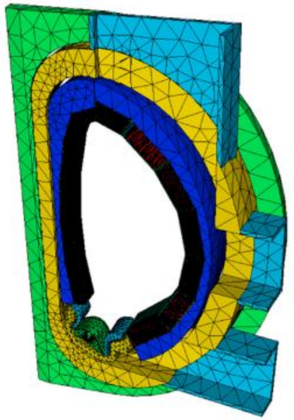
OpenMC

Challenge 5

Inside and outside need to be remotely maintained

OpenMC

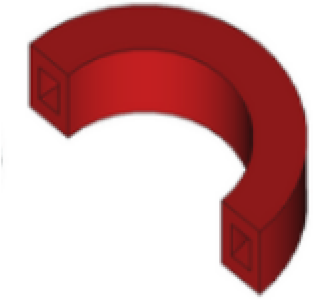
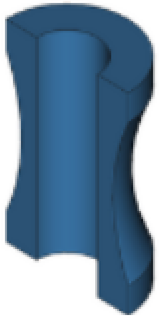
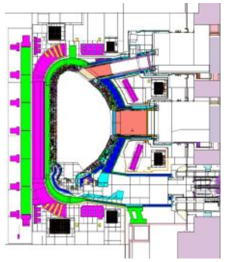
Neutronics Calculation Workflow

OpenMC

FISPACT-II

Script-generated CAD (Paramak [1]) → CAD-based transport model (DAGMC [2]) / Conversion to CSG → Radiation Transport Code (OpenMC [3]) → Inventory Codes (FISPACT II [4])

References

[1] Shimwell et al., The Paramak: automated parametric geometry construction for fusion reactor designs, Version 1. F1000Res. 2021; 10: 27

[2] https://github.com/svalinn/DAGMC

[3] Romano, Paul K. & Forget, Benoit. “The OpenMC Monte Carlo Particle Transport Code.” Annals of Nuclear Energy 51 (January 2013): 274–281

[4] FISPACT-II 5.0, NEA-1890/06, 11/01/2022

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Neutronics model approaches in the design lifecycle

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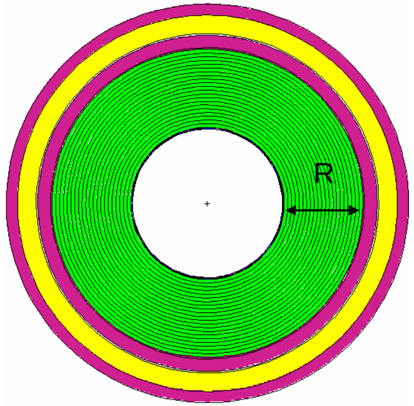
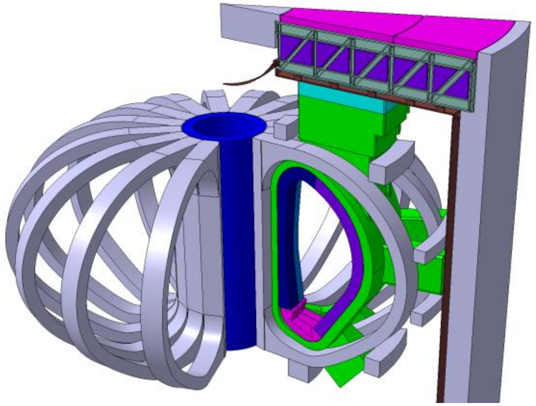
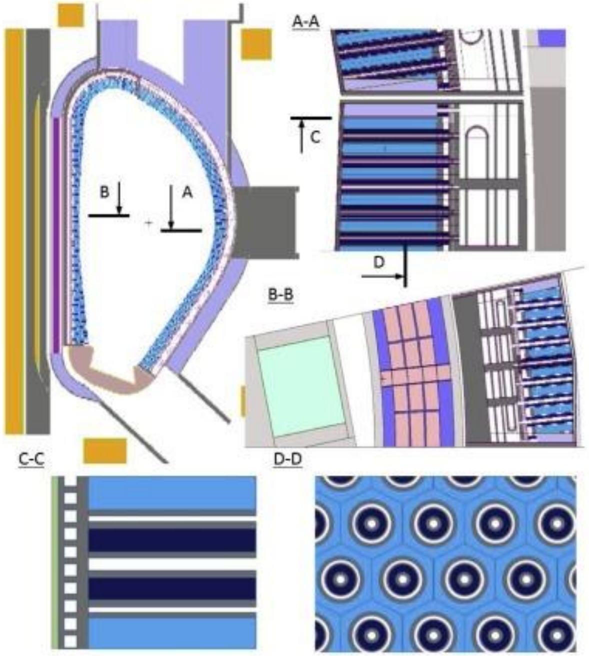
Scoping studies → Conceptual studies → Preliminary design(s) → Detailed design



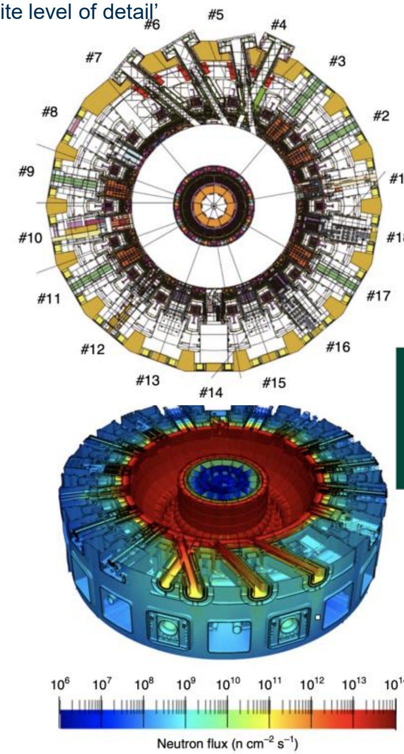




U. Fischer et al., Fus. Eng. Des. **155** (2020)

EUROfusion

'E-lite level of detail'



UNED

R. Juarez et al., Nature Energy **6** 150–157 (2021)

Homogenised materials, simplified parameter studies: down-selection, explore viability

Generally, though not always, neutronic performance reduces as designs progress (models become more detailed, gaps, structures, etc.….)

TBR – Blankets

- UKAEA blanket tools OpenMC:
  - RaBBIT – a collection of low-fidelity analysis modules for performing parameter sweeps and understanding blanket design space
  - Parablank – Parametric Blanket CAD/Volume Fractions/Flow Networks
  - Aurora [1] – Multiphysics codes
- Allow quick approximate calculations for blanket concepts and detailed analysis of single blanket modules.
- Allow different design ideas to be explored easily.

OpenMC Code for calculating TBR

```
tallies = openmc.Tallies()
tally_id = 0

# Reactor Totals

tally_id = tally_id + 1
tally = openmc.Tally( tally_id = tally_id, name = 'tbr_total')
tally.scores = ['(n,Xt)']
tallies.append( tally )


# Cell Scores

tally_id = tally_id + 1
tally = openmc.Tally( tally_id = tally_id, name = 'tbr_by_cell')
tally.filters = [all_cell_filter]
tally.scores = ['(n,Xt)']
tallies.append( tally )
```

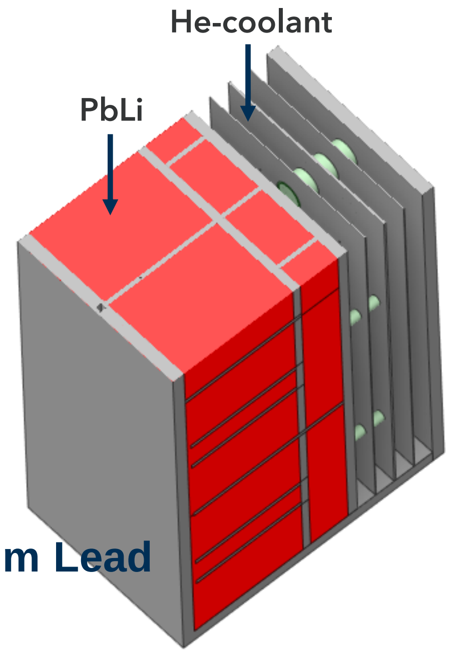
Key tritium production and multiplication reactions

$$^{6}\text{Li} + n \longrightarrow \alpha + T \quad + 4.78\ \text{MeV}$$ [1]

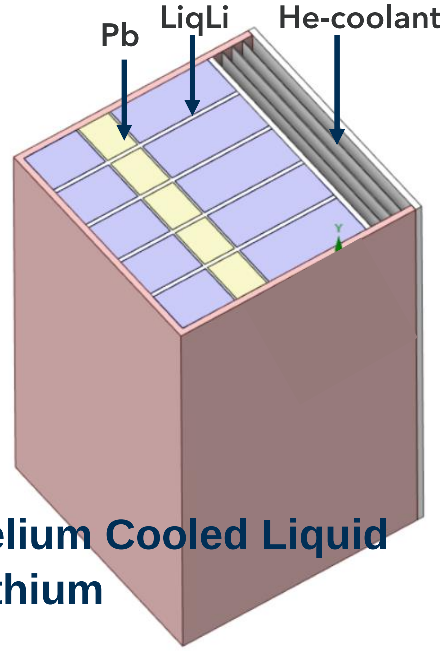
$$^{7}\text{Li} + n \longrightarrow \alpha + T + n' - 2.47\ \text{MeV}$$

$$^{9}\text{Be} + n \longrightarrow 2\alpha + 2n' \quad - 2.5\ \text{MeV}$$

$$^{208}\text{Pb} + n \longrightarrow {}^{207}\text{Pb} + 2n' \quad - 7.4\ \text{MeV}$$



Lithium Lead



Helium Cooled Liquid Lithium

References: [1] https://github.com/aurora-multiphysics

TBR Impact of Aspect Ratio and Elongation

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- A larger non-breeding central column is detrimental to TBR as neutrons are absorbed and moderated.
- The impact of aspect ratio on TBR varies depending on the inboard materials.
- A higher elongation reduces divertor coverage, which can improve TBR.
- Paramak was built to easily vary these parameters and assess changes.

