STS MRA Preliminary Design Neutronics Analysis

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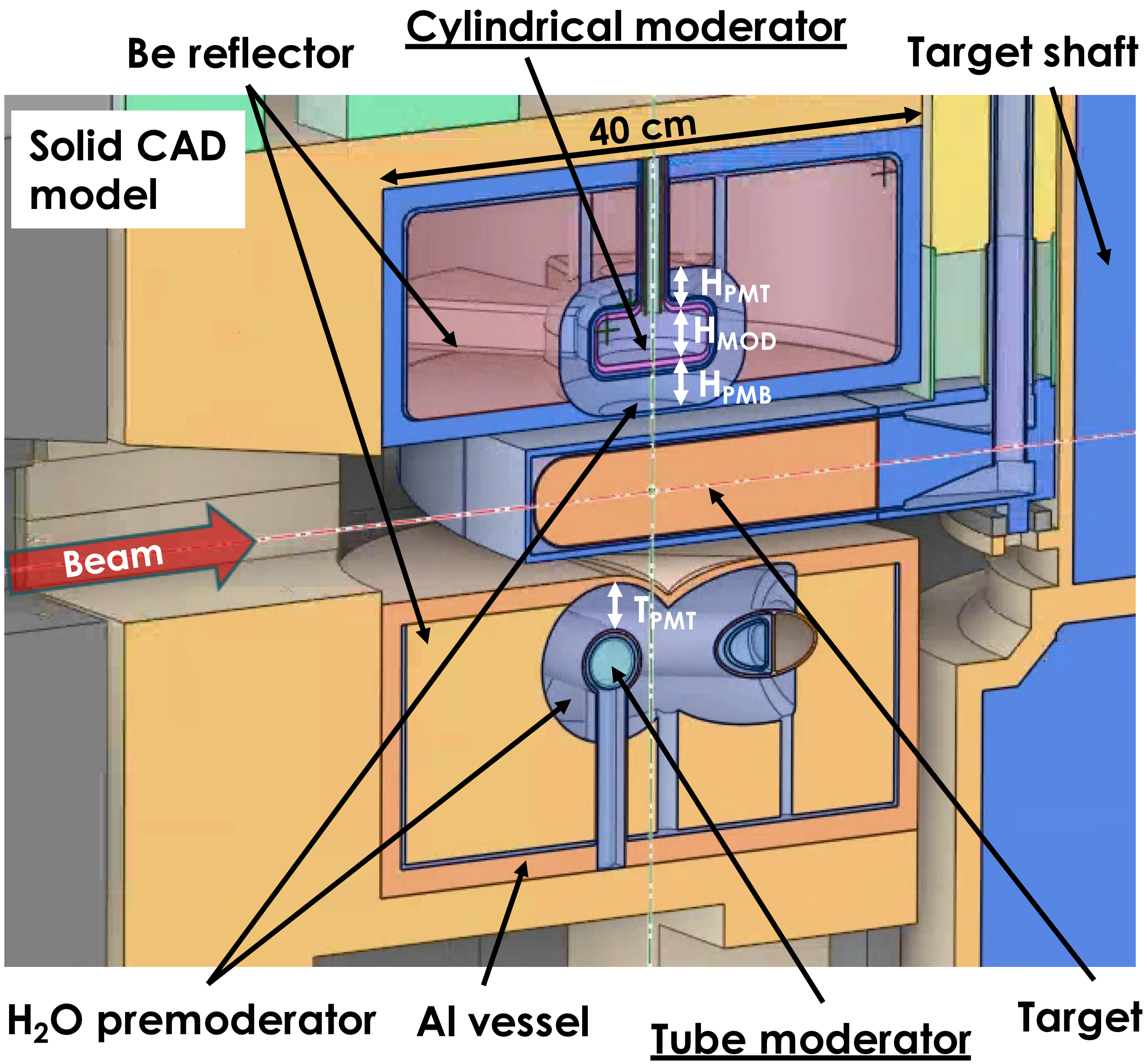
STS MRA Preliminary Design Neutronics Analysis

- The goal of this analysis is to perform MCNP radiation transport (neutronics) simulations that support the MRA preliminary design
- These simulations intend primarily to:
  - Evaluate the neutronics performance to make sure that the neutron brightness satisfies the Key Performance Parameters (KPP)
  - Provide input for the subsequent Finite Element Analysis (FEA), mainly structural stress and thermal analysis, to ensure that the structural integrity is maintained during the predicted lifetime of the MRA
  - Determine the radionuclide inventory at the end of the lifetime and provide information about activation dose rates during the MRA replacement

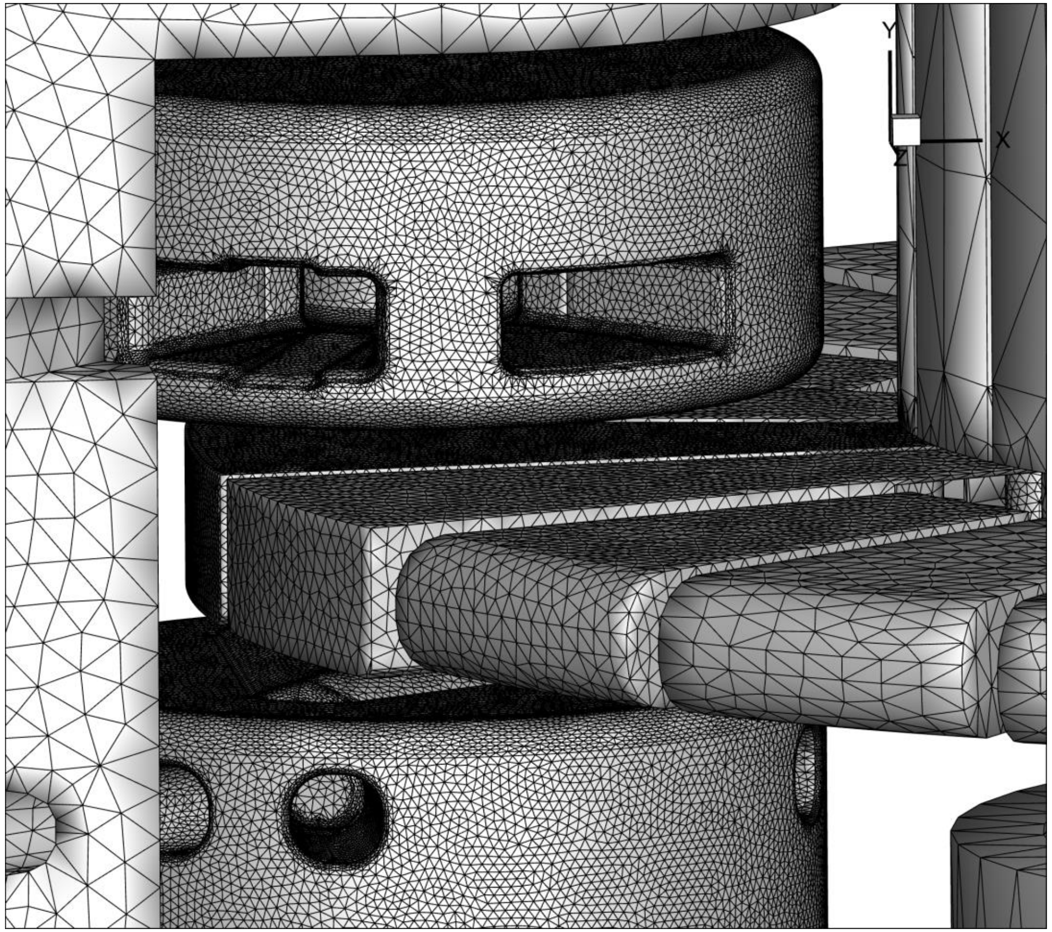
Unstructured Mesh (UM) Geometry (UMG) application

- The analysis relies heavily on the recently developed UMG capability of MCNP6 and Attila4MC' volumetric mesh generator
- UM enables conversion of the solid CAD models directly for MCNP, which significantly improves both the efficiency and quality of the neutronics models' generation
- Volumetric (3D) UM provides data with high spatial-resolution that can be conveniently processed for the subsequent FEA
- UM allows us to use an automated MRA optimization workflow
- The use of UM has been thoroughly validated against traditional MCNP's Constructive Solid Geometry (CSG) modeling

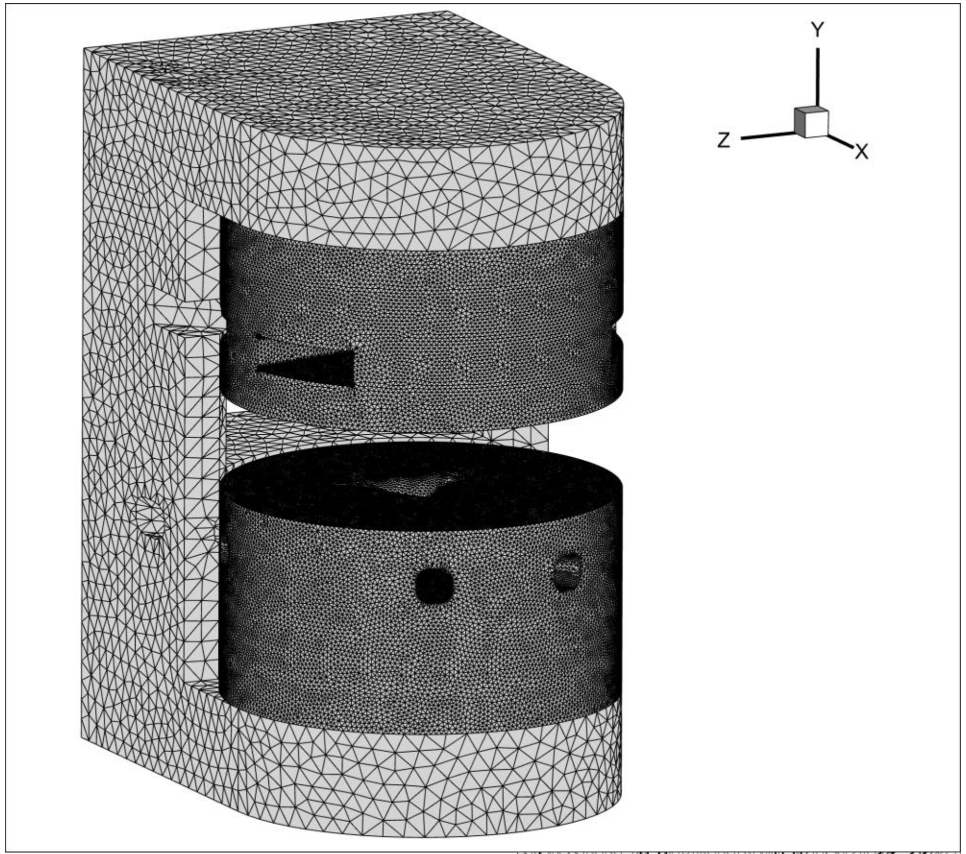
MRA UM model



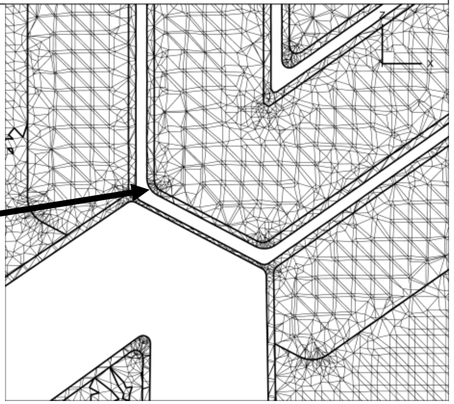
Unstructured mesh model for MCNP

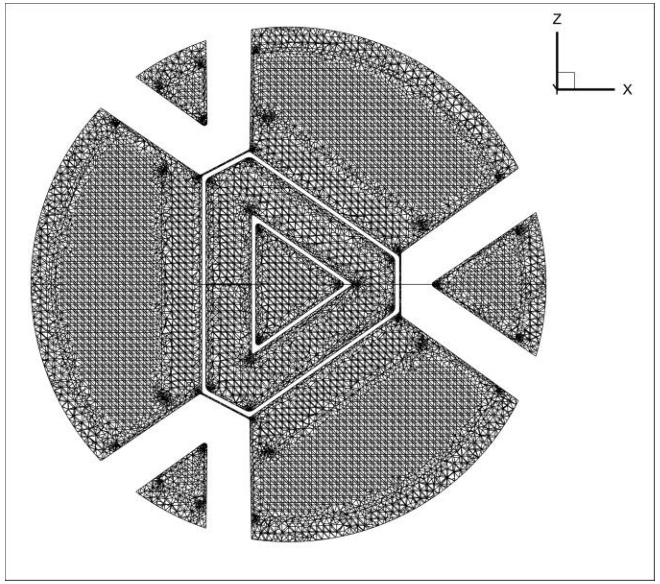


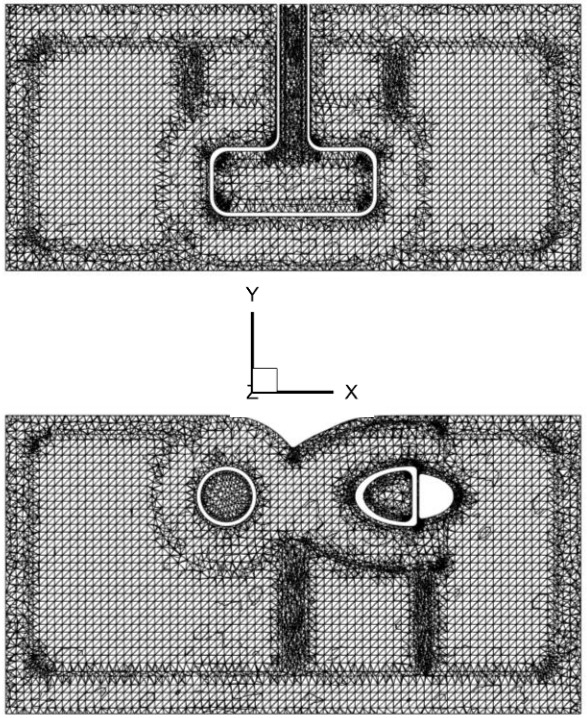
MRA UM model (cont.)



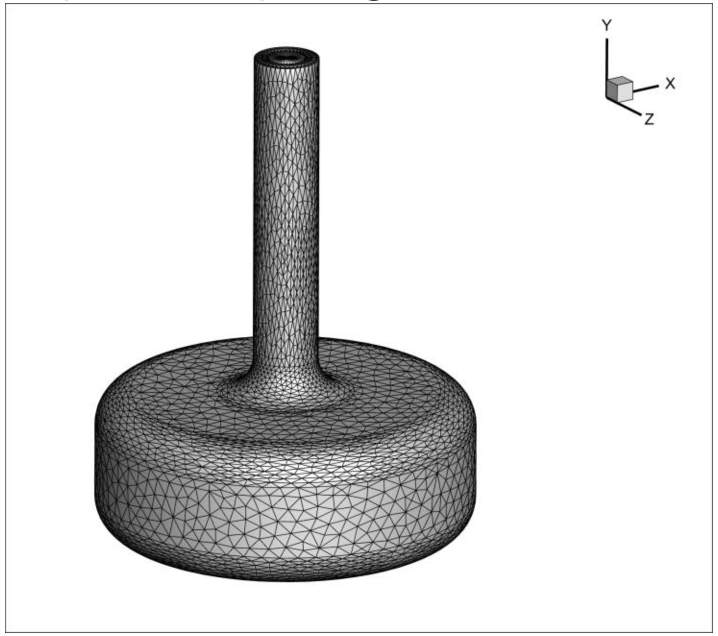
UM captures all fine curvatures (difficult to achieve with CSG)



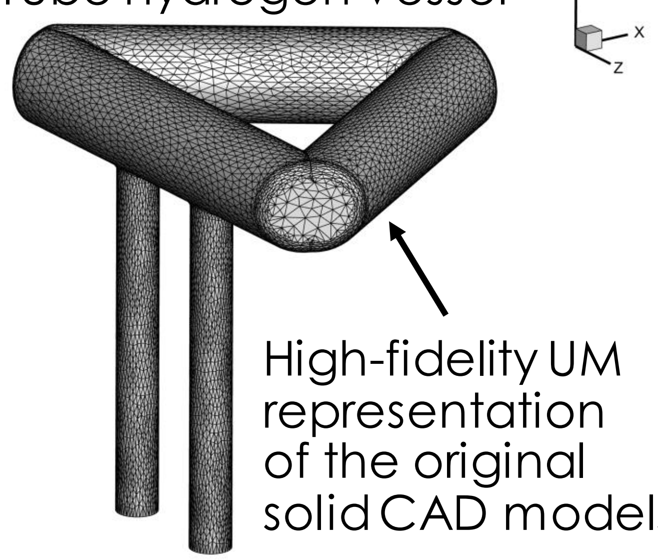




Cylinder hydrogen vessel



Tube hydrogen vessel

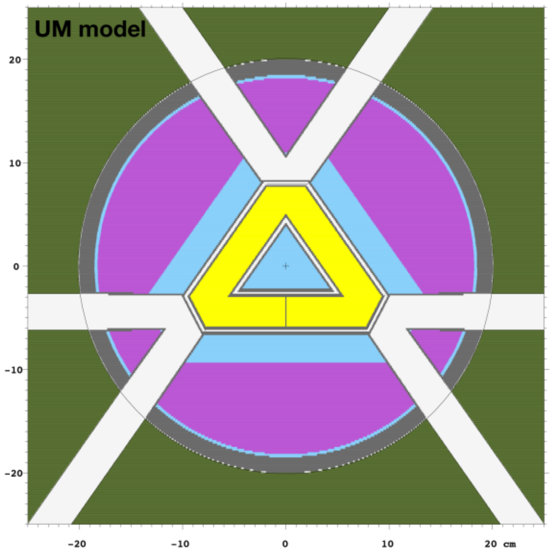


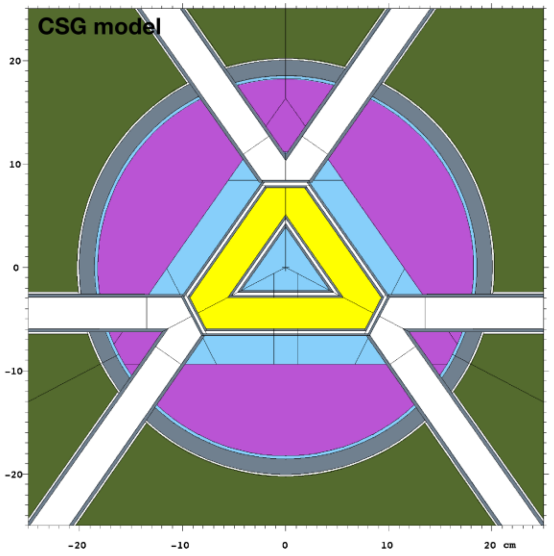
High-fidelity UM representation of the original solid CAD models

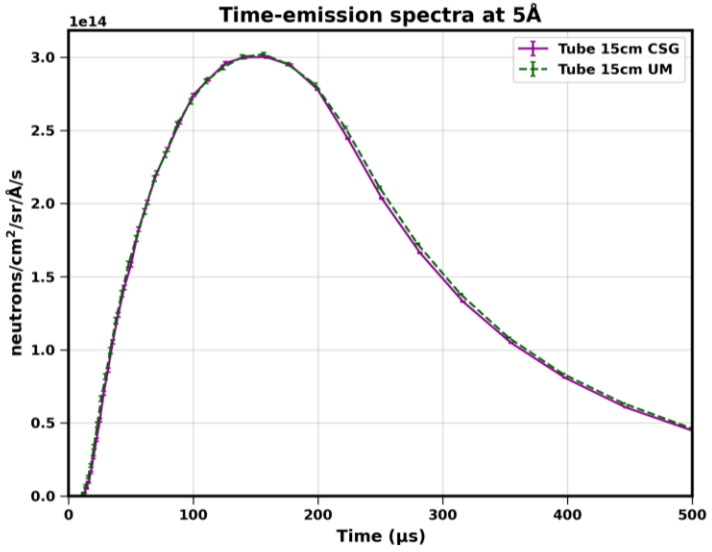
Validation of UM against CSG

- Since the use of UM is relatively new at STS (since 2020), a series of validation tests against traditional CSG was performed
- Good agreement was reached between UM and detailed CSG models for the neutronics performance of the MRA
- Other quantities, such as total energy deposition per component also resulted in consistent agreements between UM and CSG

Tube moderator (15 cm tube length) modeled as UM and CSG. Monolithic target block (V 06/2021) and 90 cm^2 proton beam used.





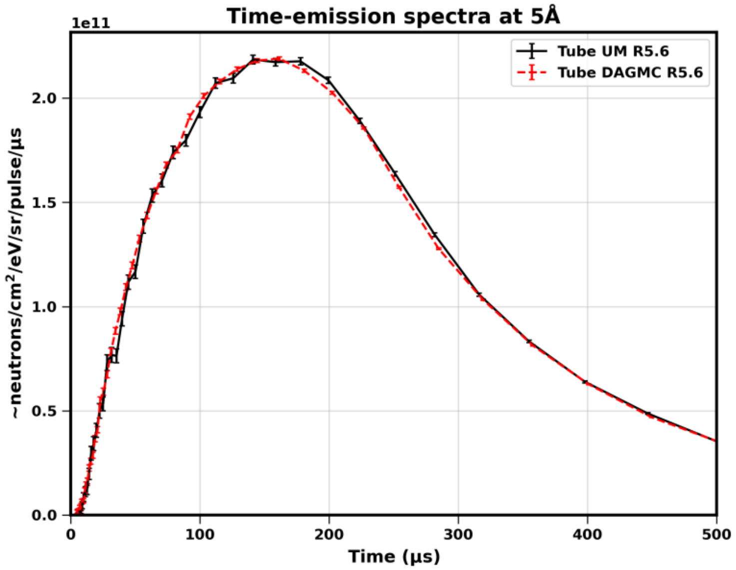


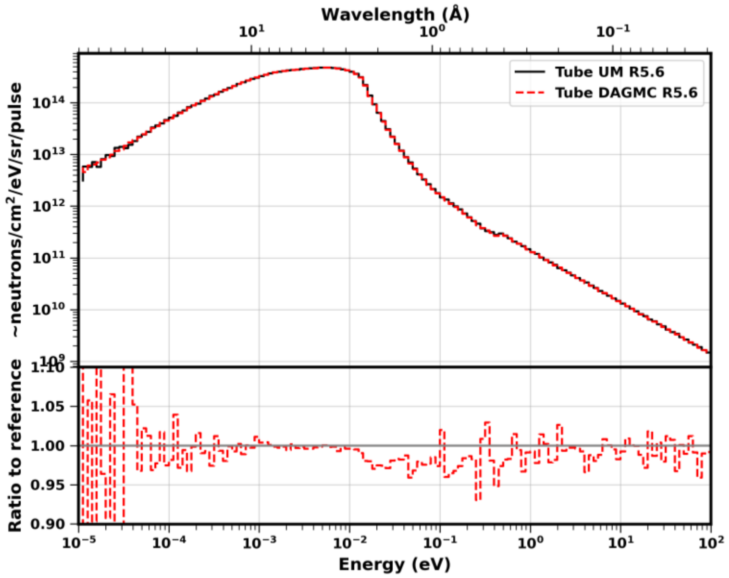
More on UM validation in the spallation environment: L. Zavorka, et al. NIM A 1052 (2023) 168252 and NIM A 1040 (2022) 167210

Validation of UM against DAGMC

- Neutronics results on volumetric (3D) UM with MCNP6.2 have also been validated against data obtained with DAGMC, which is a patched version of MCNP6 that facilitates the use of surface mesh (~2D) instead of traditional CSG. DAGMC was used in previous neutronics studies, and was validated against MCNP6/X.
- Surface mesh does not allow to obtain volumetric heating in the way the volumetric UM does, thus the use of DAGMC is limited.

Tube moderator (R5.6) performance calculated with MCNP6.2' UM and DAGMC. Monolithic target block (V 09/2022) and 90 cm^2 proton beam used.





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List of analyses

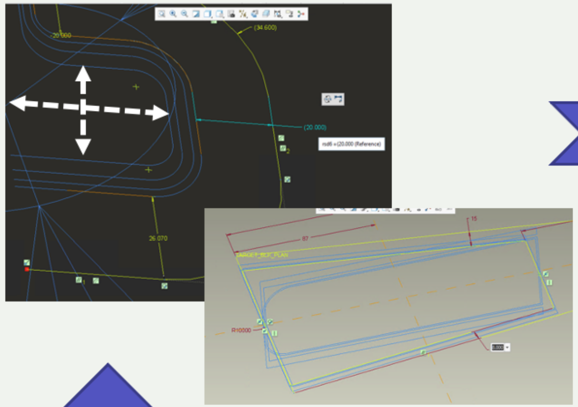
- The slides in this presentation provide information on:
  - Neutronics optimization (basics)
  - Neutronics performance of the MRA
  - Impact of the MRA misalignment on the neutronics performance
  - Energy deposition in the MRA
  - dpa rates in the MRA
  - Radionuclide inventory
  - Prompt dose rates due to the streaming up MRA pipe chases
  - Activation dose rates during the MRA replacement

Neutronics optimization

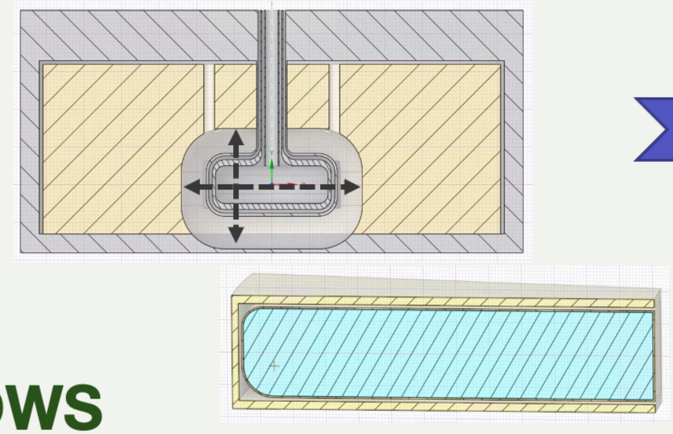
- Neutronics optimization of the MRA geometry was performed using a fully automated UM-based workflow (see next slide, excluding the structural stress analysis portion) and will be discussed in a separate presentation.
- Models and conditions used:
  - Monolithic target block (21 segments) mraanalysis-r5.scdoc
  - 90 cm^2 Super-Gaussian proton beam profile
  - Parametric MRA model based on MRA R5 mraanalysis-r5.scdoc

Unstructured mesh based neutronics optimization workflow

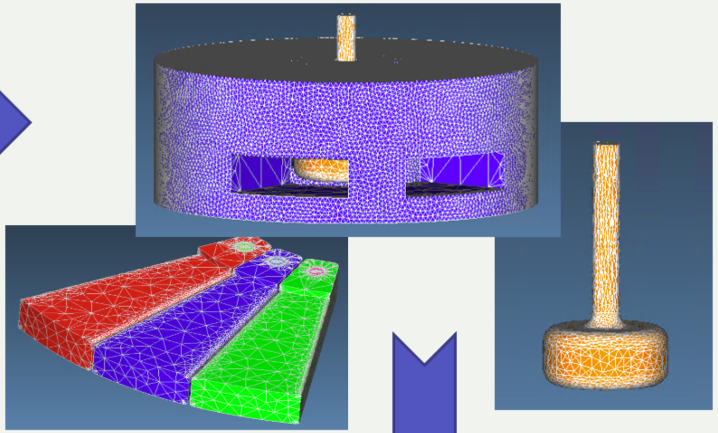
Parametrization with CREO



Filling volumes with SpaceClaim

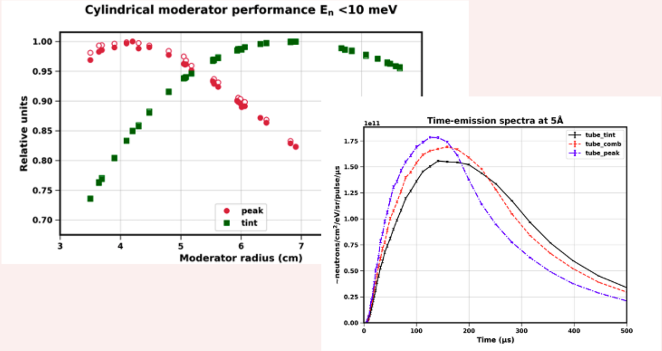


Unstructured Mesh (UM) generation with Attila4MC

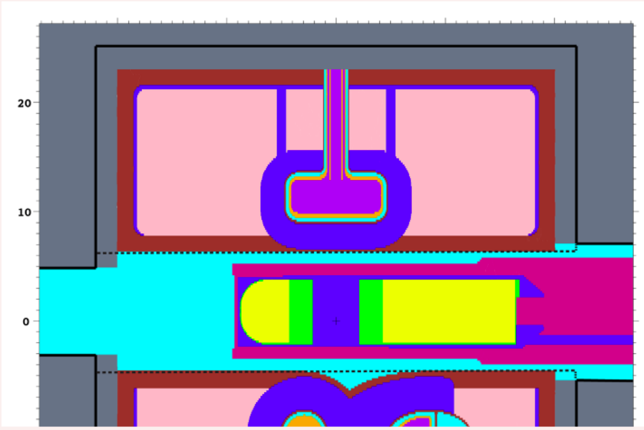


WINDOWS

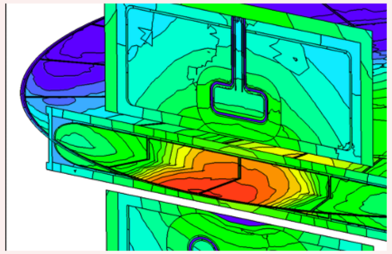
LINUX



Hybrid UM/CSG MCNP model



DAKOTA
Optimization

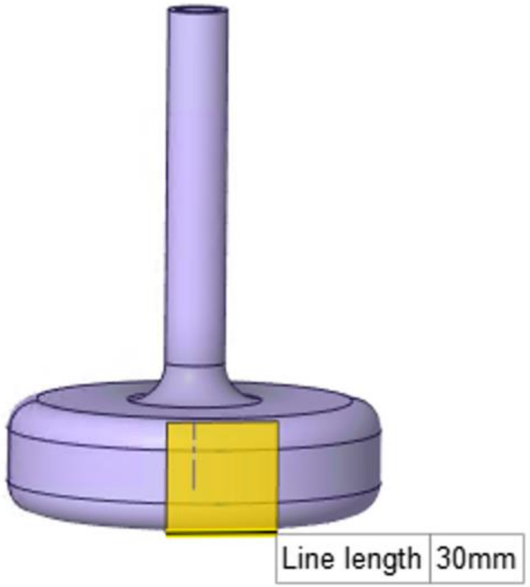


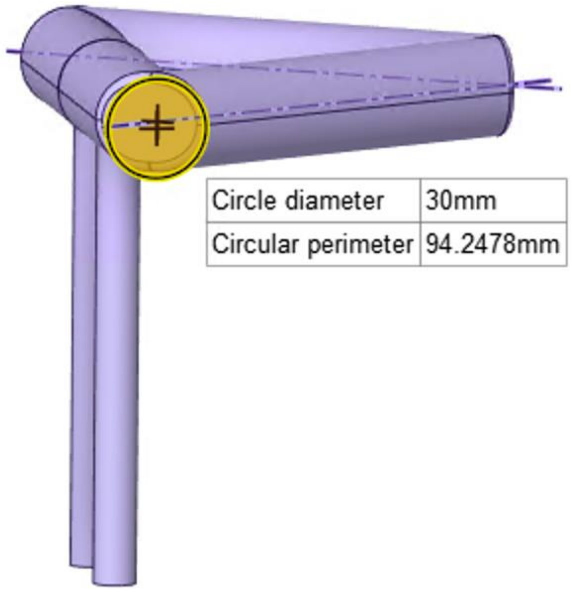
Structural stress analysis ← **Neutronics analysis** ← **MCNP6**

L. Zavorka et al., An unstructured mesh based neutronics optimization workflow, NIM A 1052 (2023) 168252.

Neutronics performance

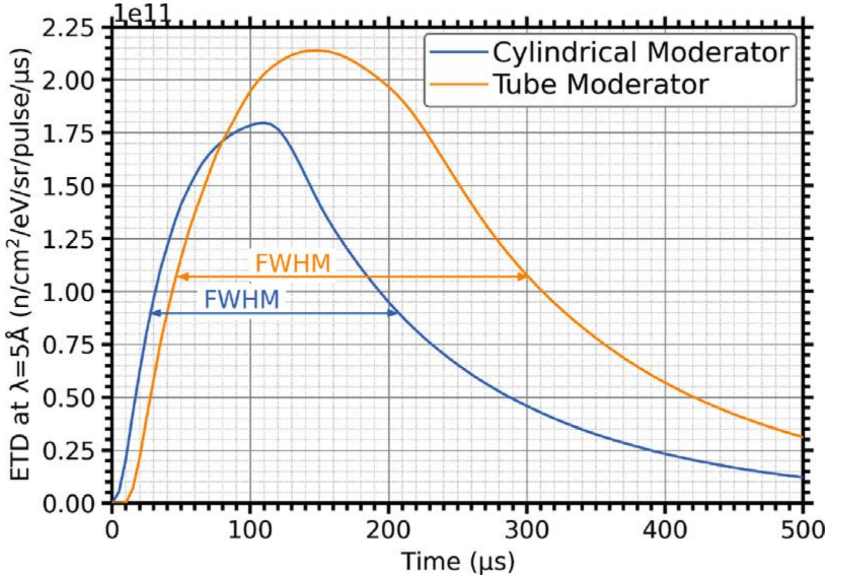
- The goal is to evaluate neutronics performance of the MRA in terms of neutron brightness
- Neutron brightness is calculated at the moderator emission surface using the MCNP6' point detector (F5 tally) located 10 m downstream the beamline, with the neutron time of flight corrected back to the emission surface. The viewed area is 3x3 cm for the cylinder moderator and 3 cm diameter for the tube moderator.

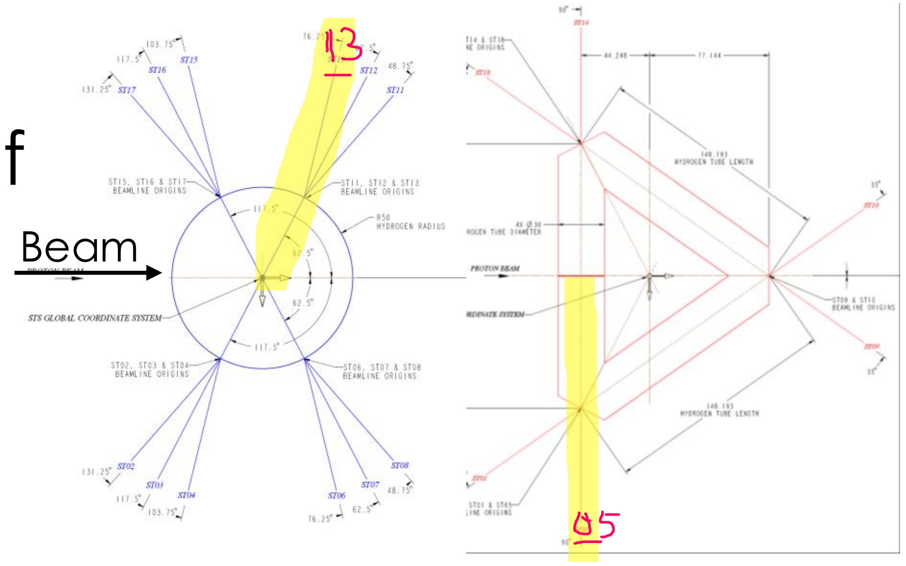




Neutronics performance (cont.)

- Important quantities are peak and time-integrated brightness. The former is the peak maximum, and the latter is the area under the curve of the time emission spectra for a given neutron wavelength.
- These are calculated for two beamlines: ST13 at 46° or 76.25° for the cylinder moderator and ST05 at 90° for the tube moderator. ST13 moved as the number of beamlines was reduced from 22 to 18.
- Key Performance Parameters require STS to generate peak neutron brightness of 2.0×10^{14} neutrons/cm2/sr/Å/s at 5Å





Neutronics performance (cont.)

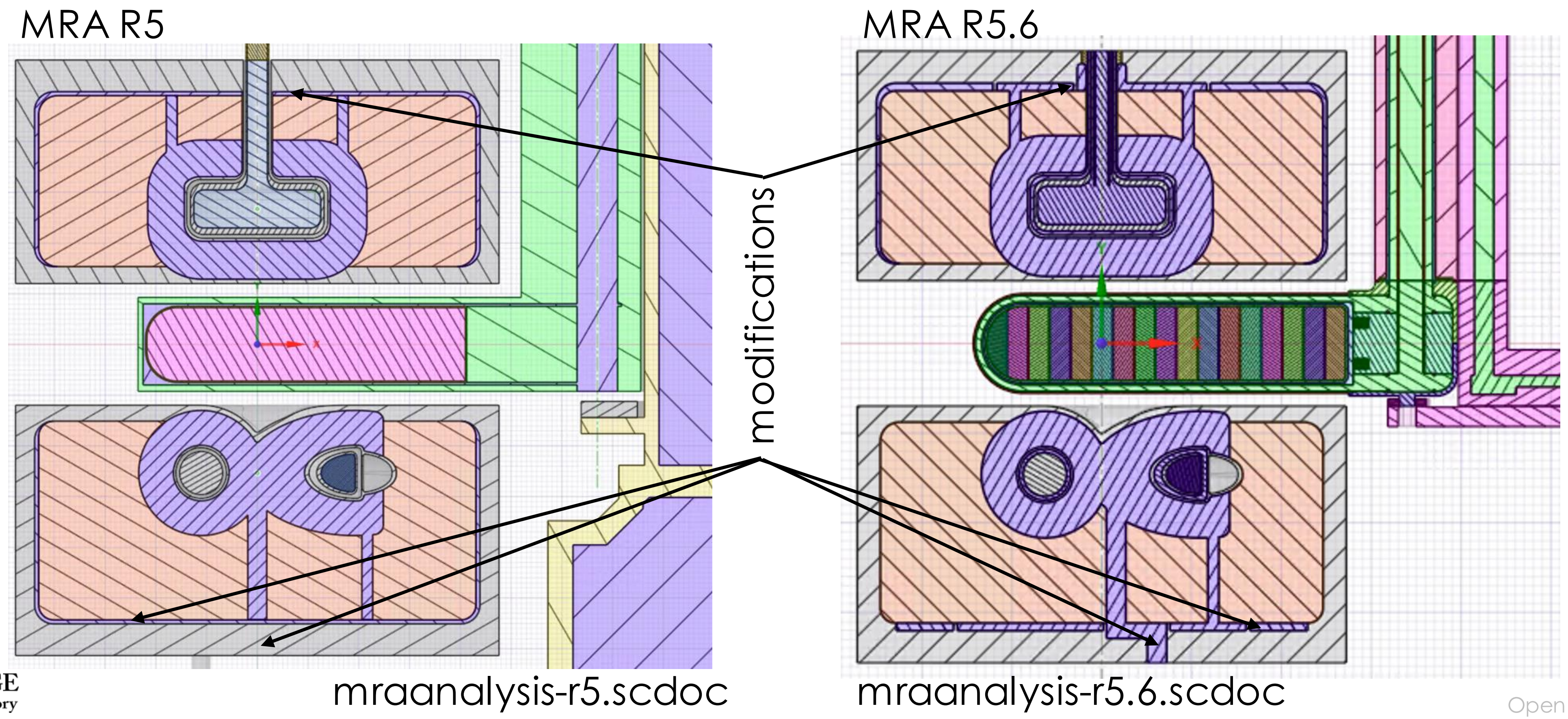
- Several modifications were implemented throughout the STS project between the original MRA/target configuration (09/2022) and the latest configuration (as of 03/2024):

MAJOR CHANGES	ORIGINAL CONFIGURATION (09/2022)	LATEST CONFIGURATION (03/2024)
MRA version	R5	R5.6
ST05 / ST13 angles	90°/46°	90°/76.25°
Target	Monolithic block	Zitti 01/2024
# of target segments	21	20
Proton beam profile	90 cm^2	60 cm^2

- We first discuss the neutronics performance of the original configuration (MRA R5) that was used for neutronics optimization and to calculate energy deposition in the MRA and the backbone to design the efficient cooling of the backbone.