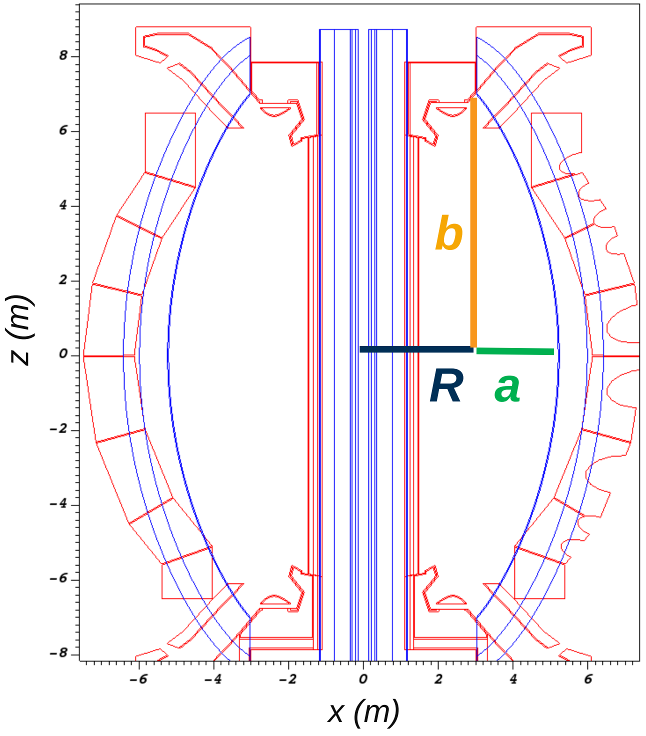
```
aspect_ratio = 2.0
minor_radius = 200.0
major_radius = minor_radius * aspect_ratio

inboard_shield_thickness = (major_radius
                            - minor_radius
                            - inner_bore_radial_thickness
                            - inboard_tf_leg_radial_thickness
                            - inner_plasma_gap_radial_thickness )

my_reactor = paramak.BallReactor(
    inner_bore_radial_thickness =            20.,
    inboard_tf_leg_radial_thickness =        60.,
    center_column_shield_radial_thickness = inboard_shield_thickness,
    inner_plasma_gap_radial_thickness =      15.,
    plasma_radial_thickness =                2 * minor_radius,
    outer_plasma_gap_radial_thickness =      20.,
    firstwall_radial_thickness =             3.,
    blanket_radial_thickness =               100.,
    blanket_rear_wall_radial_thickness =     50.,
    divertor_radial_thickness =              0.9 * minor_radius,
    elongation =                             elongation,
    triangularity =                          triangularity,

    number_of_tf_coils=                      None,

    rotation_angle =                         360,
    divertor_position =                      'both'
)
```

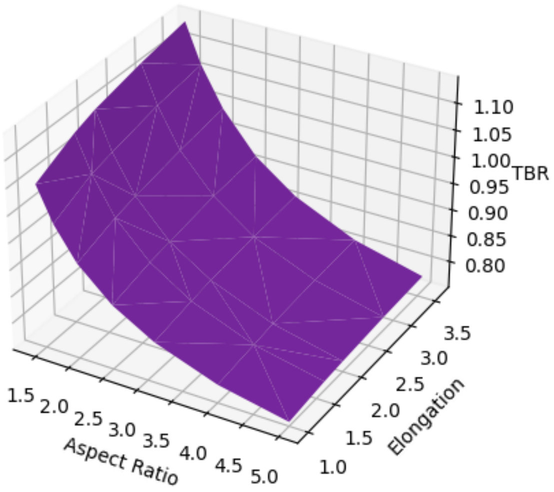


Spherical Tokamak (red) vs. ARIES-ST (blue)

$$aspect\ ratio = \frac{R}{a}$$

$$elongation = \frac{b}{a}$$

TBR sensitivity to Aspect Ratio and Elongation for a reactor without inboard or divertor breeding



$$R = major\ radius$$
$$a = minor\ radius$$

- **The aspect ratio can have a TBR impact of ~0.05**
- **The elongation can have a TBR impact of ~0.01**

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TBR Uncertainty and Experiments

Lee Packer

Discussion: concepts of required and design target TBR

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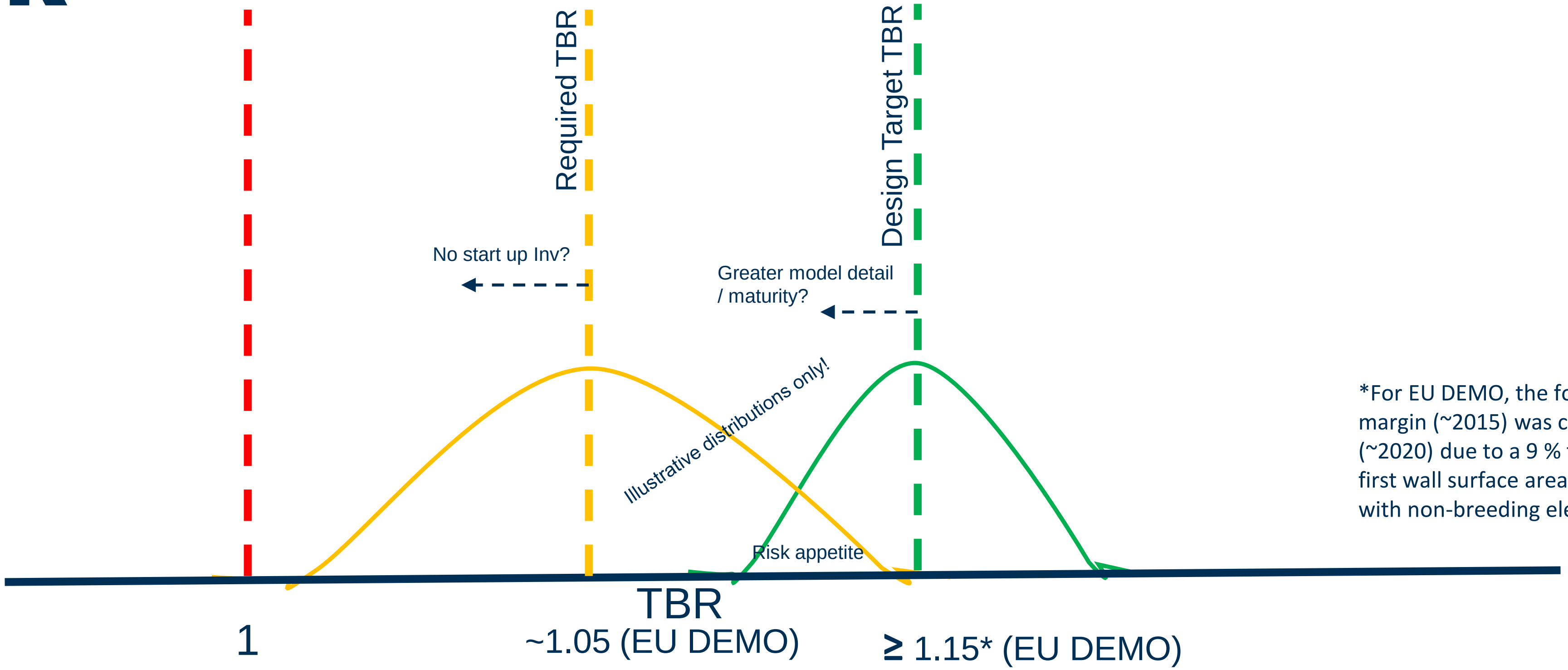


*For EU DEMO, the former 5% additional margin (~2015) was changed to 10% (~2020) due to a 9 % fraction of the DEMO first wall surface area that will be covered with non-breeding elements.