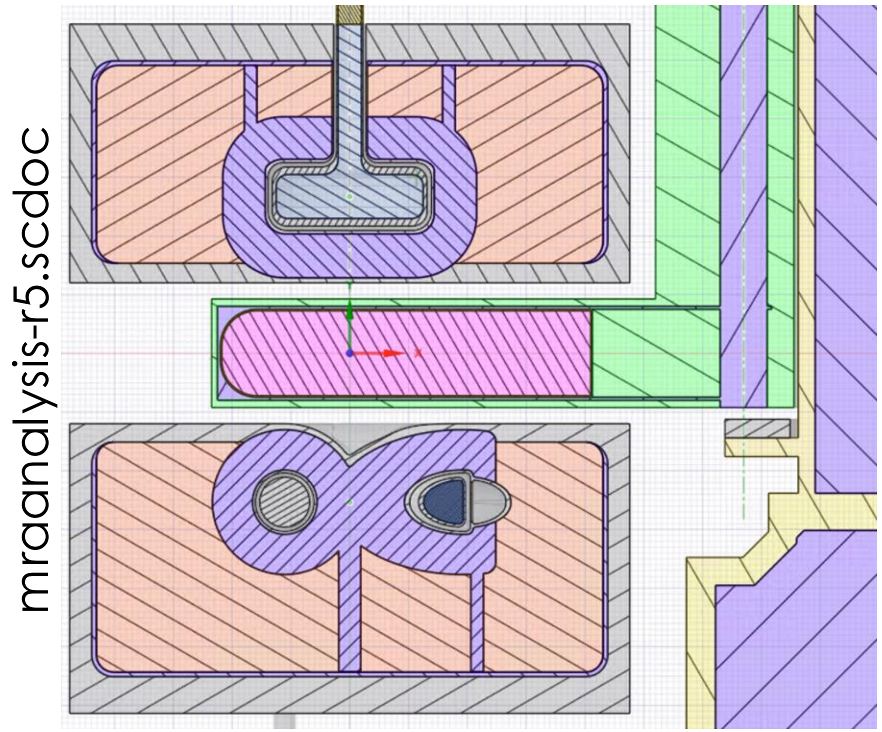
Neutronics performance (cont.)

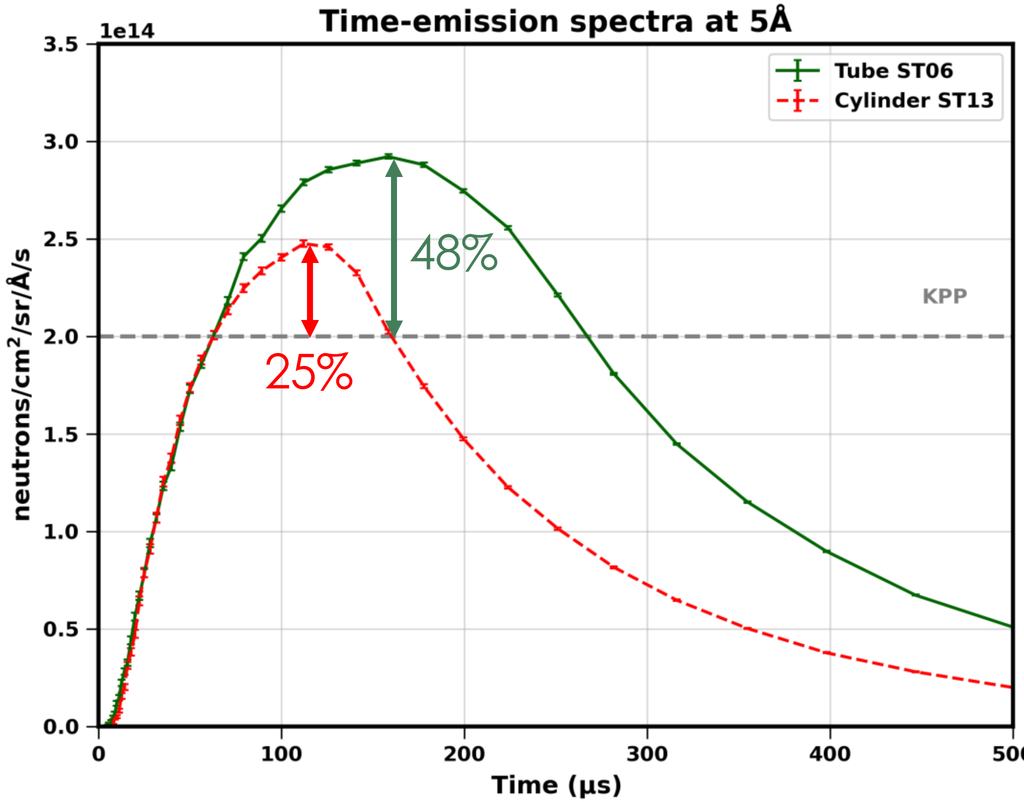
- Minor modifications were implemented between MRA R5 and MRA R5.6, such as thicker water outside the reflector, baffles in the outside water channel, and updated tube water inlet.



Neutronics performance – Original version

- Neutronics performance of the MRA R5, monolithic target, and 90 cm^2 profile used for optimization and energy deposition runs
- Cylinder moderator exceeds KPP by 25%, tube moderator by 48%





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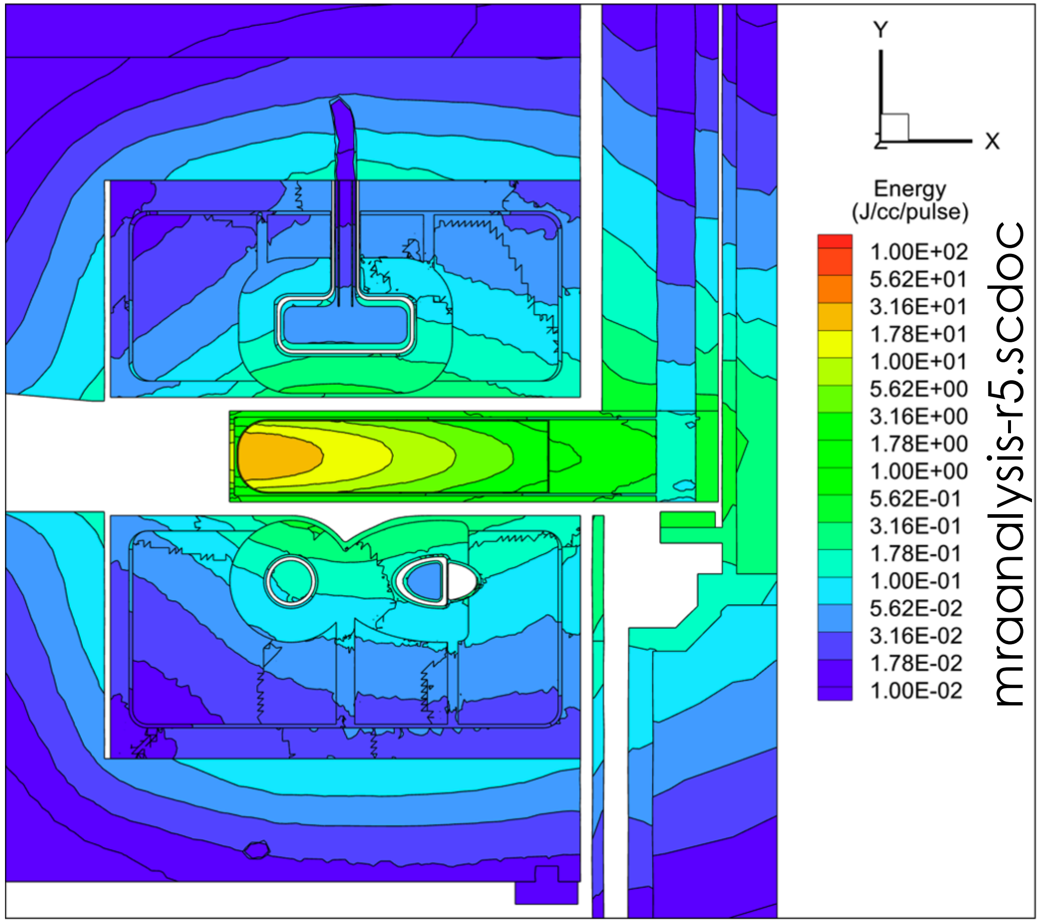
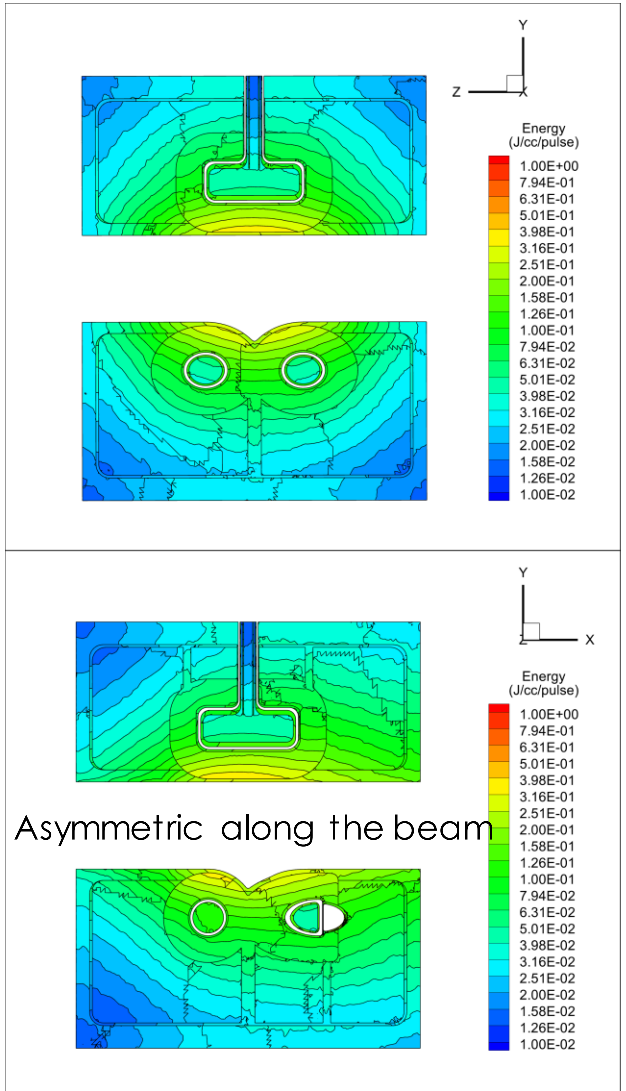
Energy deposition

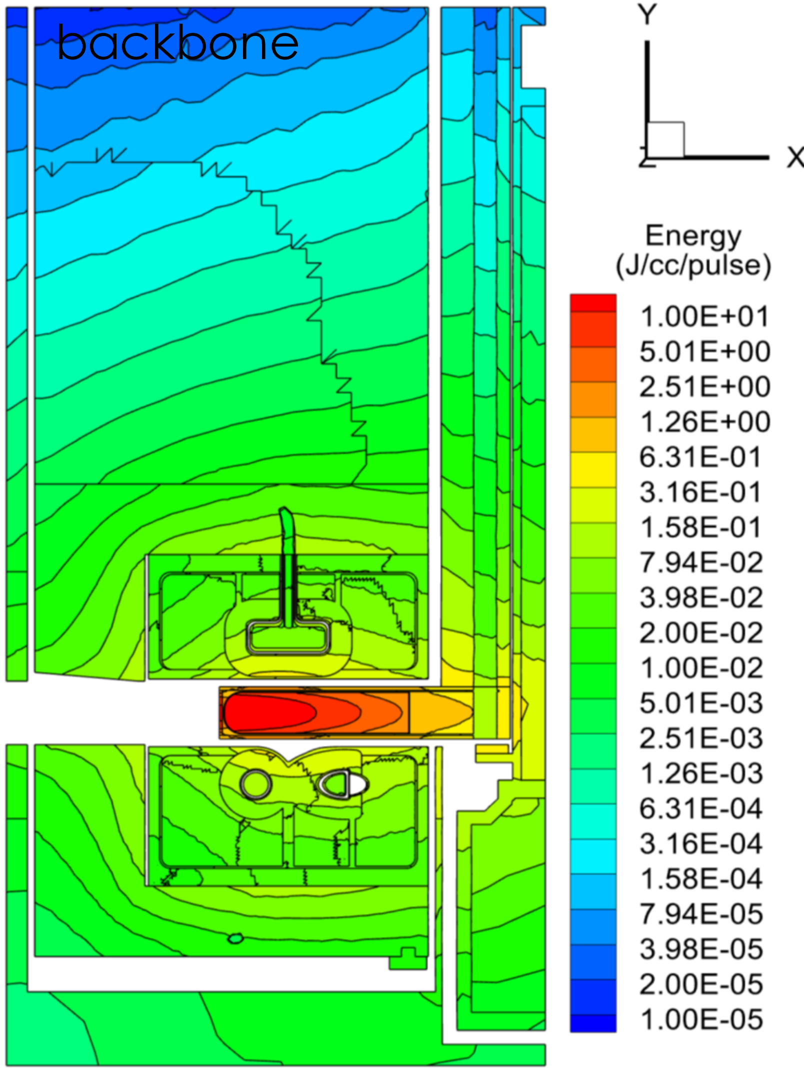
- Energy deposition was calculated using the same geometry configuration, i.e., MRA R5, monolithic target block, and the 90 cm^2 proton beam profile. Backbone assumed homogenous mixture of SS316L (95%) and water (5%).
- Energy deposition (J/cc/pulse) was calculated on volumetric UM to support the subsequent FEA by Min-Tsung Kao. Total values per individual components and materials were calculated as well.
- The use of UM is especially beneficial in this case because it allows us to depart from the original cartesian mesh tallies of MCNP6, which mix the materials across the voxels (if two or more materials are present) and have inferior spatial resolution at the boundaries of the neighboring objects.

Energy deposition (cont.)

- Data available for the MRA and the backbone







Note different axes ranges in these plots

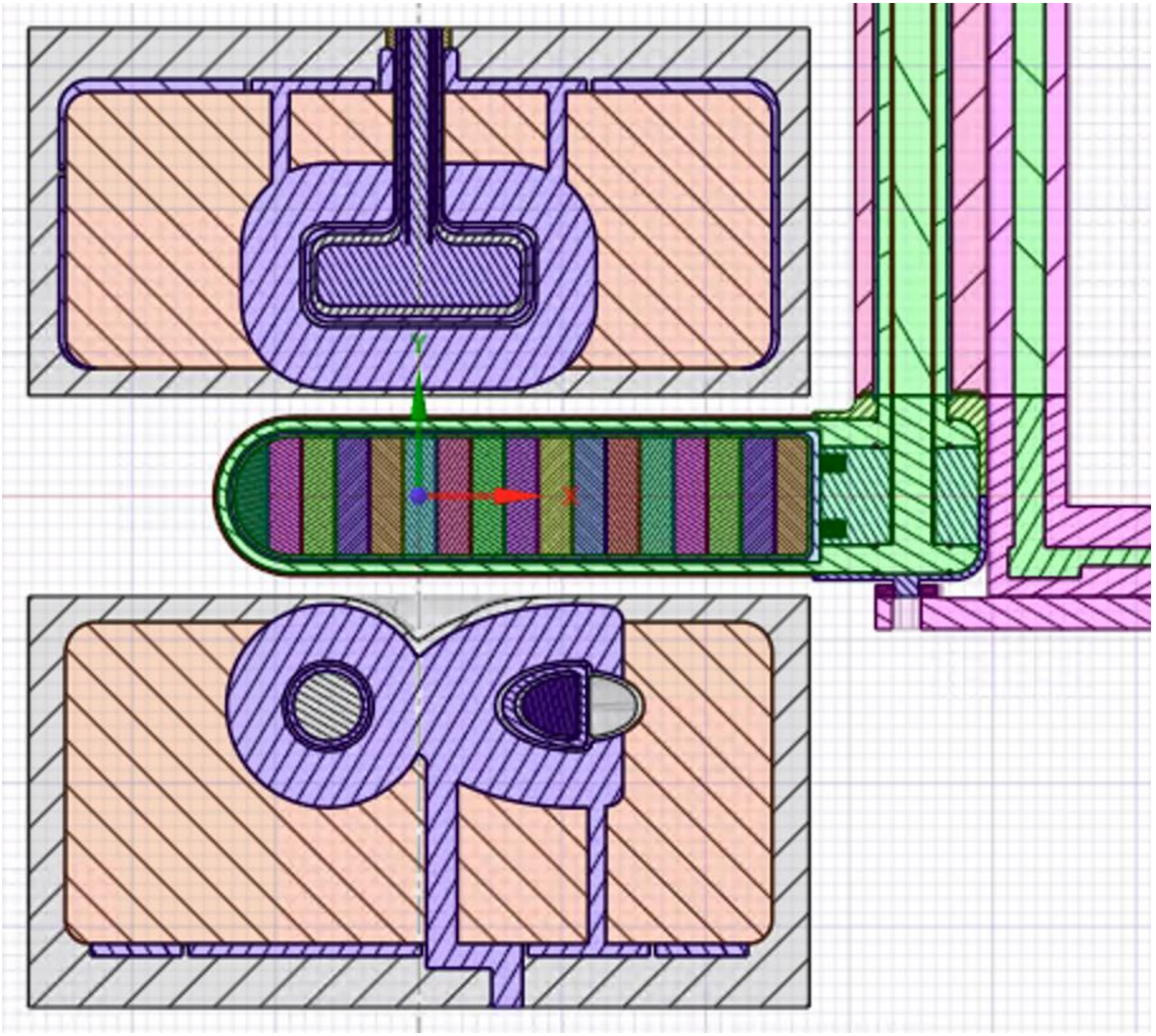
Energy deposition (cont.)