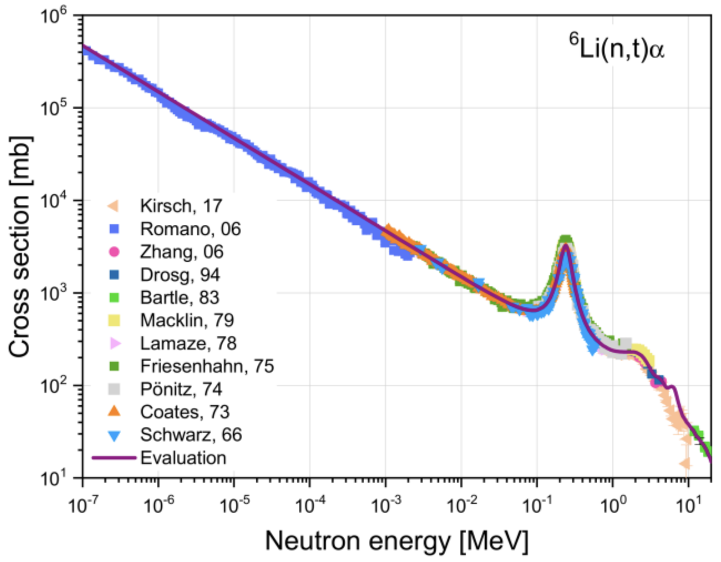
The ***required*** **TBR**, depends on several factors, well-documented in the various papers e.g. M. Abdou et al. 2021 Nucl. Fusion 61 013001, M Sawan et al., Fus. Eng. Des. **81** 1131–44. These include T extraction, plasma fuel burn-up performance, technological & temporal aspects of the fuel cycle and need for start-up inventory for example. [see analyses for reduced D–T cycle times: M Coleman, FED **141** (2019)]

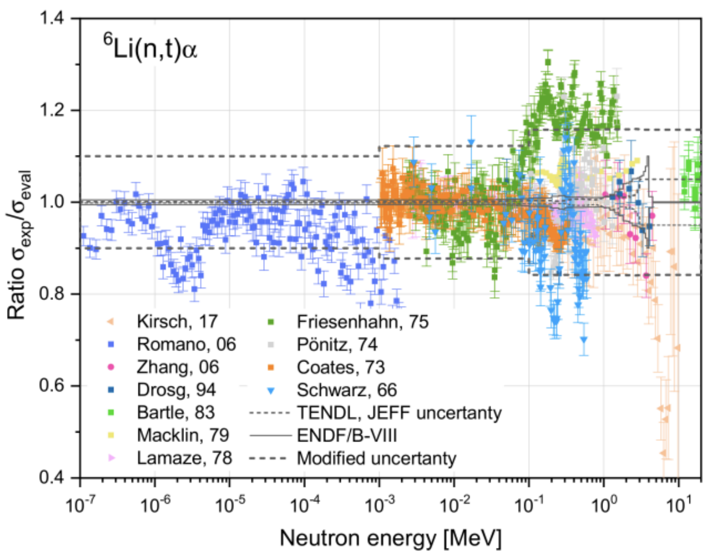
The ***design target*** **TBR** is an additional margin to the *required* TBR. It derives from the uncertainty in neutronics modelling e.g. geometry, materials, nuclear data and the maturity of design (an added margin for components not yet included/designed, ΔCM). This knowledge and an appropriate confidence level (appetite for risk) can be used to set a target TBR. [Fischer FED **155** (2020) refers to the ΔCM margin - incomplete Computational Model]

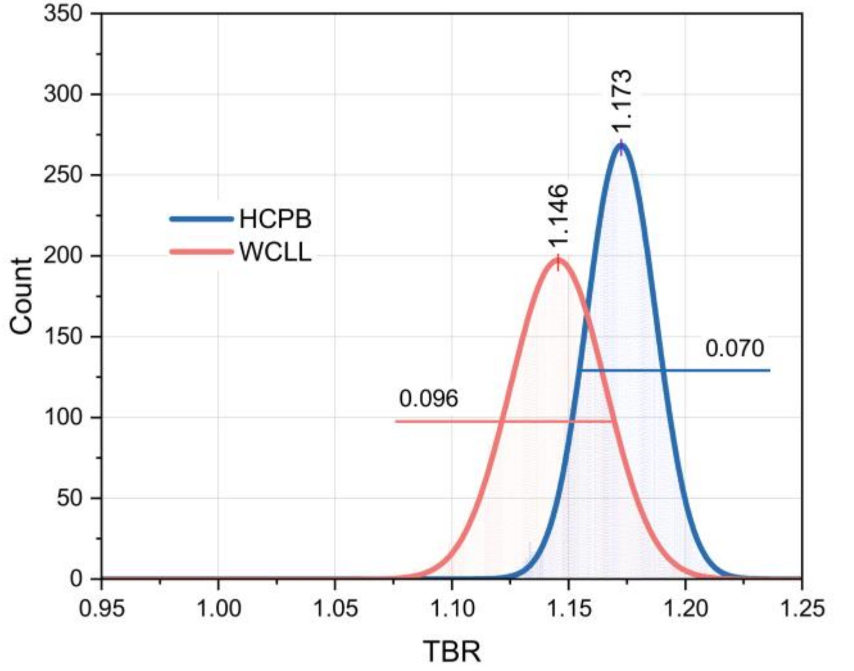
Total Monte Carlo approaches: EU DEMO TBR and uncertainty estimates for HCPB and WCLL

See J Park et al. Statistical Analysis of Tritium Breeding Ratio Deviations in the DEMO Due to Nuclear Data Uncertainties, Appl. Sci. 2021, 11, 5234. https://doi.org/10.3390/app11115234

Nuclear data uncertainties and impact on computational assessment of TBR







TBR distribution using TENDL-2017 data with random files for each nuclide and 300 random files for n+^{56}Fe from JEFF-3.2

Recommended that this type of approach is used early in the reactor TBR design lifecycle

Uncertainty +/- 0.035 & 0.048 (1 sigma) HCPB, WCLL respectively

EU Tritium breeding experiments – C/E comparisons

- Validation of **Tritium production rate** calculations for EU **breeder blanket concepts**
- Reduction of uncertainties in TBM & blanket design

▪ **Helium Cooled Pebble Bed (HCPB)**
- ✓ Be as neutron multiplier
- ✓ Li ceramics pellets as breeder material

▪ **Helium Cooled Lithium Lead (HCLL)**
- ✓ LiPb eutectic alloy as breeder/neutron multiplier

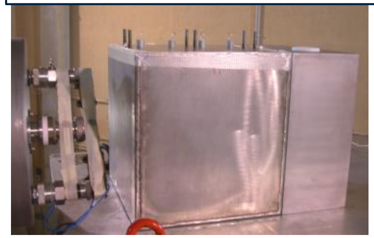
▪ **Water Cooled Lithium Lead (WCLL)**
- ✓ LiPb eutectic alloy as breeder/neutron multiplier
- ✓ Water as coolant

Current EU DEMO studies based on HCPB & WCLL concepts → ITER TBM tests

Participants: ENEA, KIT, JSI, UKAEA, JAEA

Neutronics experiment at the FNG

HCPB TBM mock-up* 2007

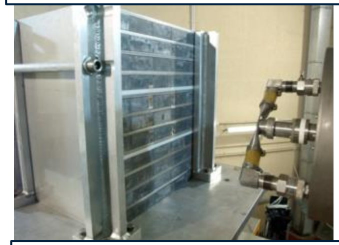


TPR C/E 0.85-0.95 – ΔC/E ~ $\pm$8 - 10% (2σ)

conservative prediction

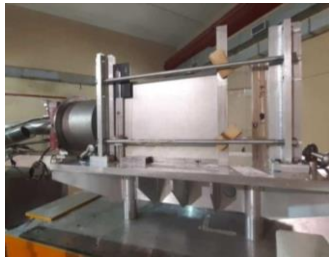
* Now installed at JET (31 cm side box)

HCLL TBM mock-up 2011



TPR C/E ~1 within the total uncertainties (~$\pm$12% -2σ)

WCLL mock-up 2021-2022



Decrease of the TPR C/E ratio with depth in the mockup

Under investigation

ENEA

EUROfusion

P. Batistoni, NF,52, 083014 (2012), Flammini, FED,156, 111600 (2020)

Slide adapted from R. Villari (ENEA), The role of FNG in fusion neutronics benchmarks, March 2023

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Japanese experiments (2006)

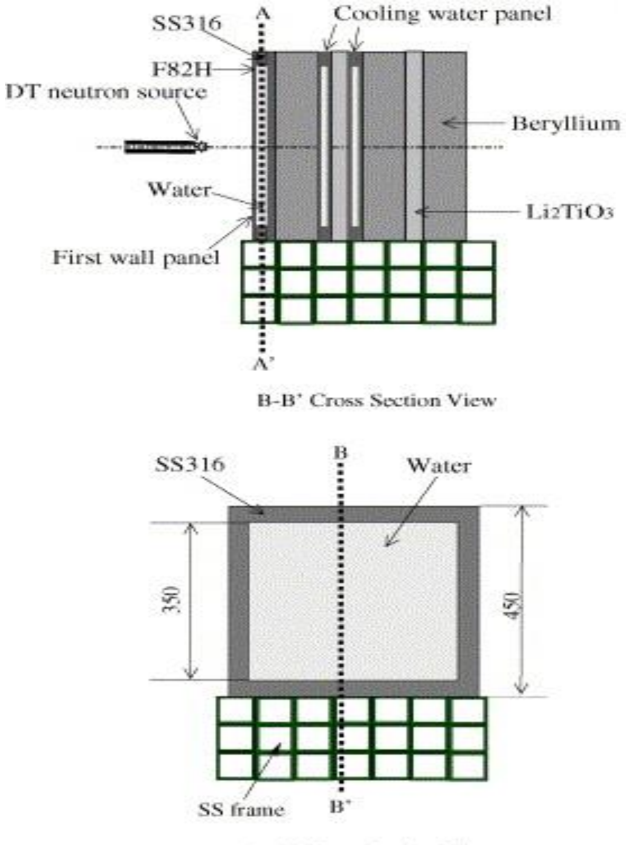
Paper: Sato et al., Progress in the blanket neutronics experiments at JAERI/FNS, FED (2006)

The conservative finding of tritium breeding experiments is not universal

Overpredictions of tritium production with C/E values up to ~1.13 were reported following experiments at the FNS in Japan by Sato et al. Fus. Eng. Des. **81** 1183–93 (2006).