- Total heating per component, including $^{27}Al(n,\gamma)^{28}Al$ decay

Component	Cylinder (kW)	Tube (kW)	Backbone (kW)
Hydrogen	0.162	0.207	
Al hydrogen vessel	0.228	0.186	
Invar pipes	0.017	0.033	0.050
Hydrogen in pipes			0.025
Water premoderator	2.901	4.035	
Water in reflector	0.357	0.345	
Be reflector	6.413	6.754	
Al reflector vessel	4.980	4.794	
SS420			0.014
SS316(95%)+Water(5%)			30.098
TOTAL	**15.058**	**16.354**	**30.187**

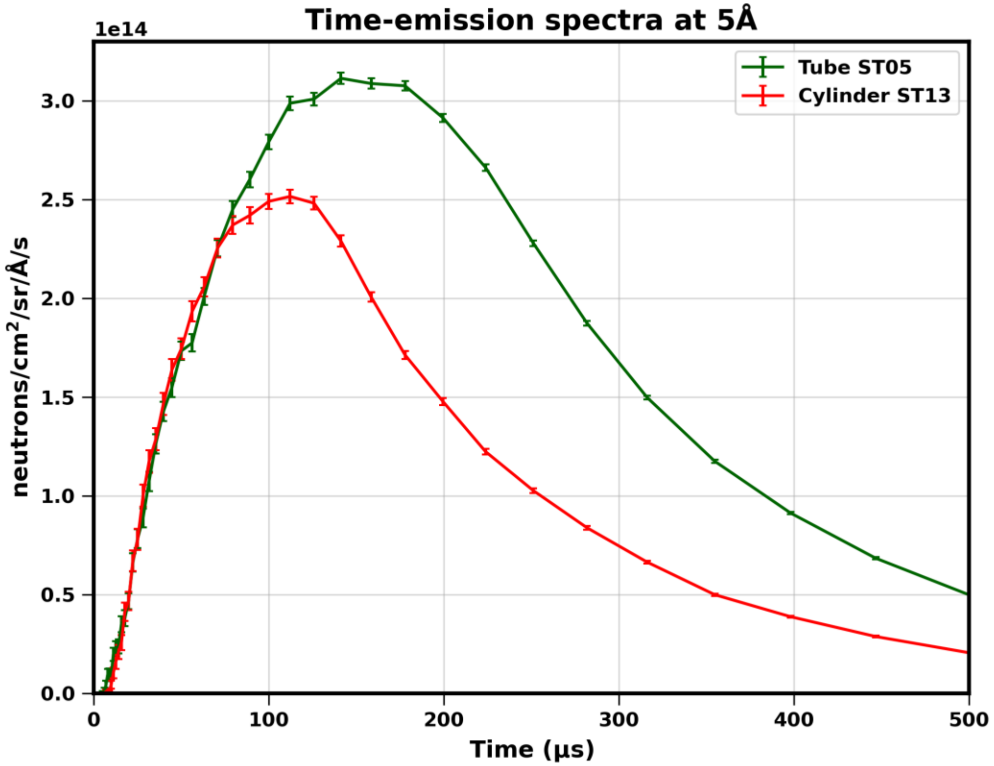
Neutronics performance – Latest version

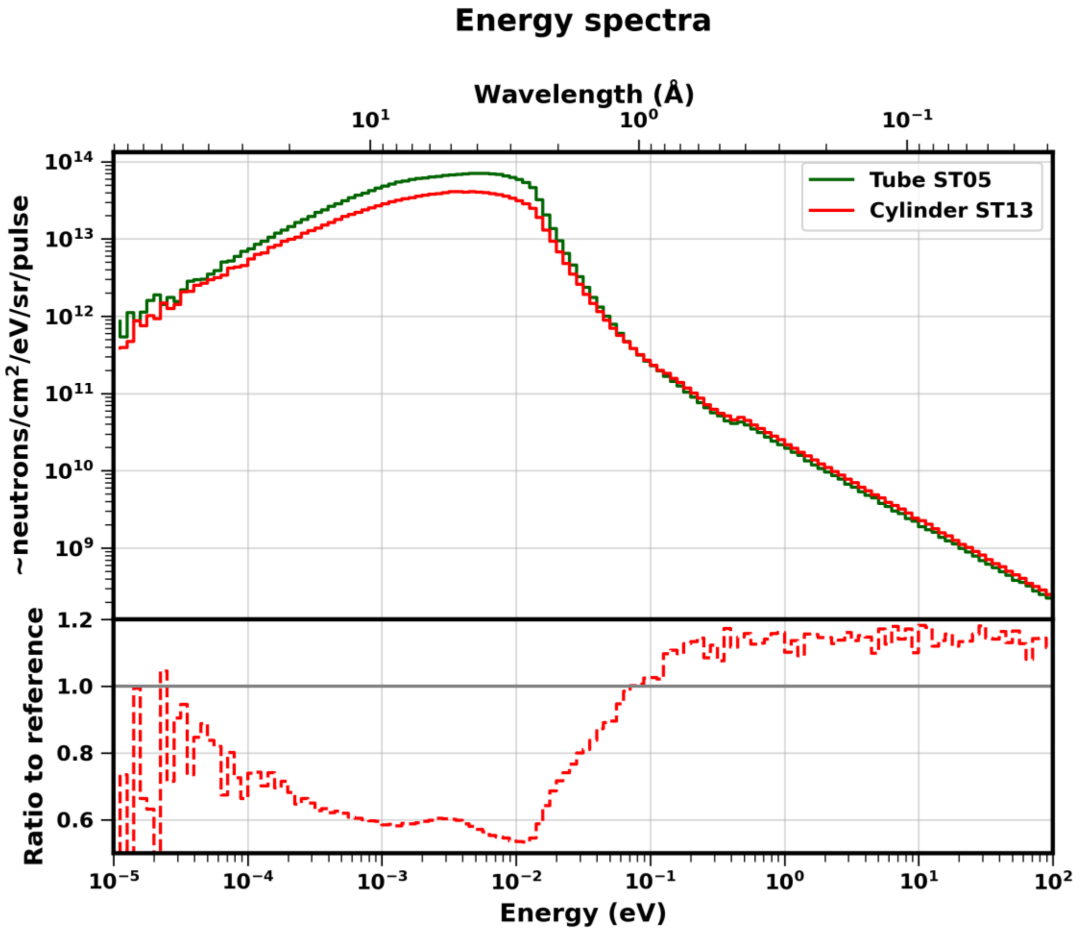
- Neutronics performance was later calculated for the MRA R5.6, the latest version of the Zitti target as of 01/2024 (20 segments) and the 60 cm^2 proton beam profile. The gap between the target and MRA stayed fixed at 10 mm.
- Files combined:
  - Mraanalysis-r5.6.scdoc
  - S03020000-m8u-8800-a10000_asm-012624.scdoc



Neutronics performance – Latest version (cont.)

- Time emission spectra for the tube (ST05) and cylinder (ST13) moderators at 5Å and time-integrated brightness as a function of neutron energy





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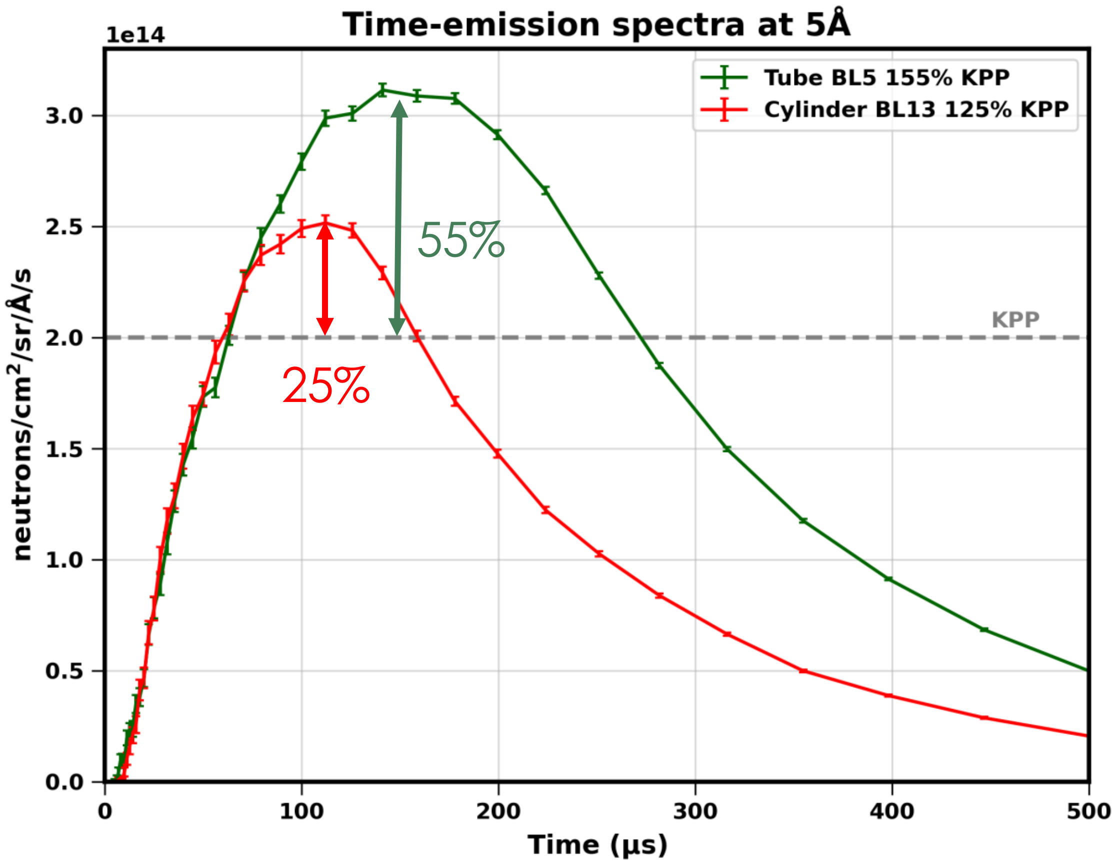
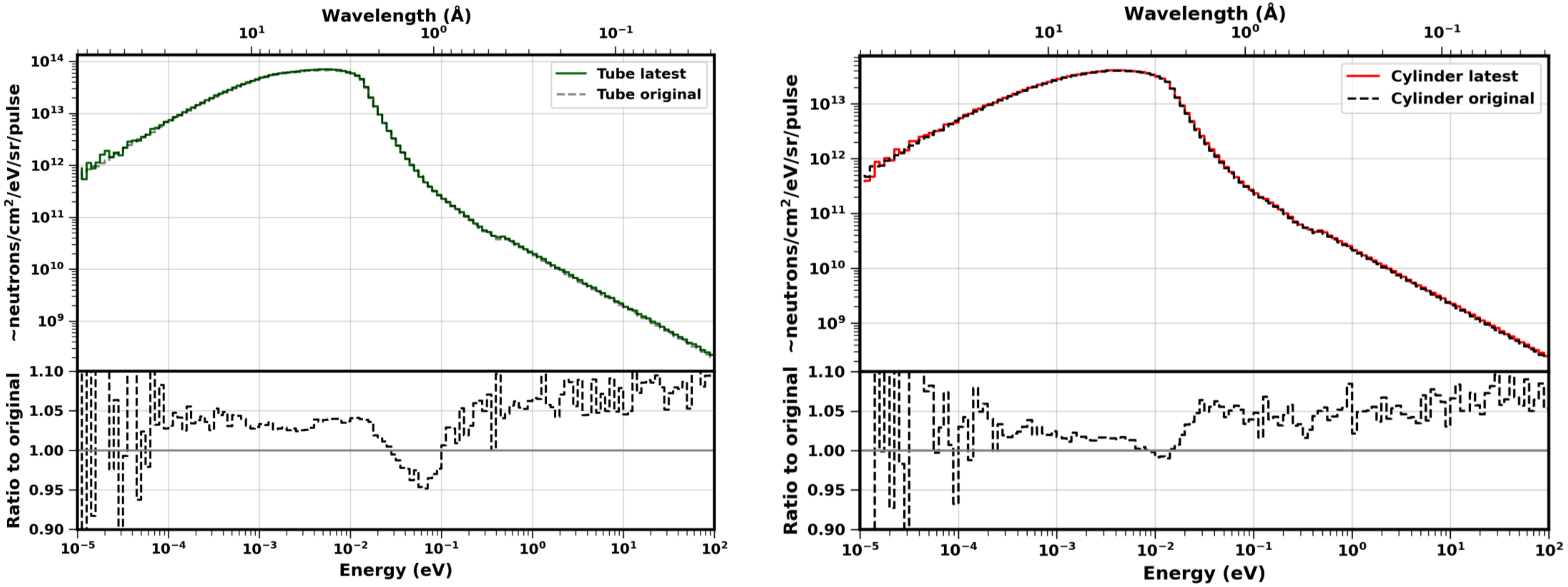
Neutronics performance – Latest version (cont.)

- In the latest configuration, cylinder moderator exceeds KPP by 25% and tube moderator by 55%, which leaves a margin to KPP.



Neutronics performance – Latest version (cont.)

- The latest MRA R5.6 performs very similarly to the original version R5. Tube performs ~4% better (mainly due to the narrower proton beam), while cylinder stays almost the same due to the change in the location of beamline ST13 – a move from 46° to 76.25°.



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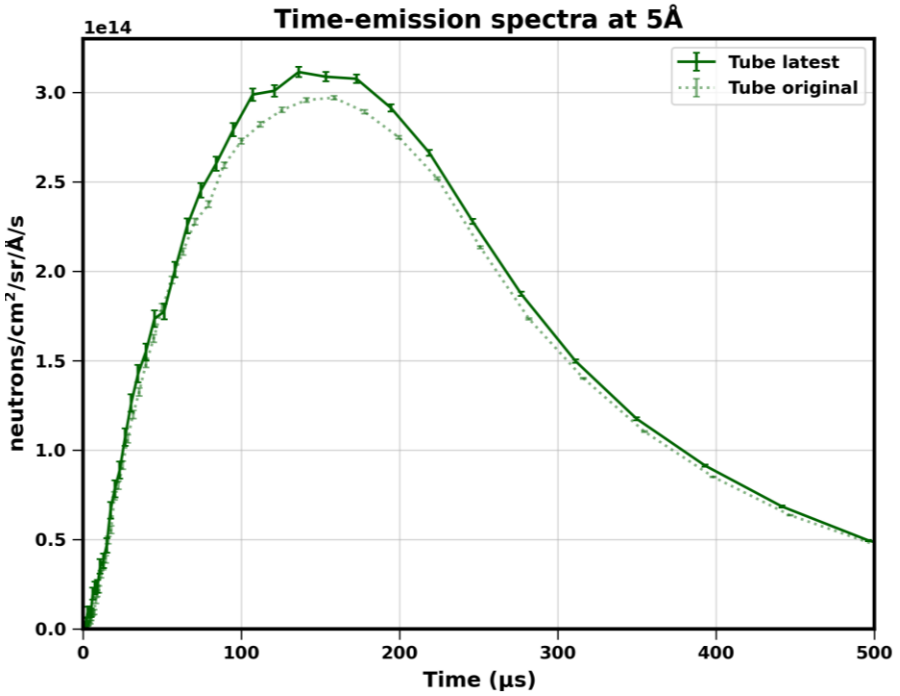
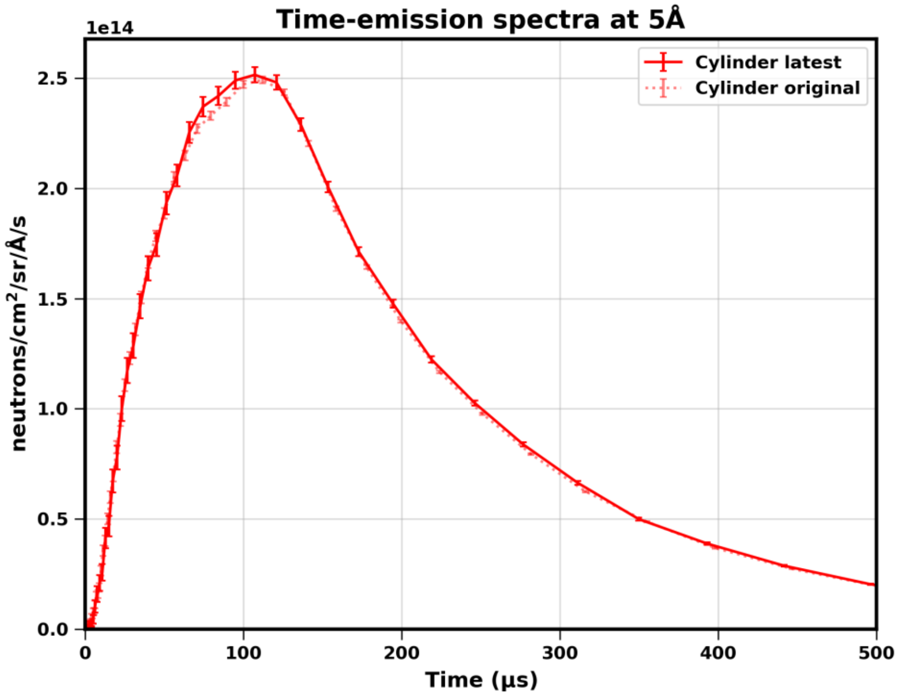
Neutronics performance – Latest version (cont.)

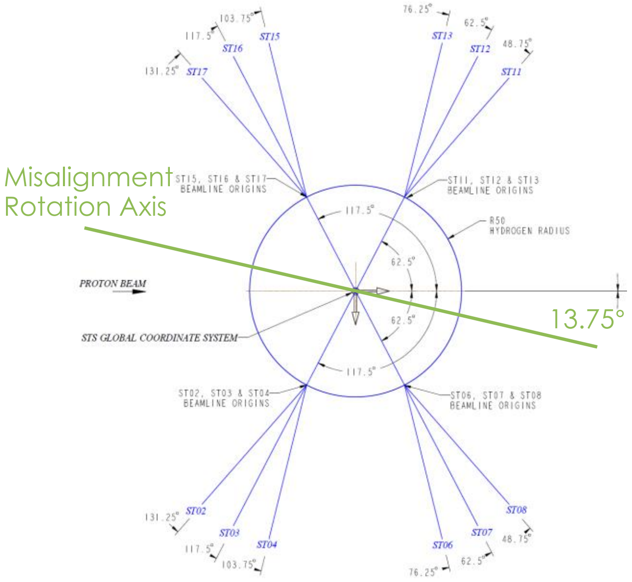
- Similar conclusion applies to the time-emission spectra at 5Å. The purpose of this comparison is to show that the performance of the two configurations is very similar, and there is no need to re-run all the analyses, such as the energy deposition, at this time. **New analyses will surely be performed for the final design**.

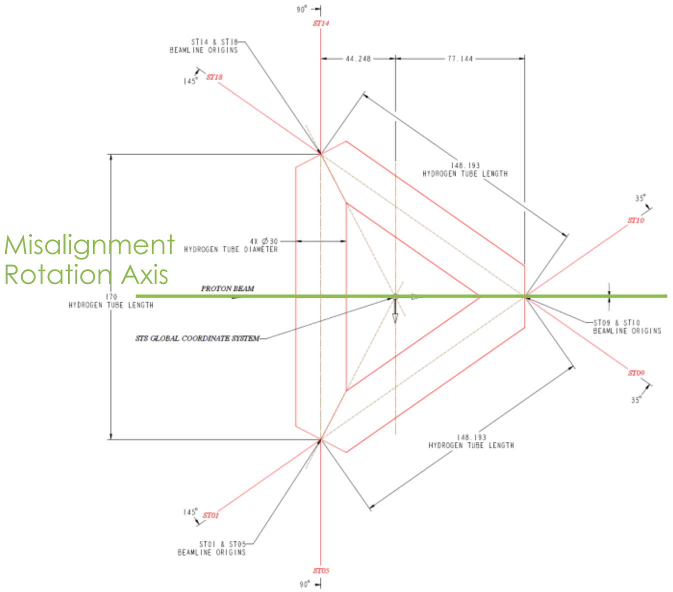




Misalignment study

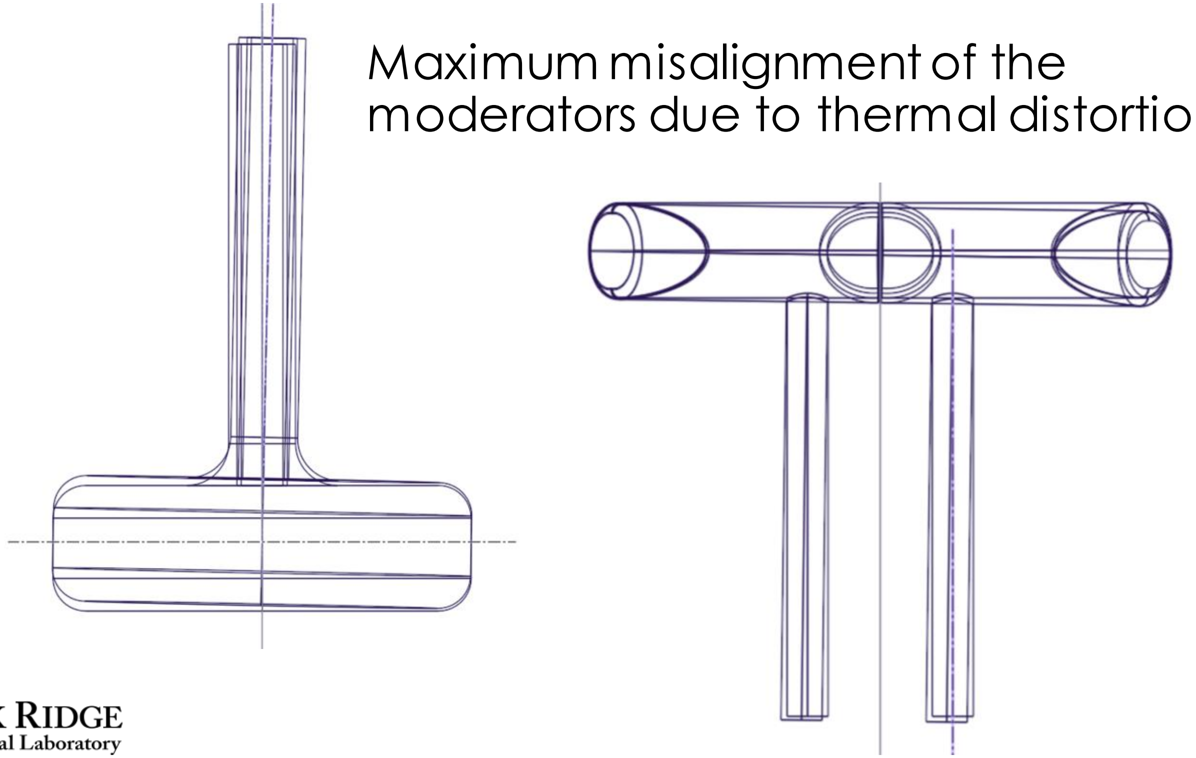
- The goal of this study with MRA R5.6 is to evaluate the decrease in the neutronics performance due to the maximum possible misalignment of the MRA with respect to the beam guides.
- Maximum misalignment is caused by installation tolerances and the thermal distortion of the core vessel shield blocks and is determined as 1.5 mm vertical shift and rotations of 1.2° and 0.75° for the cylinder and tube moderator, respectively.