The C/Es of the integrated tritium productions are 1.01–1.04 and 1.11–1.13 in the blanket mockup integral experiments without and with the neutron reflector, respectively

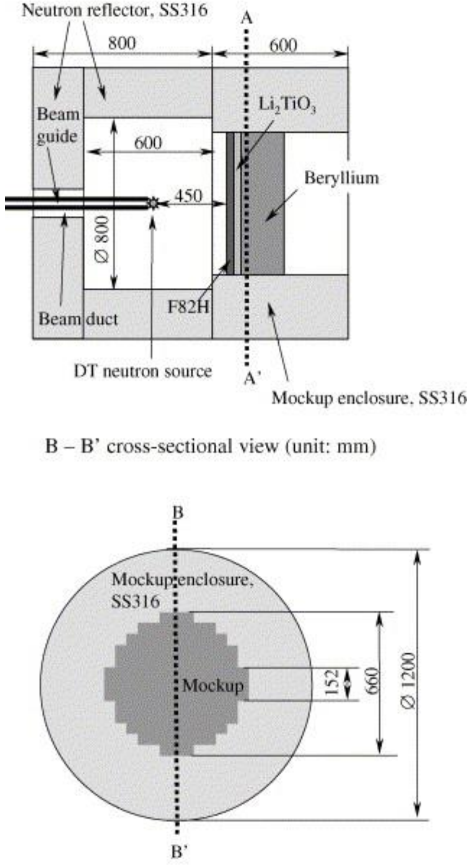
Without reflector



B-B' Cross Section View

A-A' Cross Section View

With reflector



B – B' cross-sectional view (unit: mm)

A – A' cross-sectional view (unit: mm)

In a 2008 paper by Sato et al. improved agreement was suggested considering scattering XS modifications to Fe-56 and Be-9: 'nuclear data is somewhat unreliable in the part of the angular distributions of iron and beryllium scattering in backward directions'
https://doi.org/10.1016/j.fusengdes.2008.08.004

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Further OpenMC Neutronics Calculations

James Hagues

Neutronics Models

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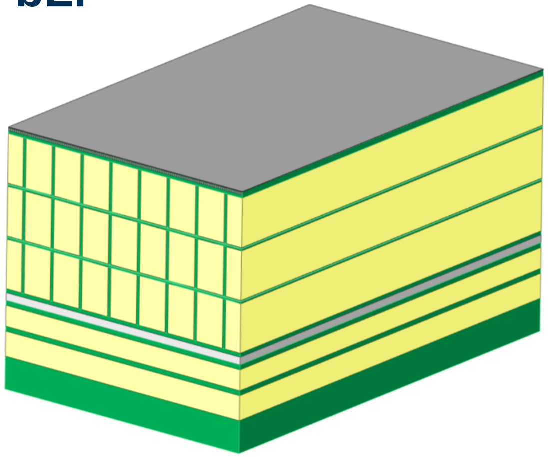
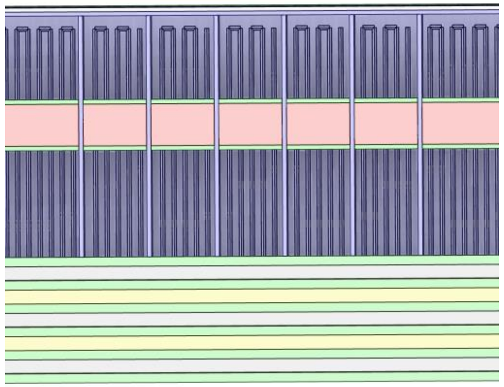
PbLi

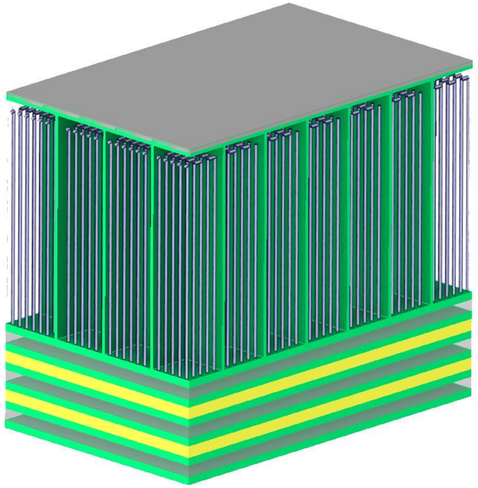


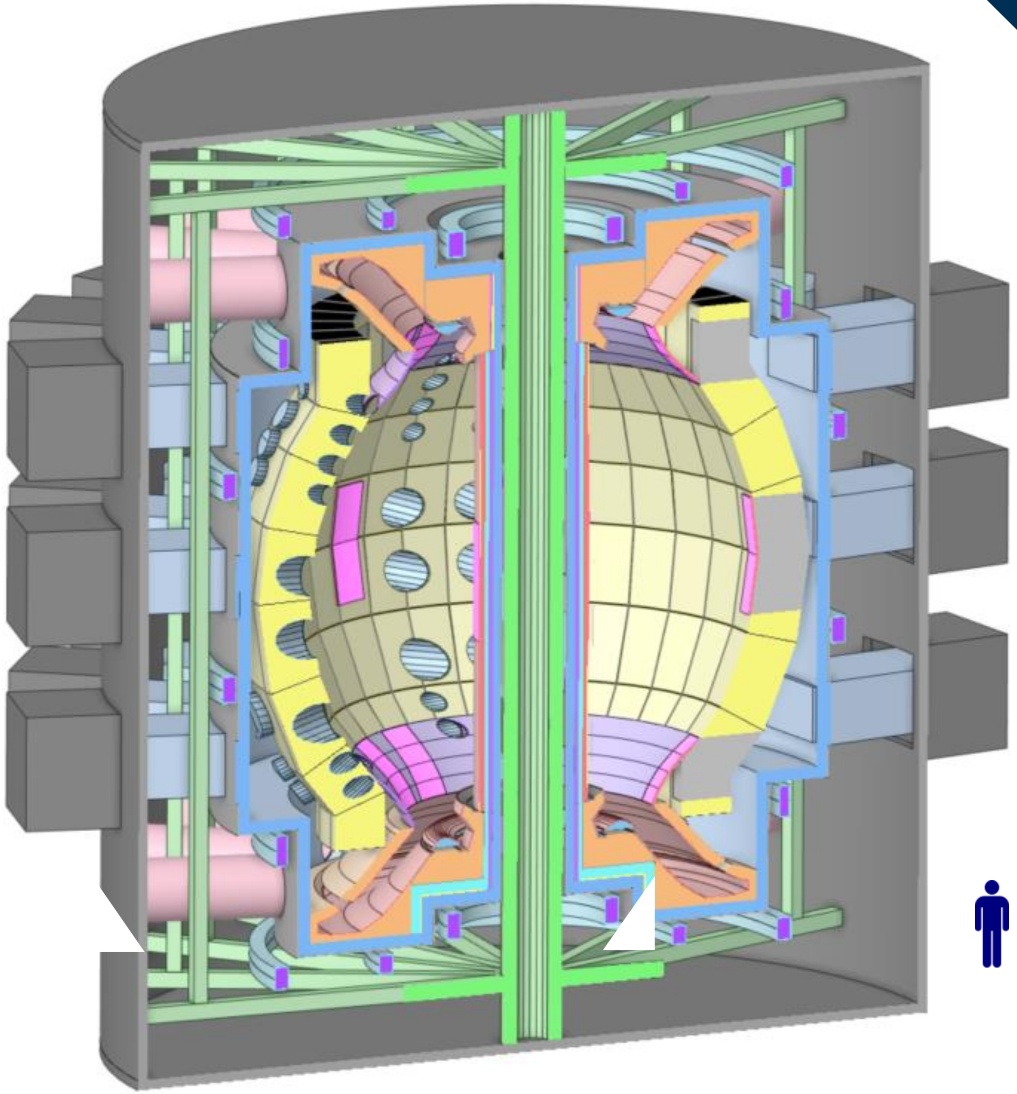
- OpenMC can be used for neutronics calculations in large and detailed models.
- Essential variance reduction weight window feature now implemented (v0.13).
- Mesh tally features and powerful source routine enabled.