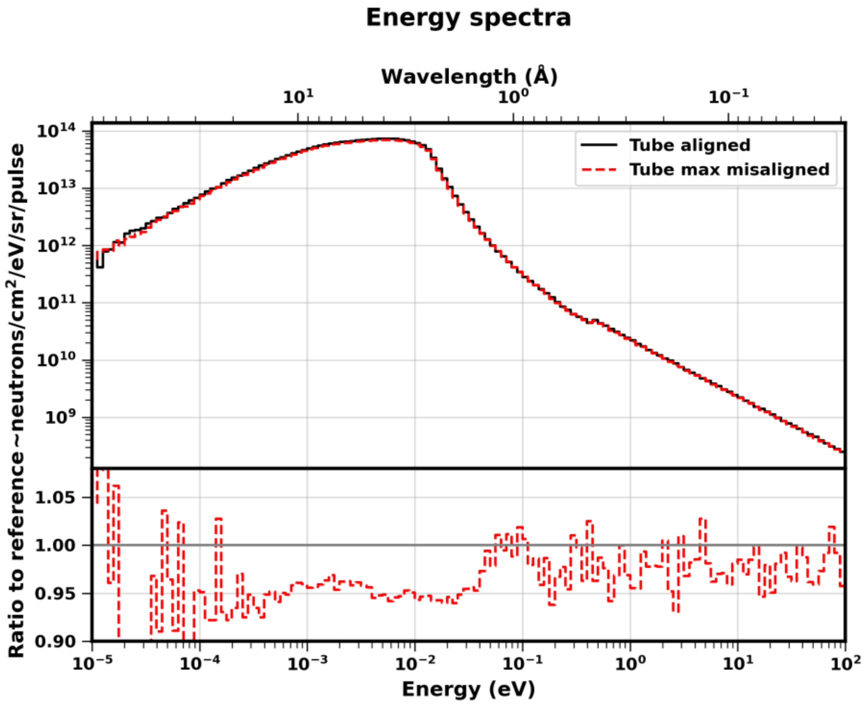


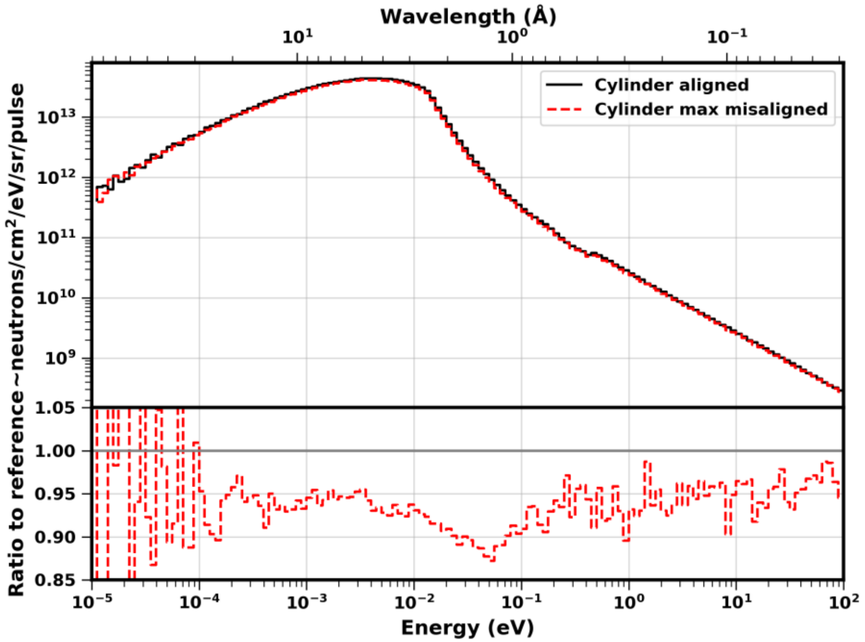
Misalignment study (cont.)

- Maximum misalignment reduces the neutronics performance on the full energy scale by up to 5% and 10% for the tube and cylinder moderators, respectively.



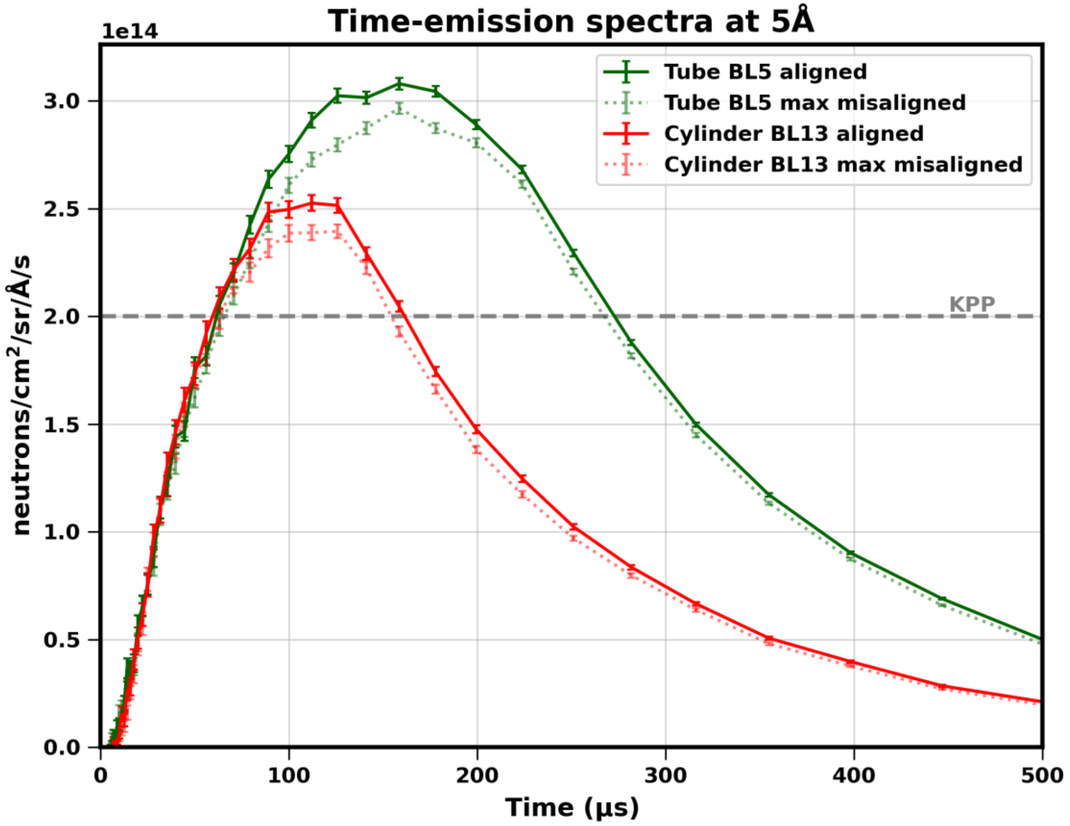
Maximum misalignment of the moderators due to thermal distortion





Misalignment study (cont.)

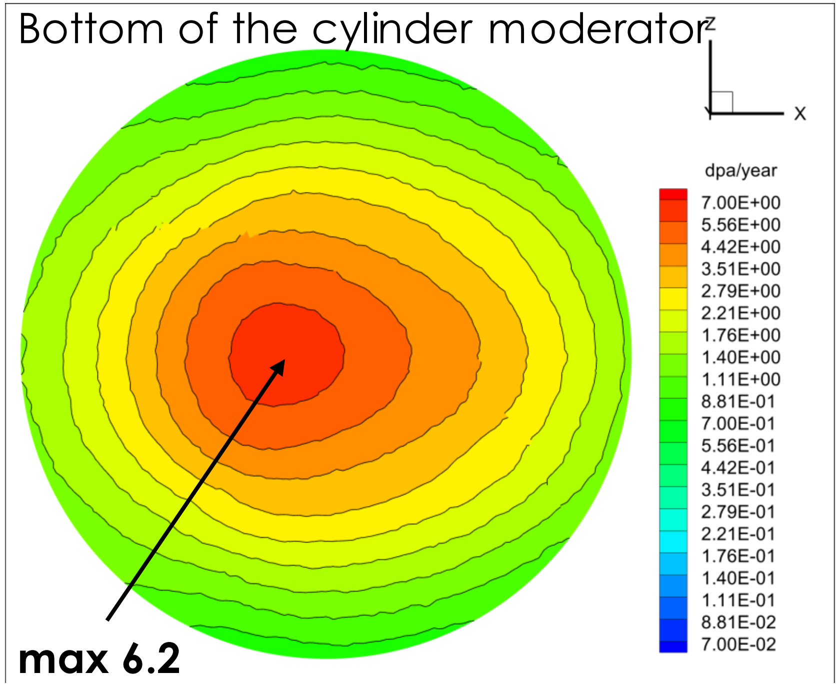
- Maximum misalignment leads to the 5% penalty in neutronics performance at 5Å, which still leaves a margin towards KPP.

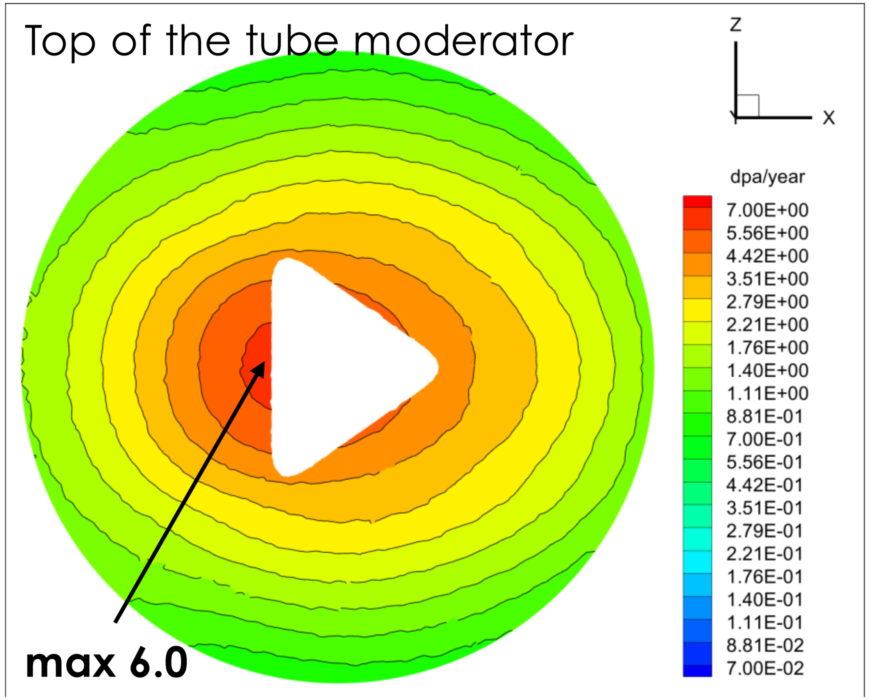


- This study used MRA R5.6, the latest version of the Zitti target as of 01/26/2024 and the 60 cm^2 proton beam profile. Combined files: Mraanalysis-r5.6.scdoc and S03020000-m8u-8800-a10000_asm-012624.scdoc

dpa and MRA lifetime

- dpa in aluminum moderator vessels determines the lifetime of the MRA. Lifetime limit is determined as 40 dpa.
- With max 6.2 dpa/year, the lifetime is predicted as 6.5 years. Lifetime due to He production is predicted as ~25 years.

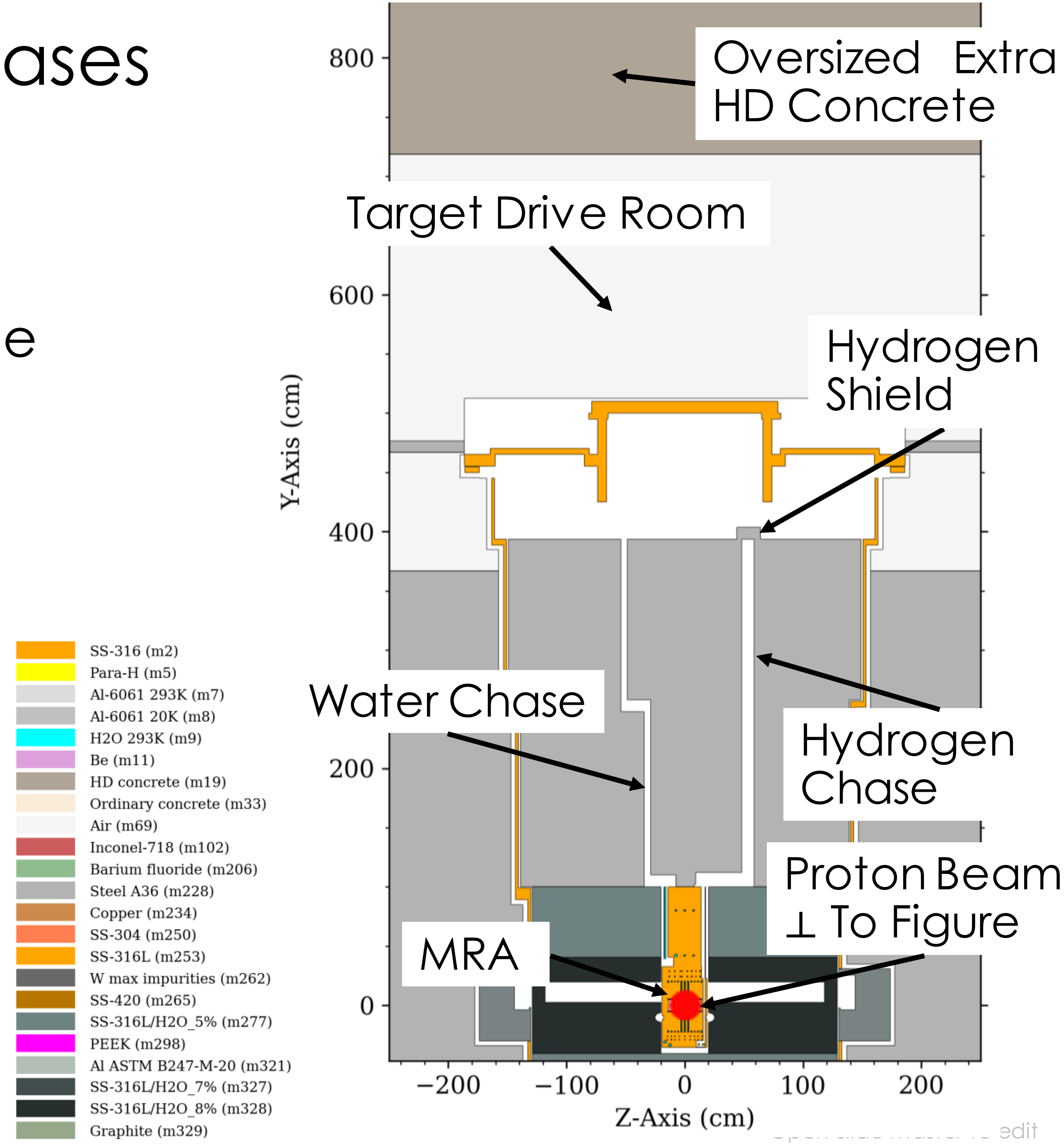




This study used MRA R5.6, the latest version of the Zitti target as of 01/26/2024 and the 60 cm^2 proton beam profile. Combined files: Mraanalysis-r5.6.scdoc and S03020000-m8u-8800-a10000_asm-012624.scdoc

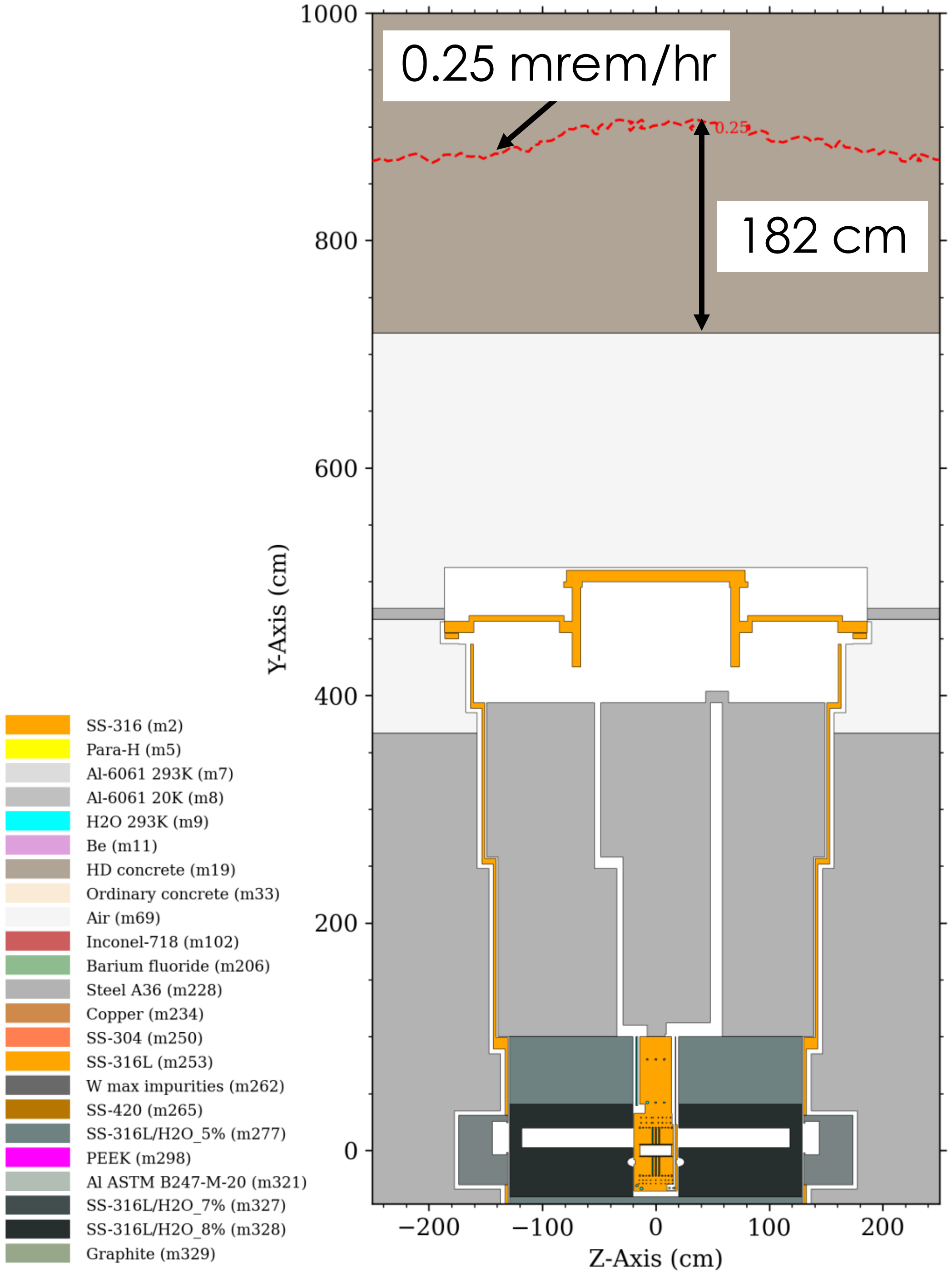
Streaming up MRA pipe chases

- Goal of Study:
  - Ensure that the streaming up the MRA hydrogen and water lines does not violate 0.25 mrem/hr limit in high bay
- BLUF:
  - The additional 10 cm thick hydrogen shield is enough to counter the streaming



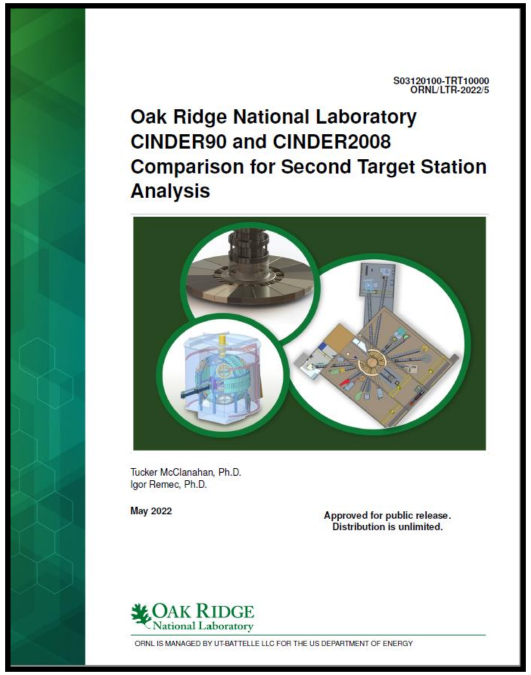
Streaming up MRA pipe chases

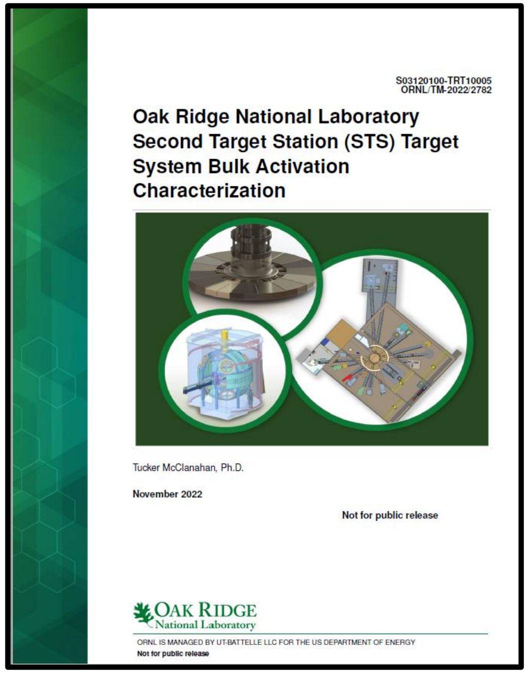
- 0.25 mrem/hr total dose rate contour shown in figure on right in red
- Thickness of the Target Drive Room Roof needs to be 182 cm of HD concrete
- Alternate Configurations:
  - Add shielding to the core vessel shield stack
  - Add shielding to the core vessel lid
  - Change the HD concrete to steel or regular concrete or layers of both

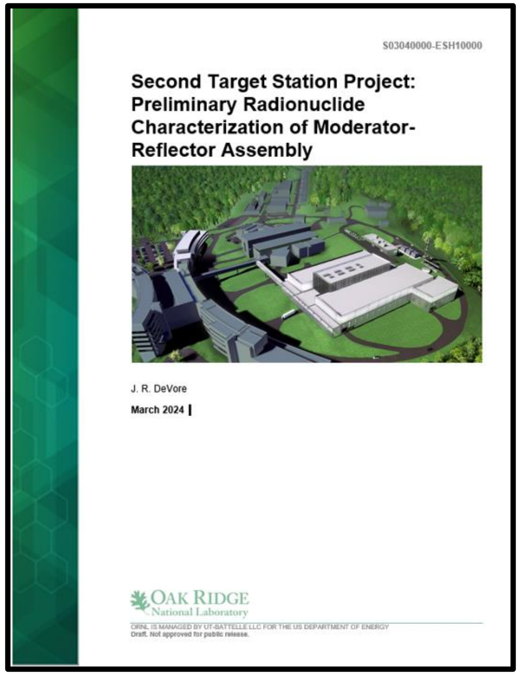


Radionuclide inventory

- The goal of this analysis is to calculate the radionuclide inventory in the MRA at the end of the lifetime and to determine the radioactive waste classification







Transmutation analysis sequence

MCNP
- Tally:
  - Neutron Fluxes
  - Spallation Products

→

Activation Script
- Processes neutron fluxes and spallation products
- Sets up CINDER2008 calculations

→

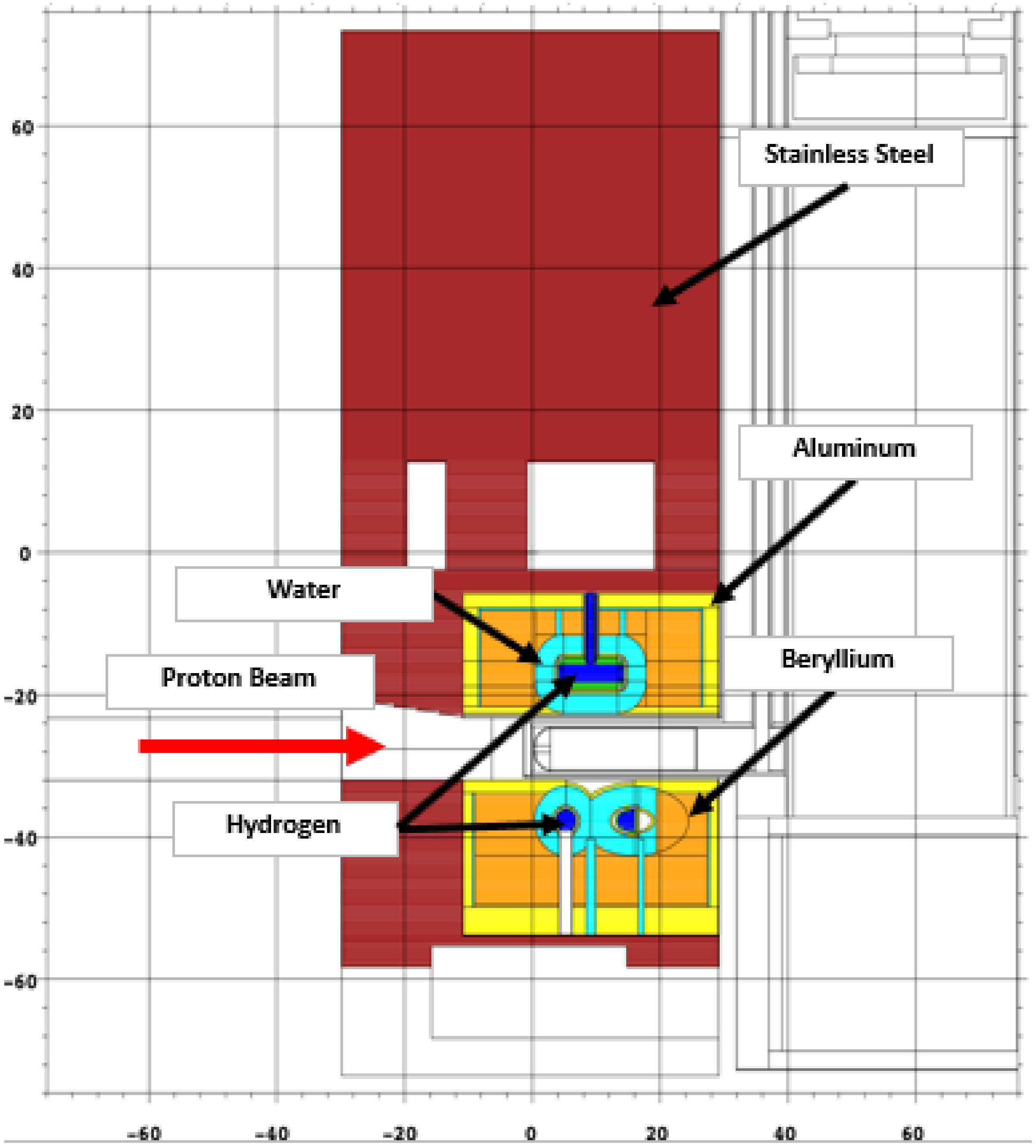
CINDER
- Outputs:
  - Nuclide Inventory
  - Decay Gamma Spectra

→

Post Process
- ACTIUM Python Toolkit

MRA Activation

- Vertical section through MRA model used for activation analysis
- Components analyzed are shown in colors, separated my materials
- Based on CSG master model



Cross section view of MCNP geometry used in the calculation where the scales are in units of cm.

Summary of the MRA activation data

Total Quantity	Shutdown	Decay 24 hr	Decay 48 hr	Decay 96 hr	Decay 1250 hr
1 Year Operation Activity (Ci)	3.47E+05	4.53E+04	4.04E+04	3.50E+04	1.57E+04
1 Year Operation Decay Power (W)	2.86E+03	1.51E+02	1.19E+02	9.75E+01	5.84E+01
1 Year Operation Decay Gamma Intensity (γ/sec)	7.66E+15	1.29E+15	1.13E+15	9.85E+14	5.24E+14
2 Years Operation Activity (Ci)	3.47E+05	4.82E+04	4.34E+04	3.83E+04	1.98E+04
2 Years Operation Decay Power (W)	2.86E+03	1.70E+02	1.39E+02	1.18E+02	7.99E+01
2 Years Operation Decay Gamma Intensity (γ/sec)	7.66E+15	1.35E+15	1.21E+15	1.06E+15	6.31E+14
4 Years Operation Activity (Ci)	3.47E+05	5.27E+04	4.82E+04	4.33E+04	2.56E+04
4 Years Operation Decay Power (W)	2.86E+03	2.00E+02	1.69E+02	1.49E+02	1.13E+02
4 Years Operation Decay Gamma Intensity (γ/sec)	7.67E+15	1.46E+15	1.32E+15	1.18E+15	7.90E+14
10 Years Operation Activity (Ci)	3.48E+05	6.18E+04	5.78E+04	5.34E+04	3.68E+04
10 Years Operation Decay Power (W)	2.85E+03	2.53E+02	2.25E+02	2.06E+02	1.75E+02
10 Years Operation Decay Gamma Intensity (γ/sec)	7.74E+15	1.70E+15	1.57E+15	1.45E+15	1.10E+15
20 Years Operation Activity (Ci)	3.52E+05	7.20E+04	6.84E+04	6.45E+04	4.87E+04
20 Years Operation Decay Power (W)	2.84E+03	2.85E+02	2.59E+02	2.42E+02	2.14E+02
20 Years Operation Decay Gamma Intensity (γ/sec)	7.80E+15	1.84E+15	1.72E+15	1.62E+15	1.29E+15

10CFR61.55 'Licensing Requirements for Land Disposal of Radioactive Waste

Characterization by Long Lived Nuclides

Radionuclide	Concentration (Ci/m^3)
C–14	8
C–14 in activated metal	80
Ni–59 in activated metal	220
Nb–94 in activated metal	0.2
Tc–99	3
I–129	0.08
Alpha emitting transuranic nuclides with half-life > 5 years	100[1]
Pu–241	3,500[1]
Cm–242	20,000[1]

[1] nano-Ci/g

If the concentration is greater than 0.1 times the value in the table, the waste is class C. If it is greater than the table value, the waste is not suitable for shallow land disposal.

Characterization by Short Lived Nuclides

Radionuclide	Class A	Class B	Class C
	(Ci/m3)		
Total of all nuclides with less than 5 year half-life	700	(1)	(1)
H–3	40	(1)	(1)
Co–60	700	(1)	(1)
Ni–63	3.5	70	700
Ni–63 in activated metal	35	700	7000
Sr–90	0.04	150	7000
Cs–137	1	44	4600

There are no limits established for these radionuclides in Class B or C wastes. Practical considerations such as the effects of external radiation and internal heat generation on transportation, handling, and disposal will limit the concentrations for these wastes. These wastes shall be Class B unless the concentrations of other nuclides in table determine the waste to be Class C independent of these nuclides.

MRA characterization by radionuclide inventory

MRA Characterization by Long Lived Nuclides

Isotope	Activity	Concentration	Waste
	Ci	Ci/m^3	Class
C-14	6.76E-03	8.76E-03	A
Ni-59	2.66E+00	3.44E+00	A
Nb-94	3.03E-03	3.93E-03	A
Tc-99	7.68E-02	9.94E-02	A
I-129	0	0.00E+00	
Total alpha	5.16E-02	2.19E+01[1]	C
Pu-241	2.64E+00	1.12E+03[1]	C
Cm-242	9.29E-01	3.94E+02[1]	A

[1] nano-Ci/g

MRA Characterization by Short Lived Nuclides

Isotope	Activity	Concentration	Waste
	Ci	Ci/m^3	Class
Total	1.89E+04	2.45E+04	B
H-3	7.77E+03	1.01E+04	B
Co-60	9.71E+03	1.26E+04	B
Ni-63	3.17E+02	4.11E+02	B
Sr-90	4.43E-03	5.73E-03	A
Cs-137	0	0.00E+00	

- **MRA activation assumed 10y operation with 1250 h decay.**
- **Shipment in TN-RAM cask assumed**
- **Based upon the total alpha and Pu-241 concentration, the MRA waste would be Class C.**

MRA in TN-RAM cask: CLASS C

- This characterization is based on a waste volume.
- The cask of choice for shipping large waste items at STS is TN-RAM.
- The volume of the liner which will ship in the TN-RAM is 0.772 m^3.

Data used in the calculation of the MRA waste form in TN-RAM cask

Parameter	Value
MRA Weight	1,361,700 g
MRA Volume	0.1925 m^3
Liner weight	998,580 g
Liner material volume	0.127 m^3
Liner ID	0.685 m
Liner inside length	1.75 m
Liner internal volume	0.645 m^3
Waste form volume	0.772 m^3
Waste form weight	2,360,280 g

Activation dose rate

- It is necessary to calculate the activation dose rate after shutdown to remove and replace the MRA after its lifetime of 6 years has passed
- Dose rate is calculated in the target drive room (TDR) and in the highbay with the goal to make work activities possible (i.e., to use remote tools to cut pipes above the backbone)
- Although the use of UM is possible with double caution (several issues identified), it was decided to use traditional approach with MCNP6' CSG geometry for this task
- Uses CSG master model as of 12/31/2023

Activation dose rate (cont.)

Irradiation times:
MRA 6 years
Target 10 years
Shielding 40 years
assuming
5,000hr/year
operation

High bay

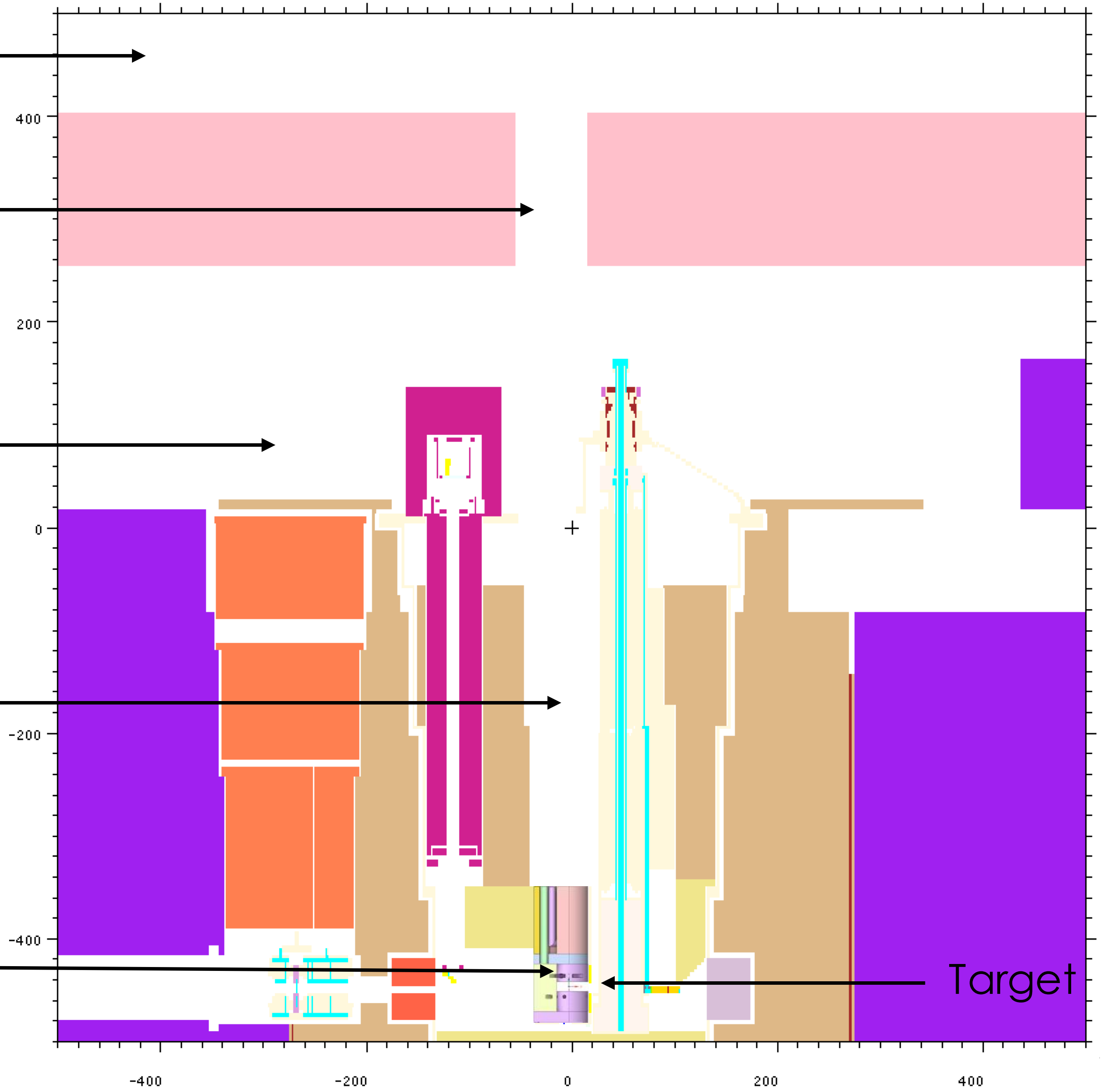
Roof with opening

Target drive room (TDR)