HCLi w/ Pb multiplier



HCLi





OpenMC Universe Structure for a Fusion Reactor

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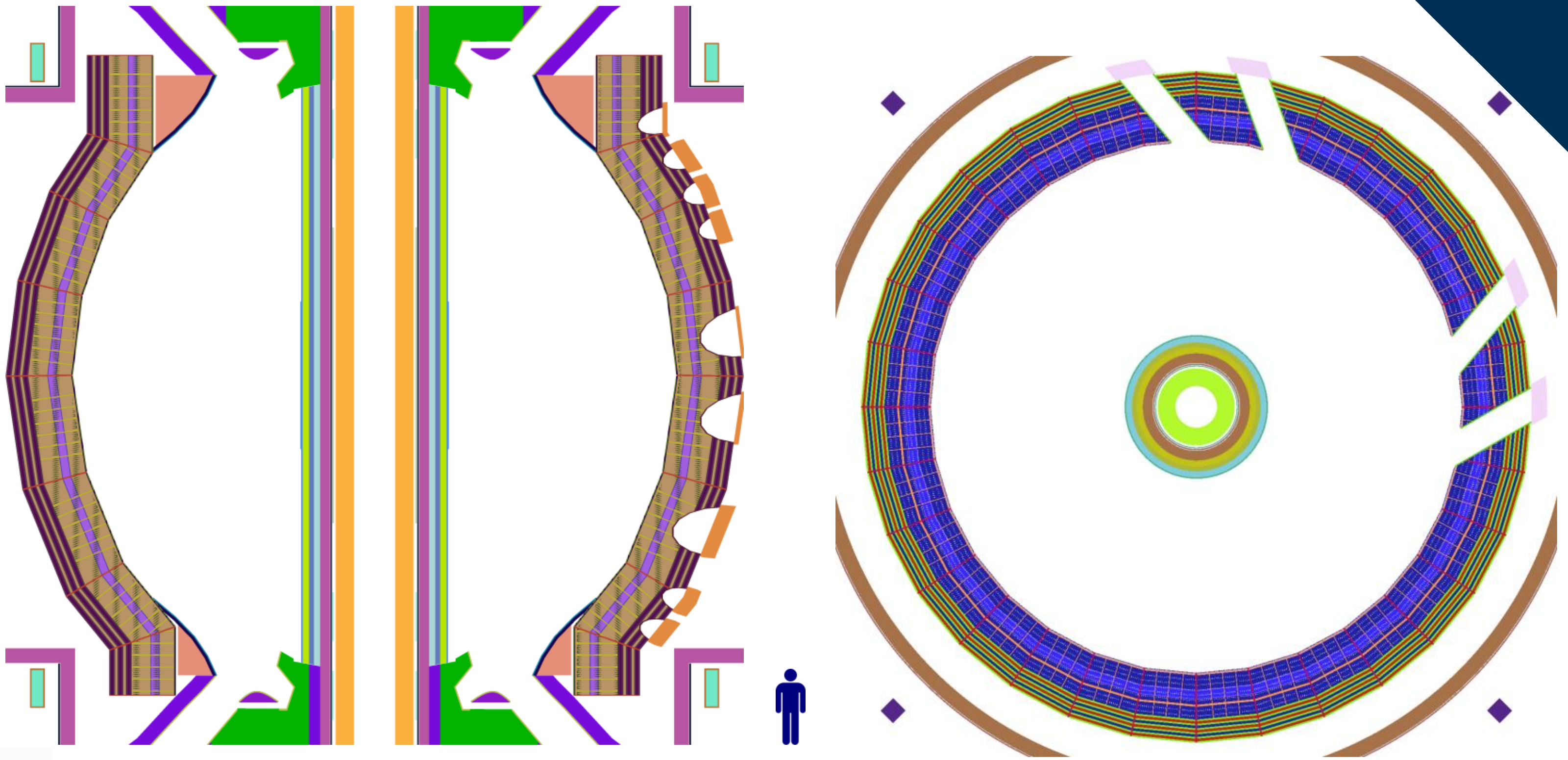
- The OpenMC universe capability allows repeated structures to be efficiently defined by the code.
- This example shows a detailed breeder blanket structure translated and rotated through each module of the reactor.
- Rotation is specified by a rotation matrix and translation by a vector.
- A DAGMC universe can fill a container cell.



In the python API the rotation applied is an intrinsic rotation with specified Tait-Bryan angles:

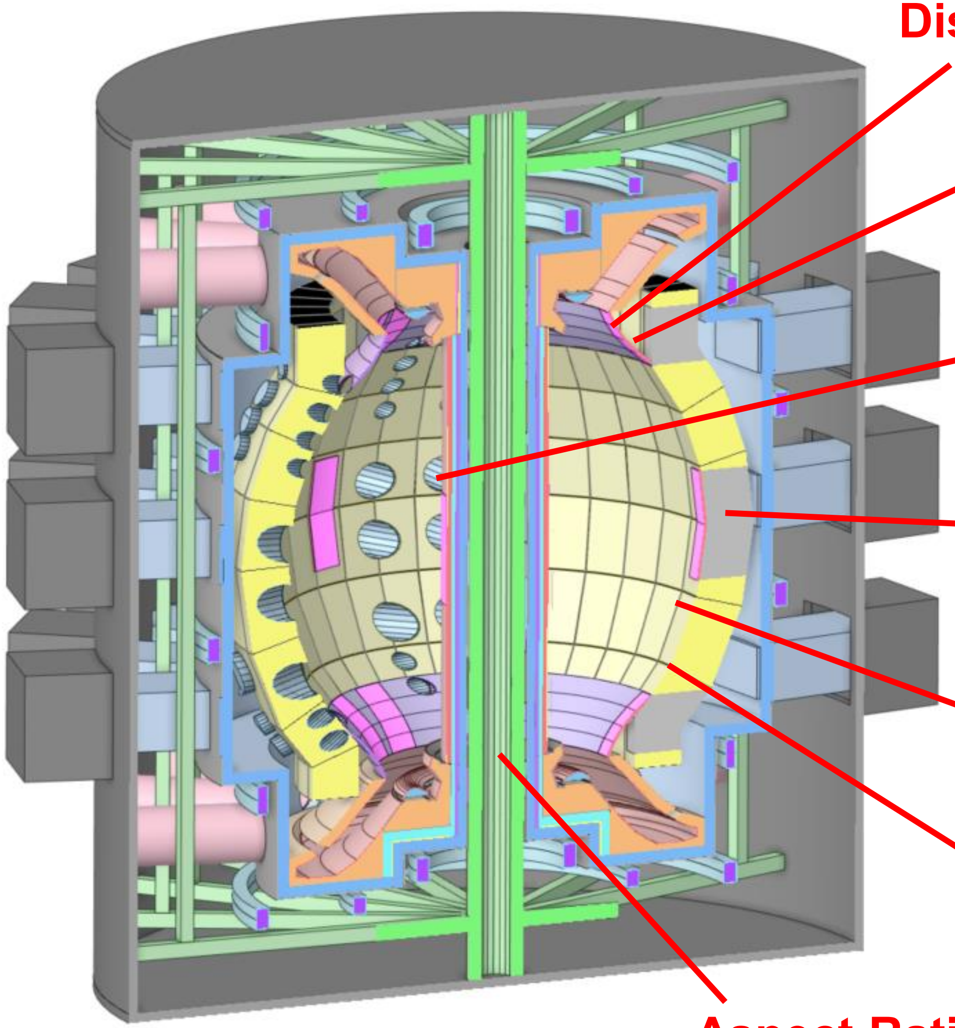
$$R_z(\psi)R_y(\theta)R_x(\phi)$$

$$\begin{bmatrix} \cos\theta\cos\psi & -\cos\phi\sin\psi + \sin\phi\sin\theta\cos\psi & \sin\phi\sin\psi + \cos\phi\sin\theta\cos\psi \\ \cos\theta\sin\psi & \cos\phi\cos\psi + \sin\phi\sin\theta\sin\psi & -\sin\phi\cos\psi + \cos\phi\sin\theta\sin\psi \\ -\sin\theta & \sin\phi\cos\theta & \cos\phi\cos\theta \end{bmatrix}$$

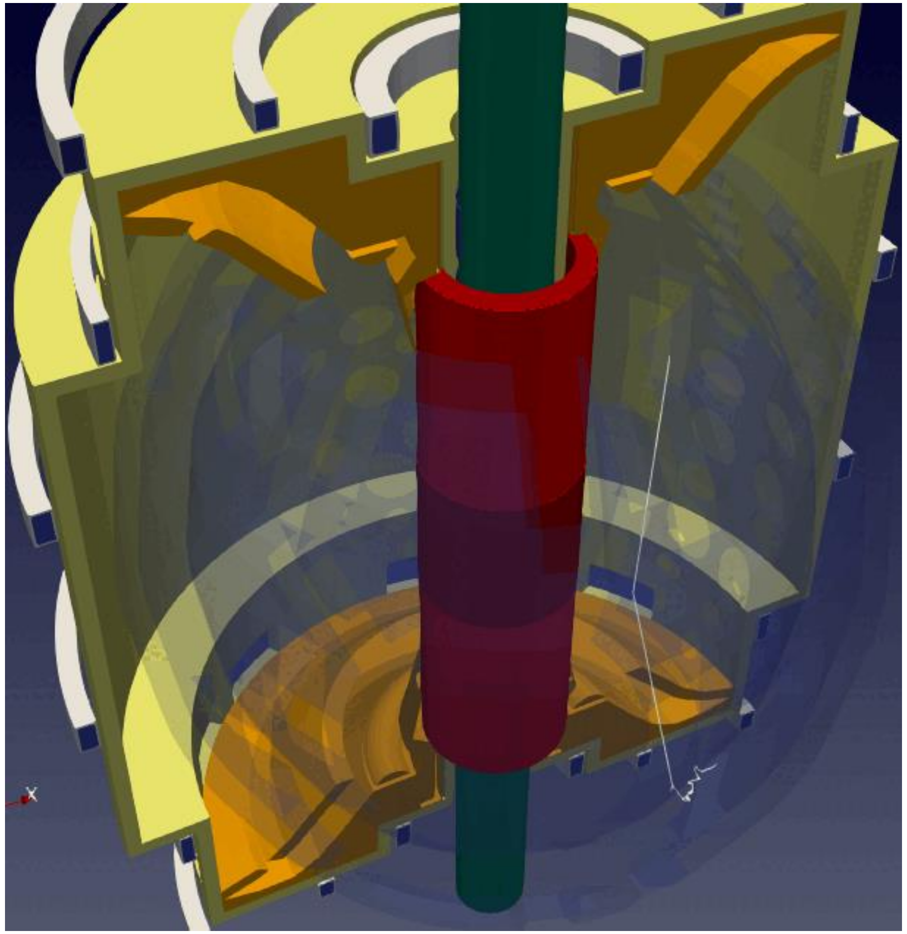
```
<dagmc_universe id="1" filename="blanket_module.h5m"/>
<cell id="1000000" fill="1" translation="-421.1814412766555 -345.6546759463979 -288.2150000000003"
 rotation="   6.34393284e-01 -7.73010453e-01 -2.77555756e-16
             -2.89788696e-01 -2.37823437e-01  9.27072017e-01
             -7.16636360e-01 -5.88128261e-01 -3.74883282e-01  "
 region="-2001738 -2004464 -2004465 -2003974 ((2004466 -2004467) | 2004467) -2001767 -2004672 2004673"
 universe="0" />
```

Impact of Spherical Tokamak Systems on TBR

ΔTBR for reactor systems



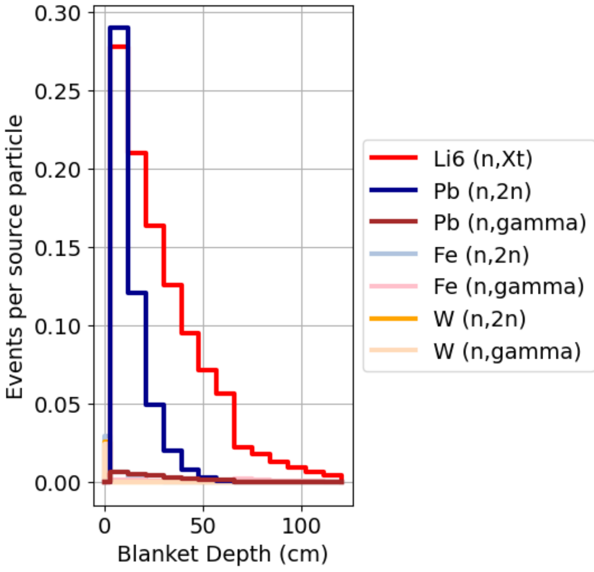
openmc-track-to-vtk



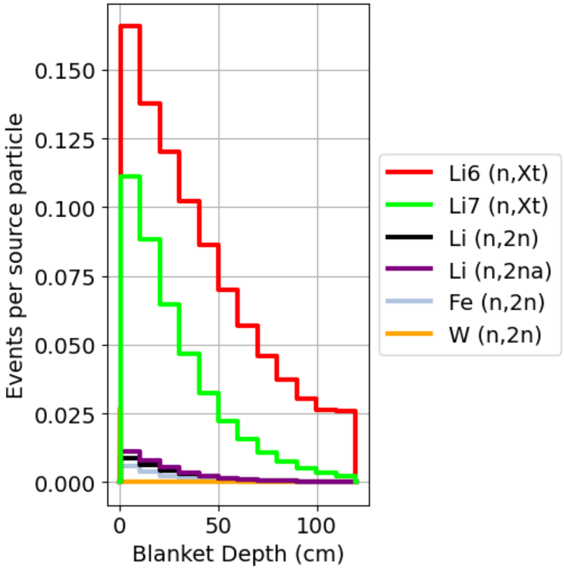
Note: the full sum of all these changes may not add linearly

TBR Assessments

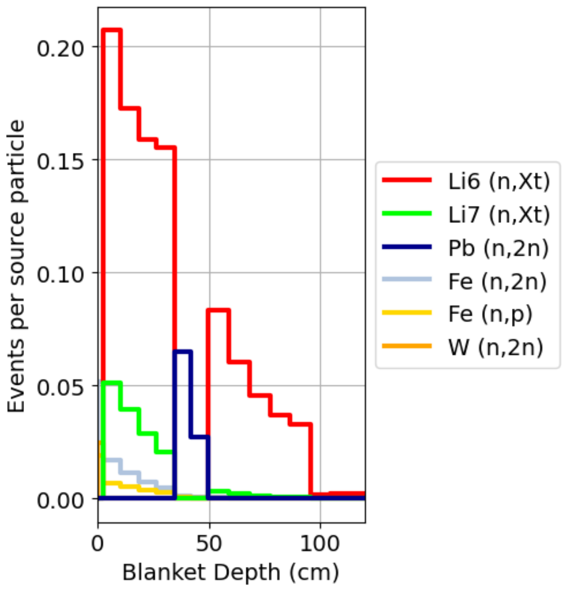
- OpenMC has the capability to record reaction rates in materials and regions.
- This can provide analysis to guide the design and calculate gas production rates or specific activation rates.
- Reaction rates decrease dramatically through the blanket as the neutron flux decreases and the energy spectrum softens.
- The 7 MeV energy threshold for Pb(n,2n) means that reaction rates reduce much more quickly than for ^{6}Li(n,Xt).



Helium-Cooled Lithium Lead



Liquid Lithium



Liquid Lithium with lead multiplier

```
# Nuclear reactions

tallies = openmc.Tallies()
tally_id = 0

nuclide_reactions = ["(n,2n)",
                     "(n,3n)",
                     "(n,2na)",
                     "(n,gamma)",
                     "(n,p)",
                     "(n,d)",
                     "(n,3He)",
                     "(n,a)",
                     "(n,2a)",
                     "(n,3a)",
                     "(n,pa)",
                     "(n,pd)",
                     "(n,da)",
                     "(n,Xt)"]

nuclides = ["Li6",
            "Li7",
            "Fe54",
            "Fe56",
            "Fe57",
            "Fe58",
            "Pb204",
            "Pb206",
            "Pb207",
            "Pb208"]

tally_id = tally_id + 1
tally = openmc.Tally( tally_id = tally_id,
                      name = 'reactions' )
tally.filters = [all_cell_filter]
tally.scores = nuclide_reactions
tally.nuclides = nuclides
tallies.append( tally )
```

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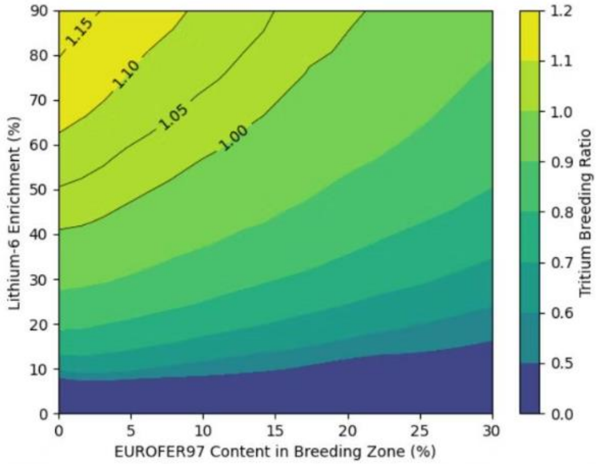
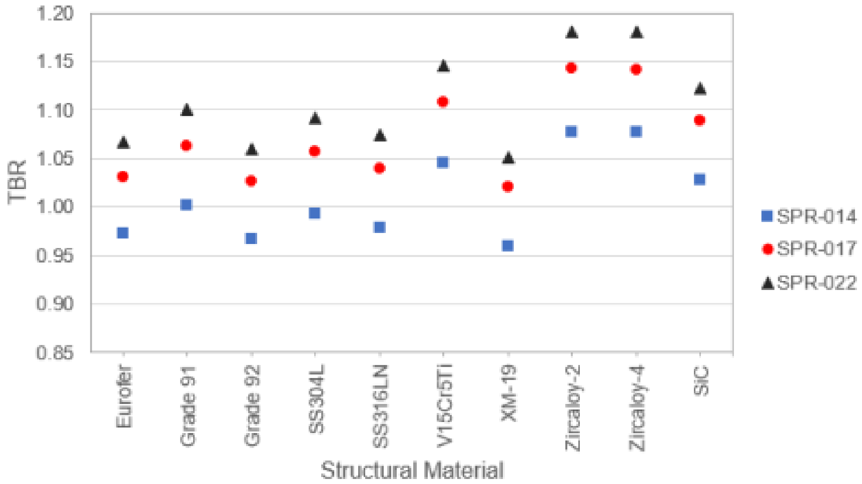
TBR Impact of First Wall & Blanket

- The first wall design and structural requirements of the breeder zone have a highly significant effect on tritium production.
- The amount and choice of structural material has a significant impact on TBR (e.g. stiffener impact ~0.04 and the choice of structural material ~0.1).
- The blanket must be designed to maximise the volume of breeder and multipliers while meeting structural, chemical, and safety requirements.