Removed shielding blocks for MRA replacement, which represents a streaming gap

MRA + backbone

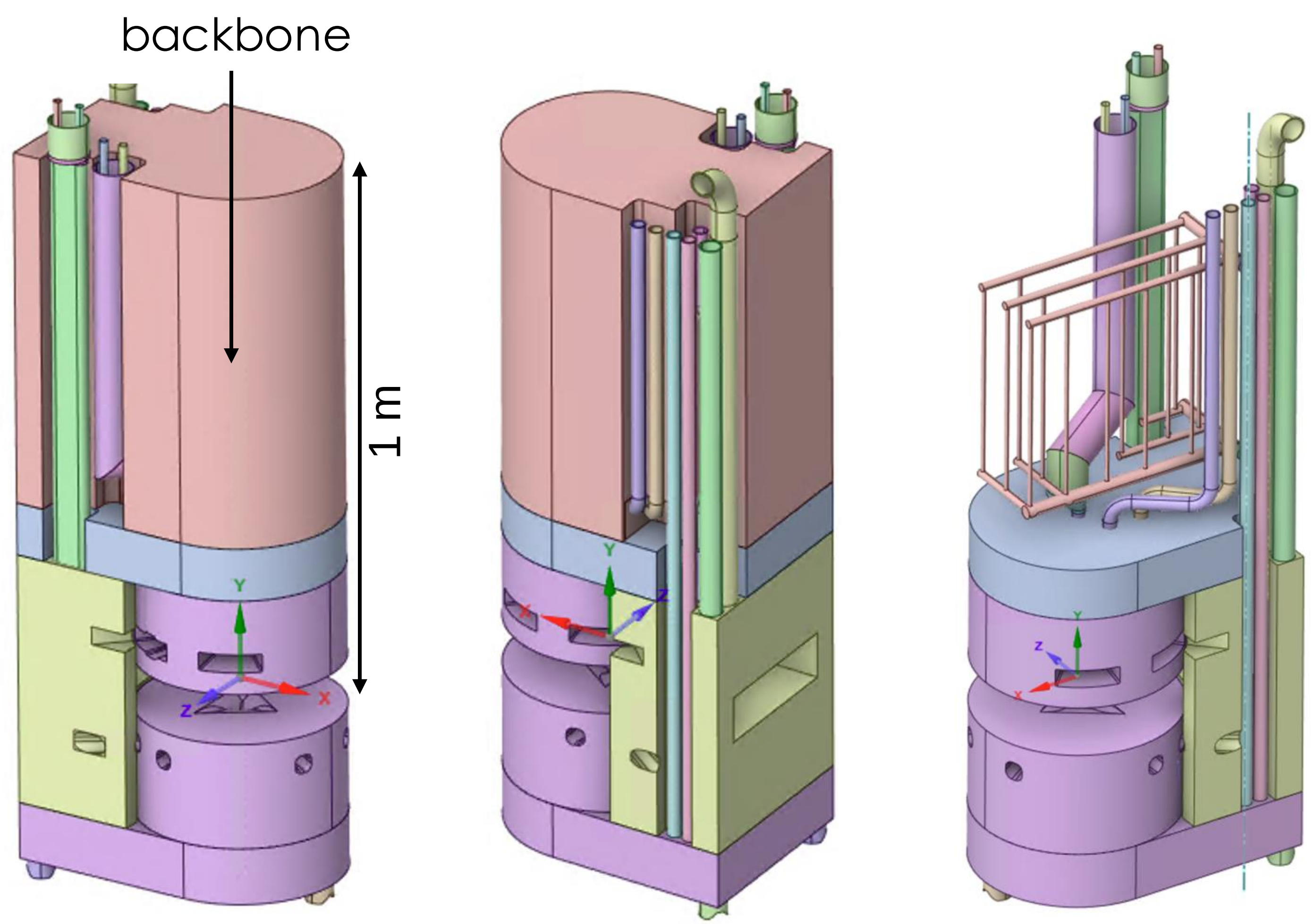
Target



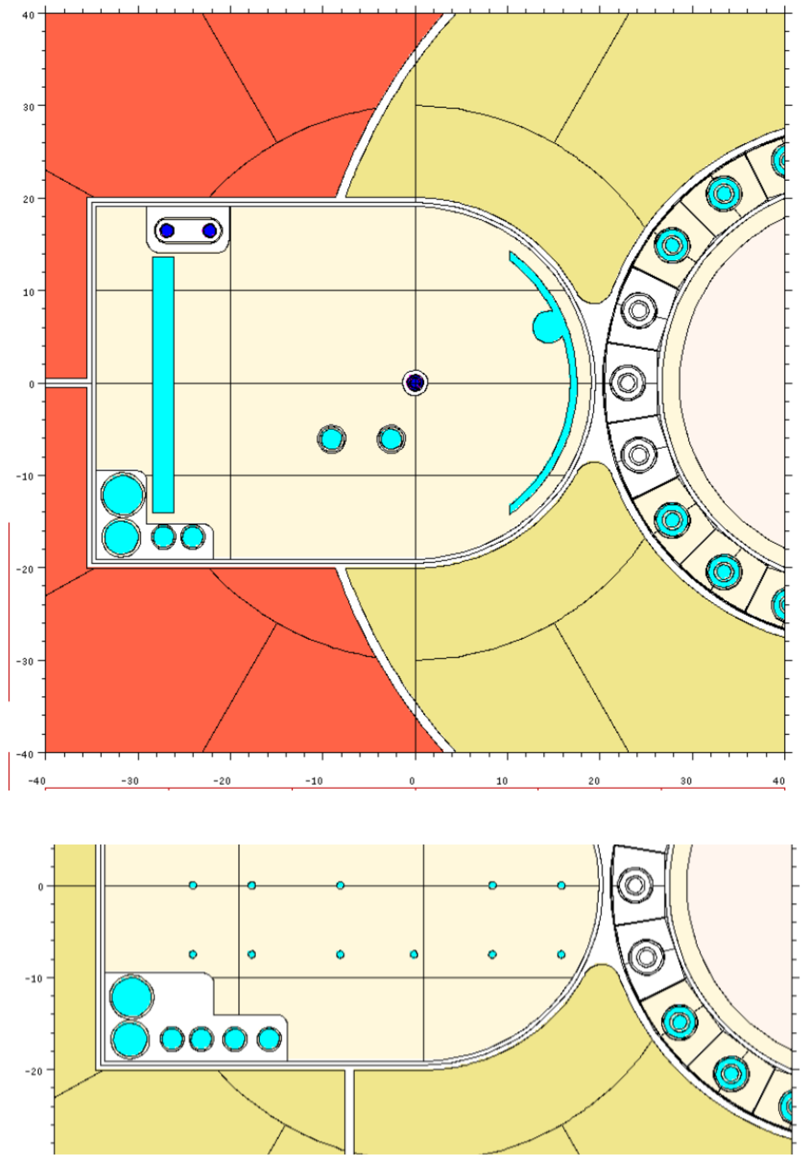
This elevation view used in the subsequent plots

Activation dose rate (cont.)

- MRA will be replaced together with the water-cooled steel backbone



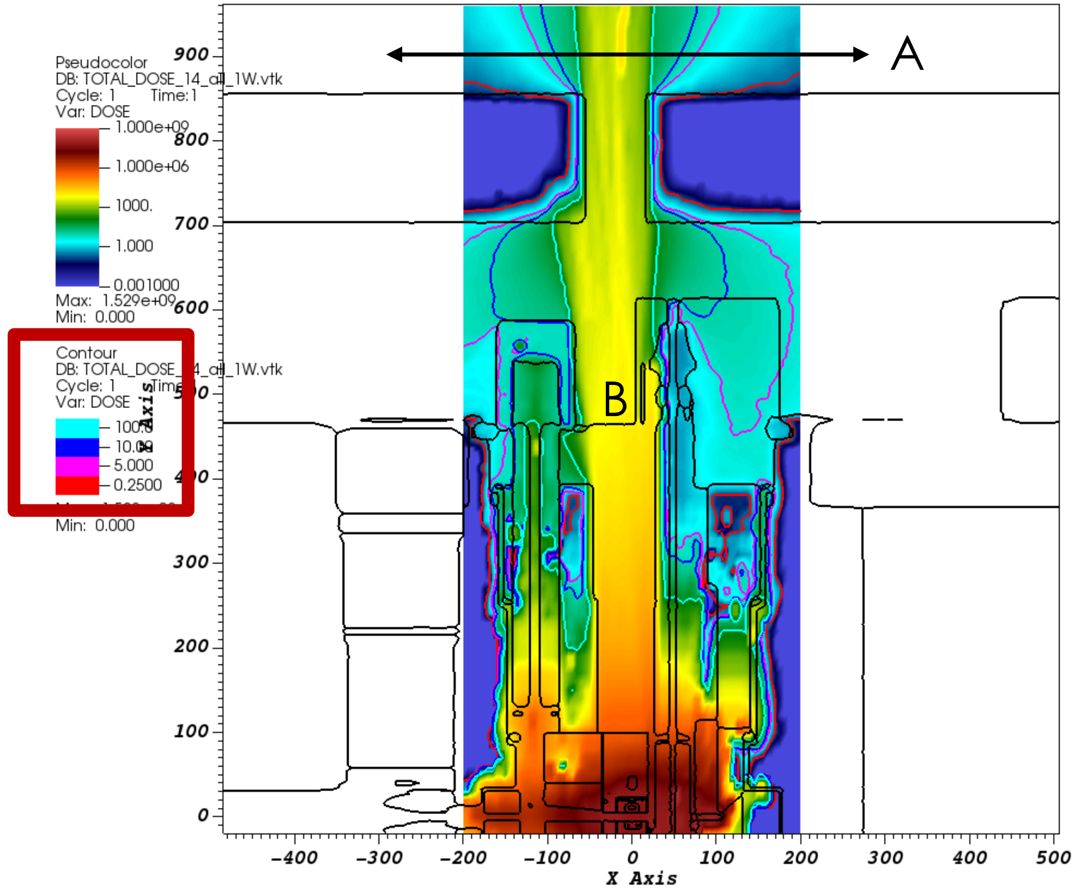
Detailed CSG model



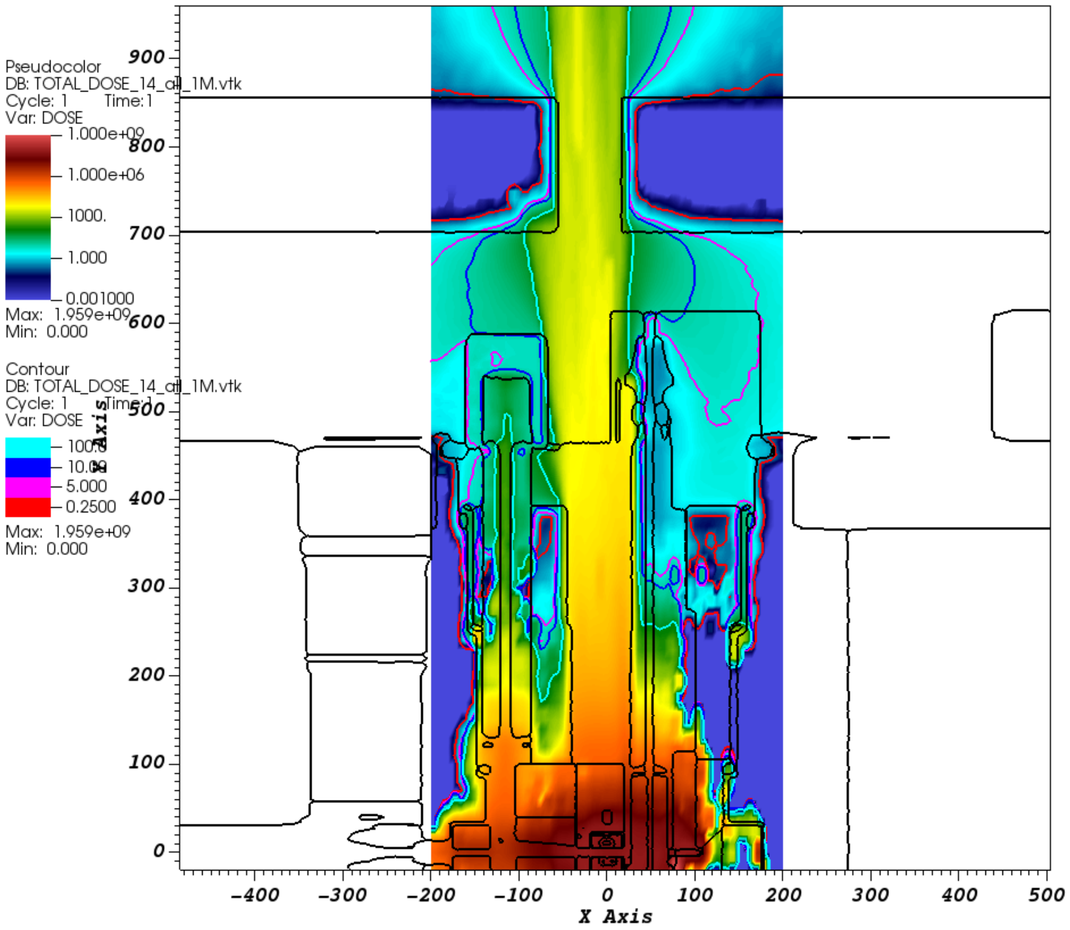
Activation dose rate (cont.)

High activation dose rates of 10 rem/hr in the streaming gap in TDR (point B) prohibit from work activities in TDR. The only potential location for work is the high bay above TDR roof. See next slide for the horizontal cross sections through plane A at the elevation of 9 m.

1-week decay time



1-month decay time

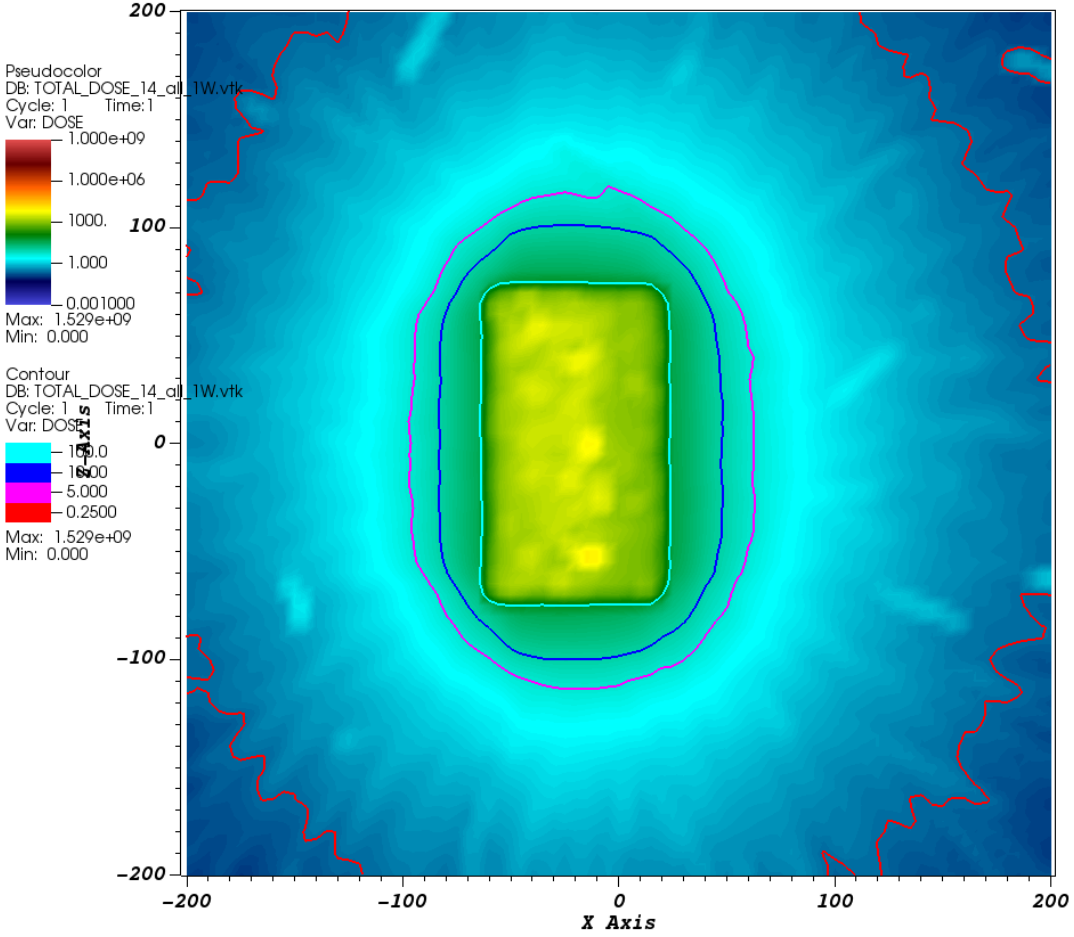


Important contour lines mrem/hr

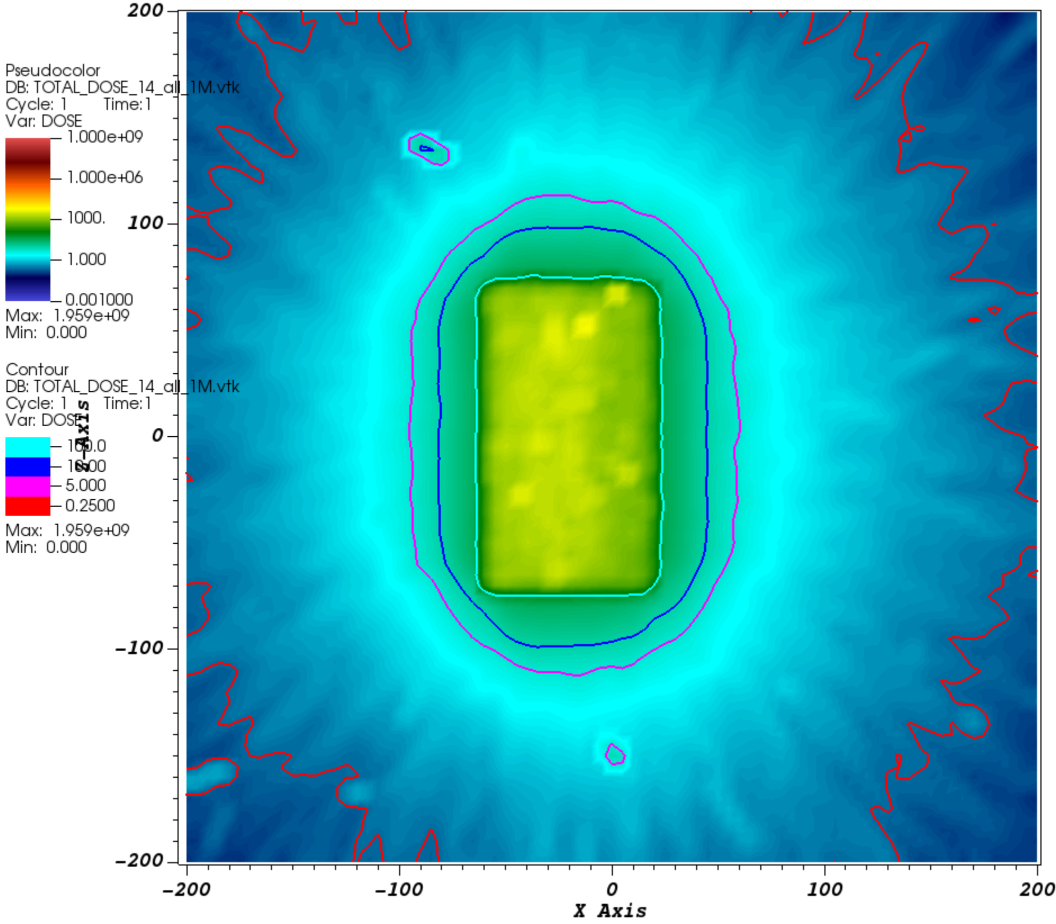
Activation dose rate (cont.)

These contour plots represent activation dose rates in the high bay, 30 cm above the floor. Dose rate is 100 mrem/hr at the edge of the roof opening and is 0.25 mrem/hr at 2 m from the opening. No significant reduction of the dose rate as a function of the decay time (1 week vs. 1 month).

1-week decay time

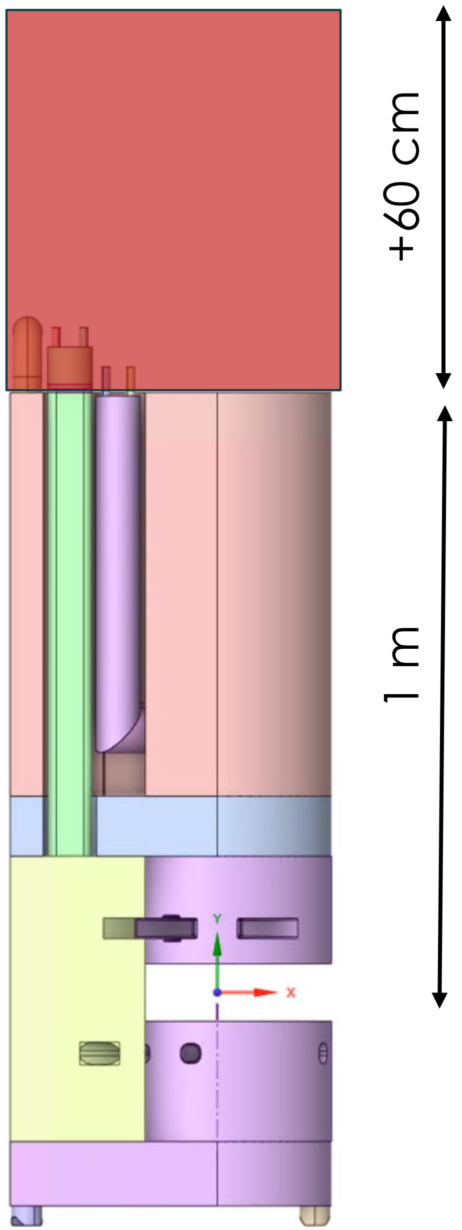


1-month decay time



Activation dose rate (cont.)

- Previous results indicate that work is possible only in the high bay, and not in the TDR.
- Dose rate does not decrease significantly as a function of the decay time.
- It was therefore decided to increase the thickness of the backbone by additional 60 cm to provide more shielding when the shield blocks above the backbone are removed for MRA replacement.
- 60 cm is max additional thickness without changing the design of the bearings.