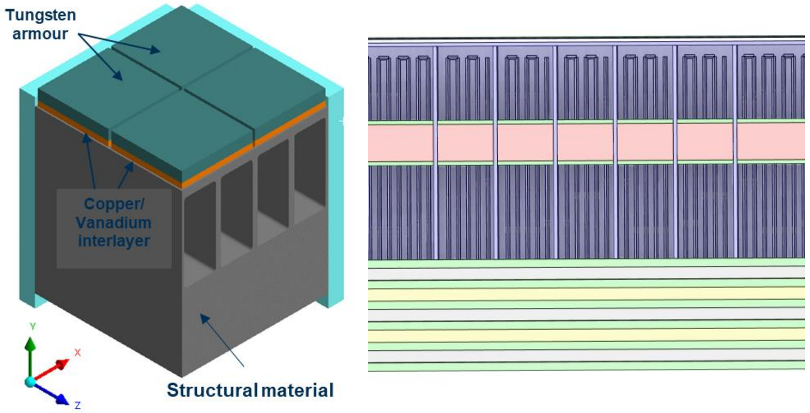
TBR for different BZ structural content



Blanket and First Wall Structural Material Impact on TBR



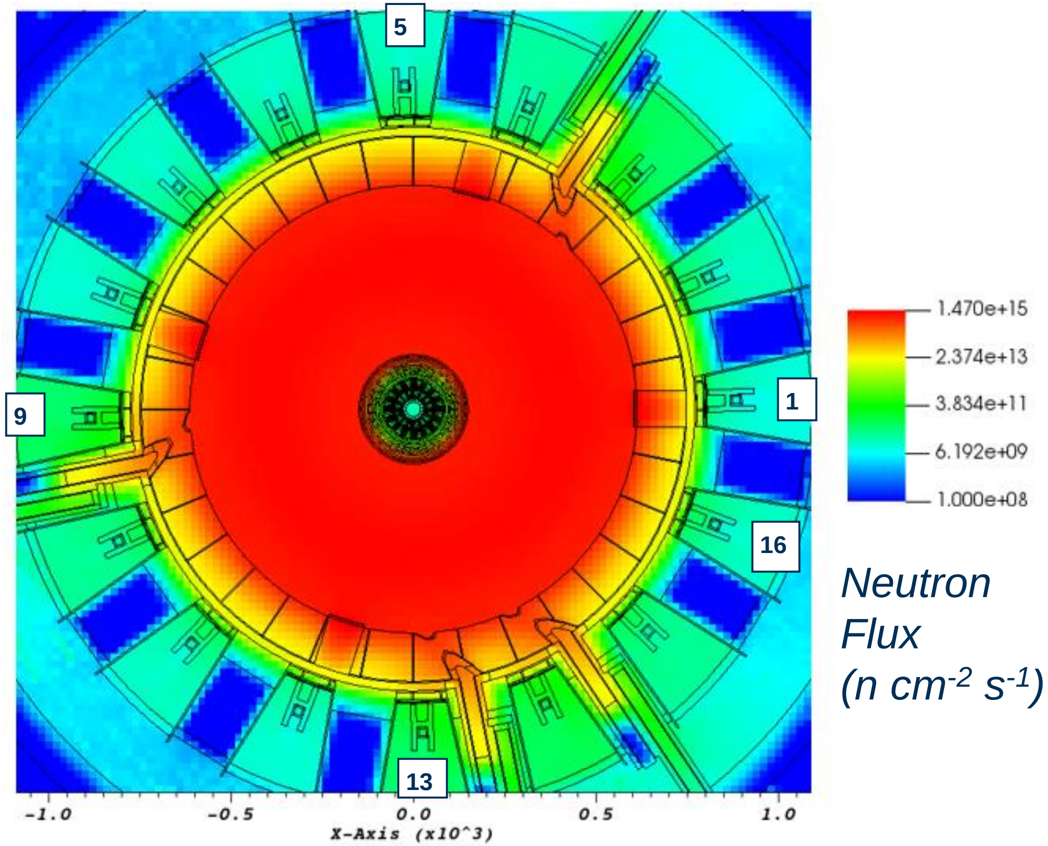
First Wall and Blanket Design

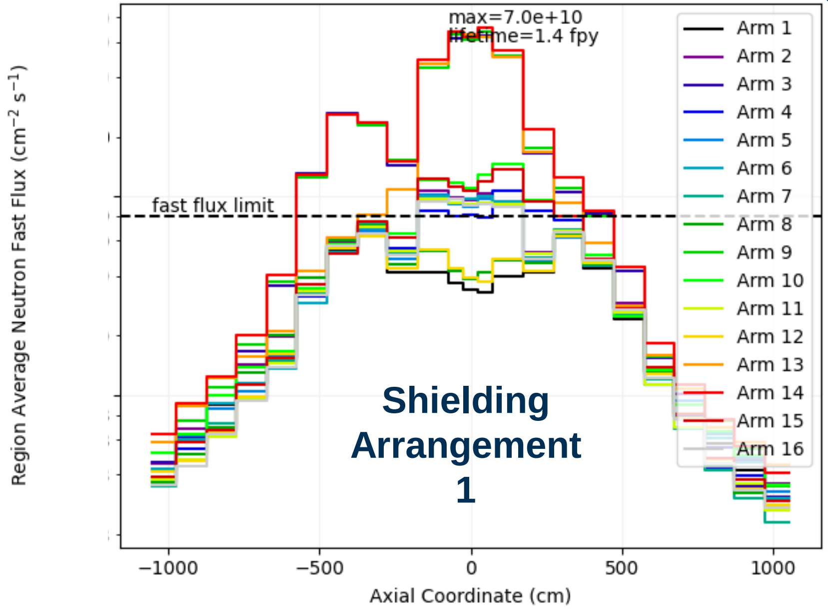


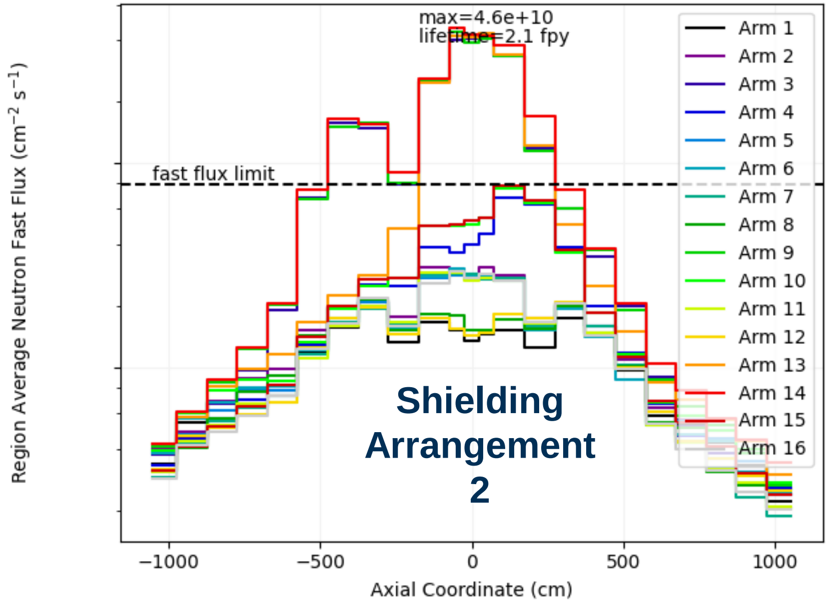
- **Structural and Coolant Requirements have a large impact on blanket design**
- **Vanadium and zirconium alloys are most favourable for TBR as they are relatively neutron transparent.**

Shielding Calculations - Magnets

- Shielding calculations are critical to the design of a fusion reactor – superconducting magnets are sensitive to neutron damage.
- Many ports are required for plasma heating, diagnostics, and fuel injection and are weak spots in the shield.

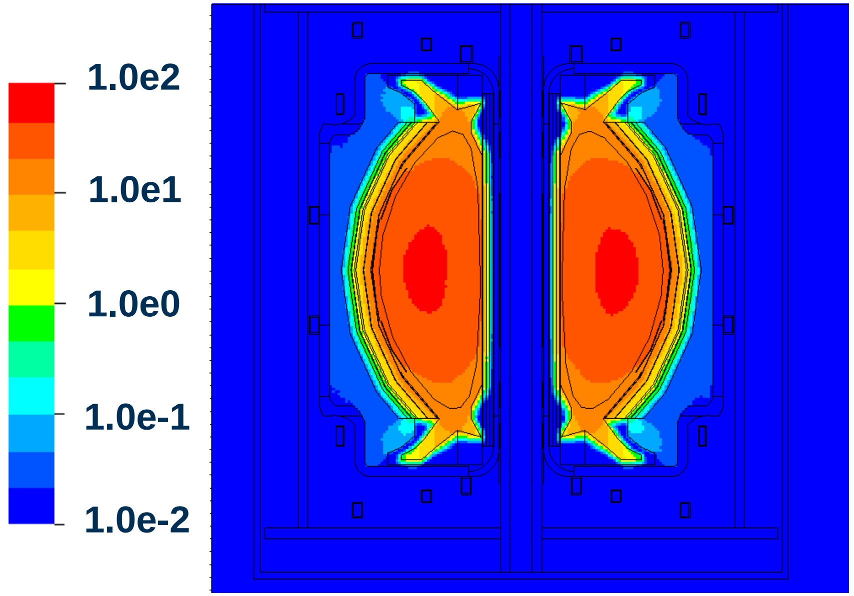




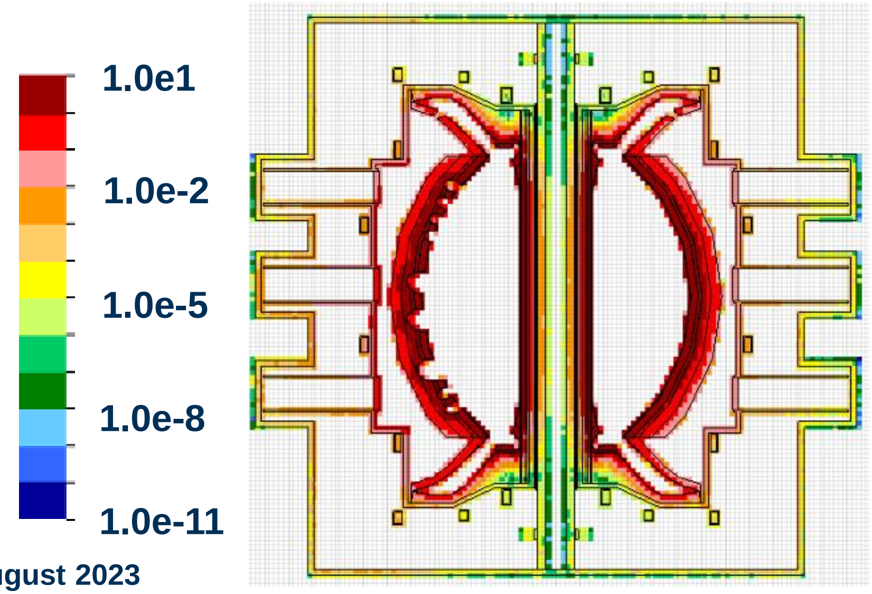


Shielding Calculations – Heating and Damage

- The dpa is considerable at the first wall so novel materials and structures are being developed to maximise first wall lifetime.
- Additionally, there is a stringent dpa target for the vacuum vessel which results in the need for careful shielding design around the larger ports.
- Heating is important for net electricity output of the power plant. The design requires as much neutronic heating as possible to be in usable .
- 20K superconducting magnets are in close proximity to 1e8 K plasma! The better the shielding, the smaller the cryoplant can be. However, the plasma control improves the closer the magnets are to the surface.



Eurofer Damage Rate (dpa/fpy)



Material Heating (W cm^{-3})

Waste Assessments

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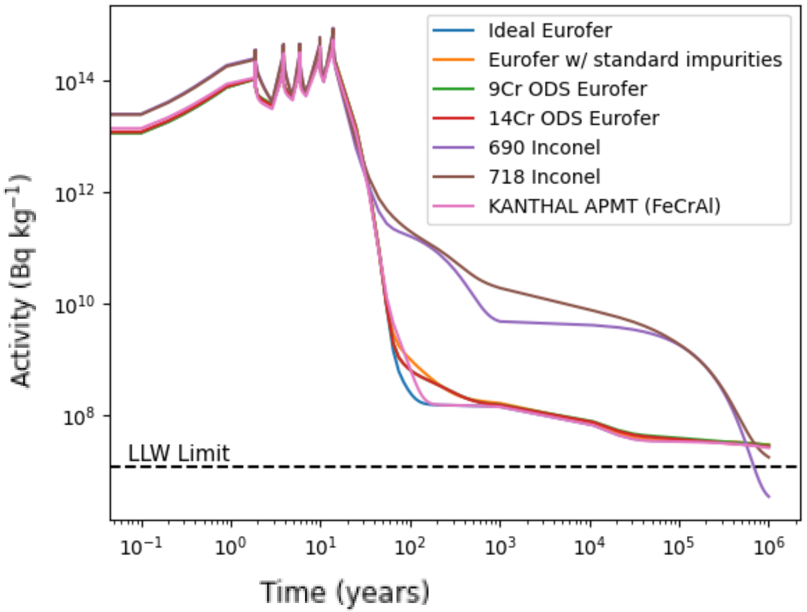
- OpenMC can be used to calculate neutron flux spectra for activation calculations.
- OpenMC Python API can be coupled with FISPACT II Python API.
- In example, the components were irradiated for 4 FPY over a 14 year period. First wall will be ILW for all cases so material selection should not be guided by waste requirements.
- However, Blanket back support structure can be LLW within 100 years if low-activation steels are chosen.

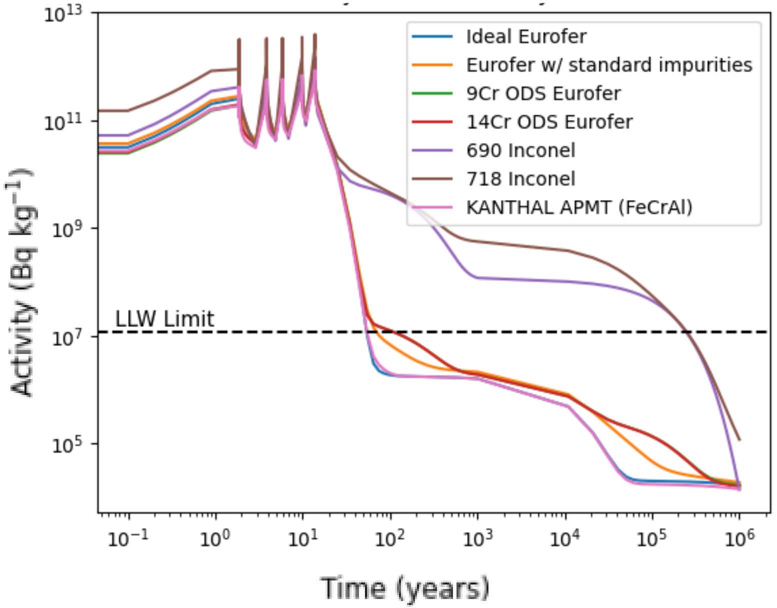
OpenMC Code for calculating neutron flux spectra

```
# Energy spectra

tallies = openmc.Tallies()
tally_id = 0

energy_bins = openmc.mgxs.GROUP_STRUCTURES['CCFE-709']
energy_filter = openmc.EnergyFilter(energy_bins)

neutron_particle_filter = openmc.ParticleFilter(['neutron'])

all_cell_filter = openmc.CellFilter(cells)

tally_id = tally_id + 1
cell_tally = openmc.Tally( tally_id = tally_id, name = 'neutron flux spectra')
cell_tally.scores   = ['flux']
cell_tally.filters = [all_cell_filter, neutron_particle_filter, energy_filter]
```

First Wall



Blanket Support Structure



OpenMC Areas of Development

- OpenMC has been benchmarked against other codes with successful comparisons [1] [2] [3].
  - DAGMC-UWUW [4] can be used to perform calculations on an identical mesh geometry and material definitions in OpenMC and MCNP.
  - OpenMC Adaptor [5] can be used to convert MCNP CSG to OpenMC CSG for comparison calculations.
- However, there are still areas for development:
  - OpenMC has no test validation suite for the user to validate their installation against experiment.
  - OpenMC is not yet accepted by regulatory bodies for safety assessment.
  - Statistical convergence checks provided by radiation transport codes such as MCNP are not available in OpenMC.
  - Variance reduction techniques for deep shielding problems are not as well-developed.
- The use of OpenMC will become more and more widespread as features are added and organisations update their workflows.

IAEA nuclear fusion

PAPER

Shutdown dose rate benchmarking using modern particle transport codes

To cite this article: T.

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Fusion Engineering and Design
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Benchmarking of emergent radiation transport codes for fusion neutronics applications

A. Valentine, T. Berry, S. Bradnam, J. Hagues, J. Hodson

Modeling and simulation of VERA core physics benchmark using OpenMC code

Abdullah O. Albugami a b, Abdullah S. Alomari a c, Abdullah I. Almarshad a

MCNP tally statistical checks

```
===========================================================================================================
      results of 10 statistical checks for the estimated answer for the tally fluctuation chart (tfc) bin of tally    4

tfc bin    --mean--    ---------relative error---------    ----variance of the variance----    --figure of merit--    -pdf-
behavior   behavior    value   decrease   decrease rate    value   decrease   decrease rate    value     behavior    slope

desired    random      <0.10     yes      1/sqrt(nps)      <0.10     yes       1/nps           constant  random      >3.00
observed   random       0.00     yes         yes            0.00     yes        yes            increase  increase     3.96
passed?     yes          yes     yes         yes             yes     yes        yes               no        no         yes
===========================================================================================================
```


References

[1] Valentine et al., Benchmarking of emergent radiation transport codes for fusion neutronics applications, Fusion Engineering and Design, Vol 180, July 2022, 113197

[2] Eade et al., Shutdown dose rate benchmarking using modern particle transport codes, Nucl. Fusion, **60** 056024

[3] Albuhami et al., Modeling and simulation of VERA core physics benchmark using OpenMC code, Nuclear Engineering and Technology, Volume 55, Issue 9,2023,

[4] https://svalinn.github.io/DAGMC/usersguide/uw2.html

[5] https://github.com/openmc-dev/openmc_mcnp_adapter

Summary

- OpenMC is used as a powerful design tool for fusion reactor concepts. All the key features have been implemented for its use as the primary design tool for fusion neutronics.
- TBR is an important metric for fusion reactors and OpenMC can be used to explore design options:
  - Blanket structural material choice can influence TBR by 0.1,
  - A 5% increase in structural material content can reduce TBR by 5%.
- It is always important to validate predictions from calculations using experiments. For tritium production experiments, the C/E ranges from ~0.9 to 1.12 (±10% 2σ).
- The Python API allows easy coupling with FISPACT II Python API:
  - The reactor first wall will be classed as ILW even if low activation materials are selected.
  - At the back of the blanket, low activation material will allow disposal as LLW.
- The use of OpenMC will become more and more widespread as features are added and organisations update their workflows.