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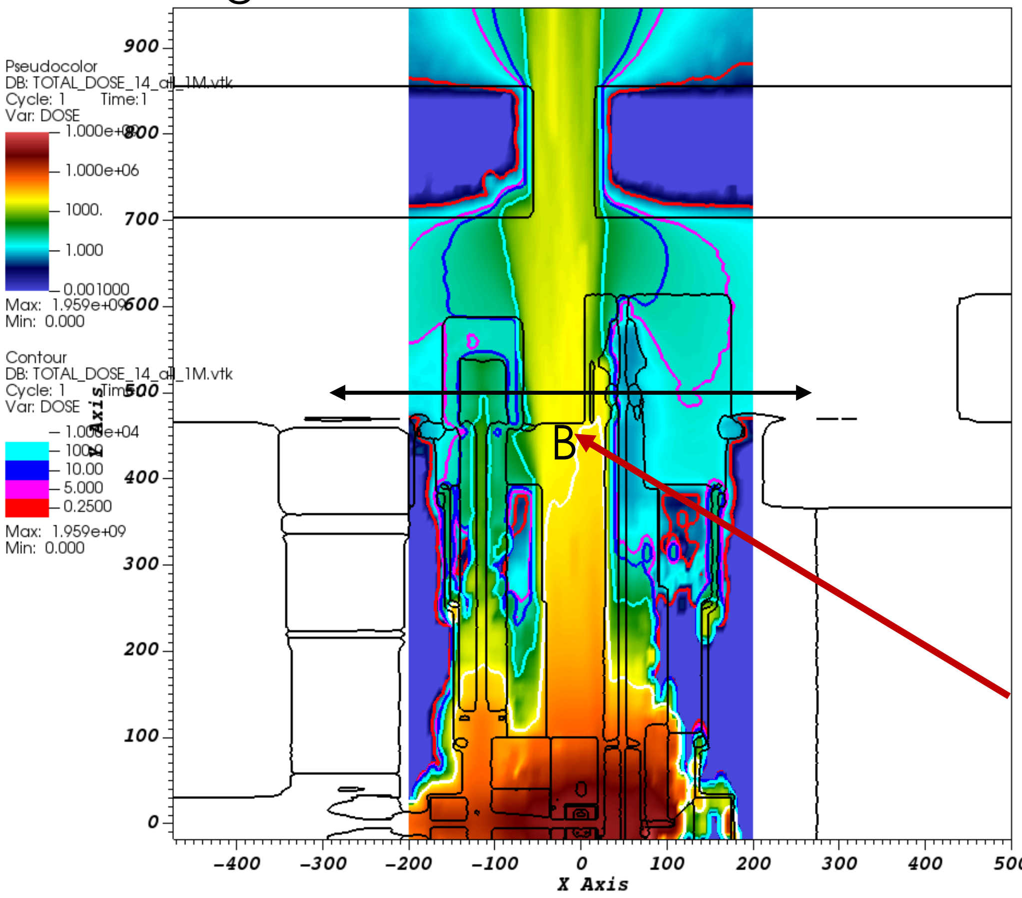
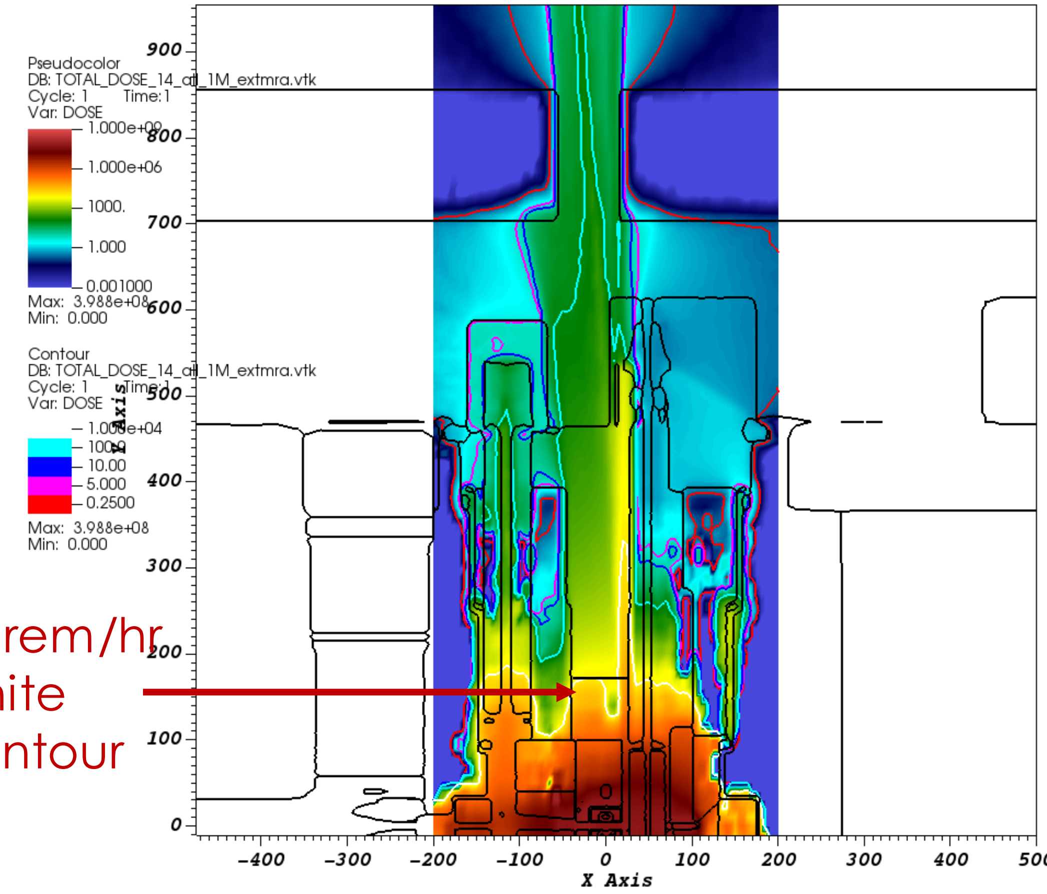
Activation dose rate (cont.)

Streaming through the gap has been reduced by more than a factor of 100 with the extended backbone, which makes work activities in TDR possible. See next slide for the horizontal cross sections through plane B at the elevation of 5 m.

1-month decay time, original backbone



1-month decay time, extended backbone



10 rem/hr white contour

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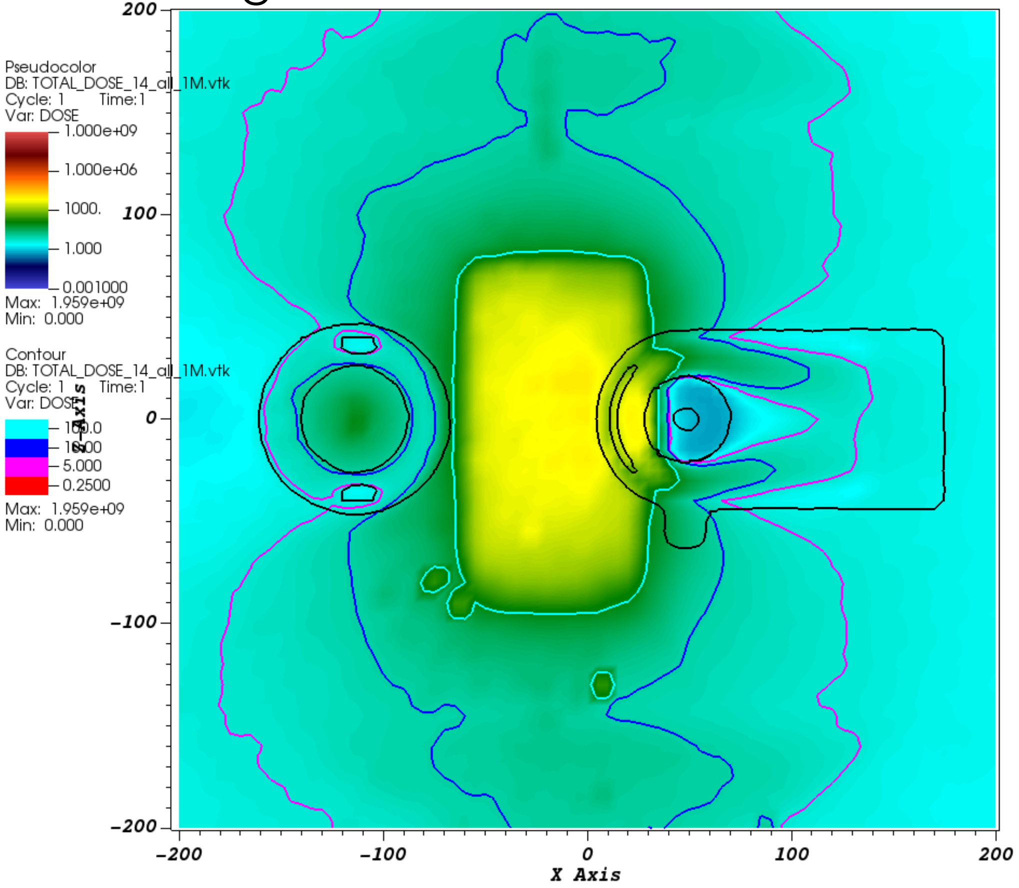
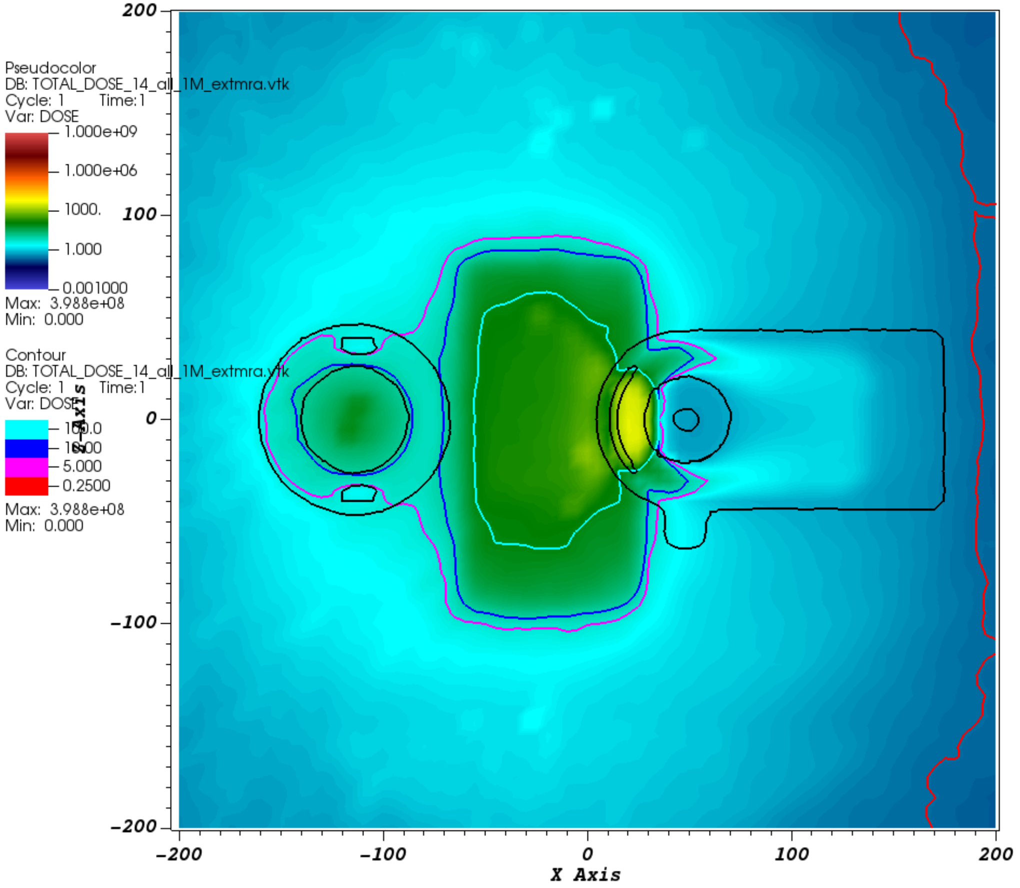
Activation dose rate (cont.)

These contour plots represent activation dose rates in the TDR, 30 cm above the floor. With the extended backbone, streaming through the gap corresponds to 100 mrem/hr and the dose rate is 5 mrem/hr at the edge of the gap, which makes work activities in the TDR possible.

1-month decay time, original backbone



1-month decay time, extended backbone



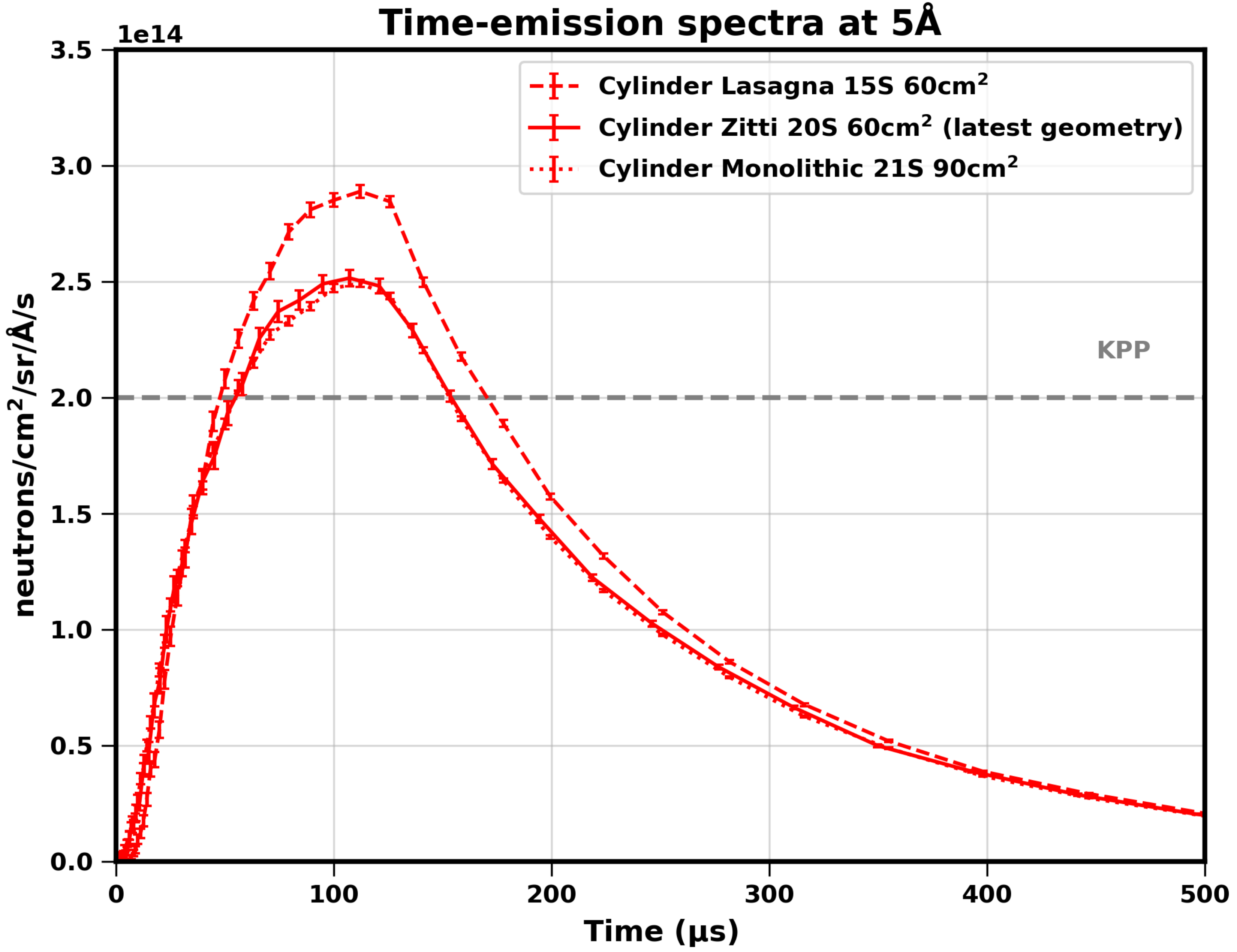
Activation dose rate (cont.)

- The increased thickness of the backbone enables work activities in the TDR associated with the MRA replacement.
- Work continues on additional geometry configurations related to MRA replacement.

Thank you.

- Backup slides follow

Cylindrical moderator performance comparison



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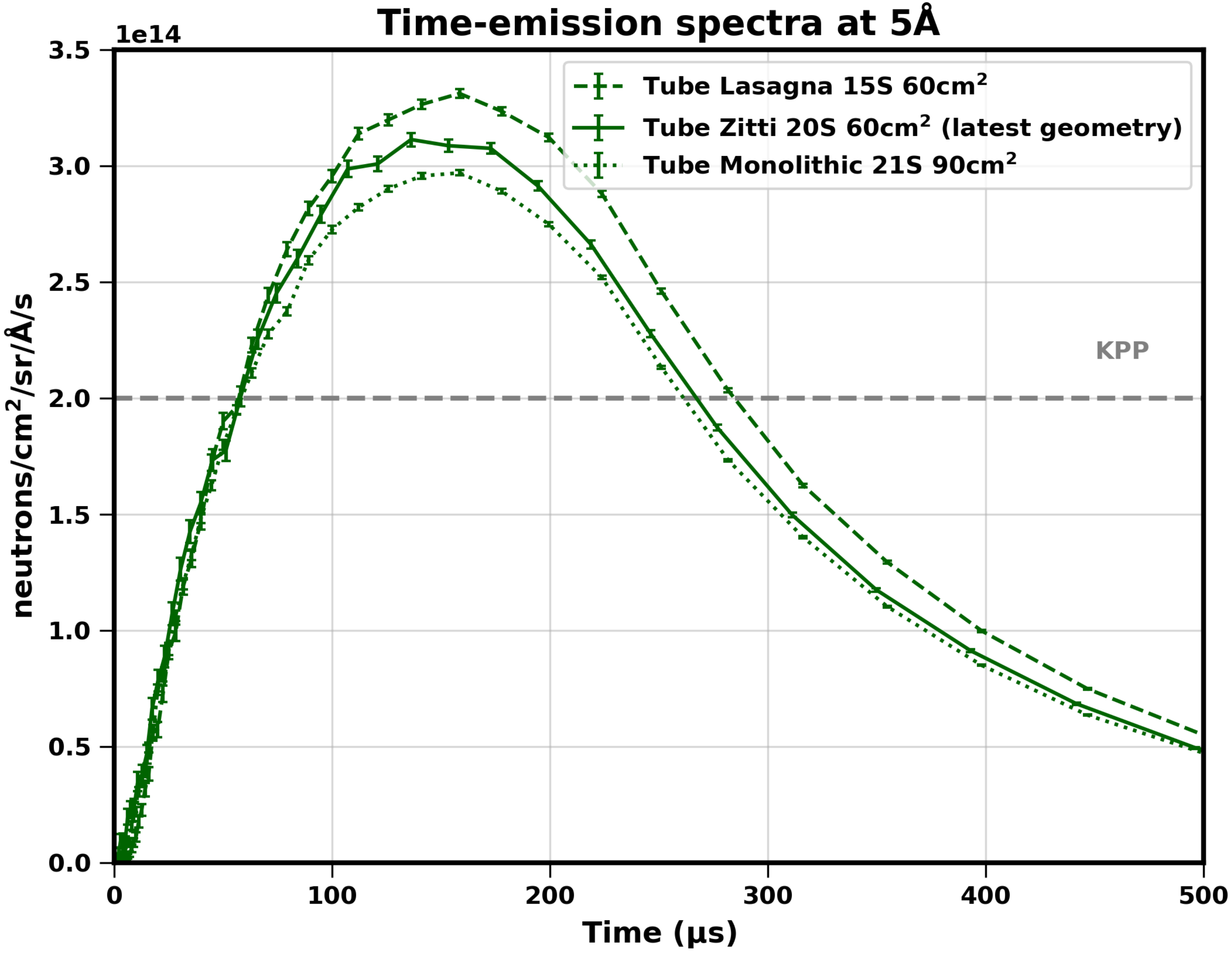
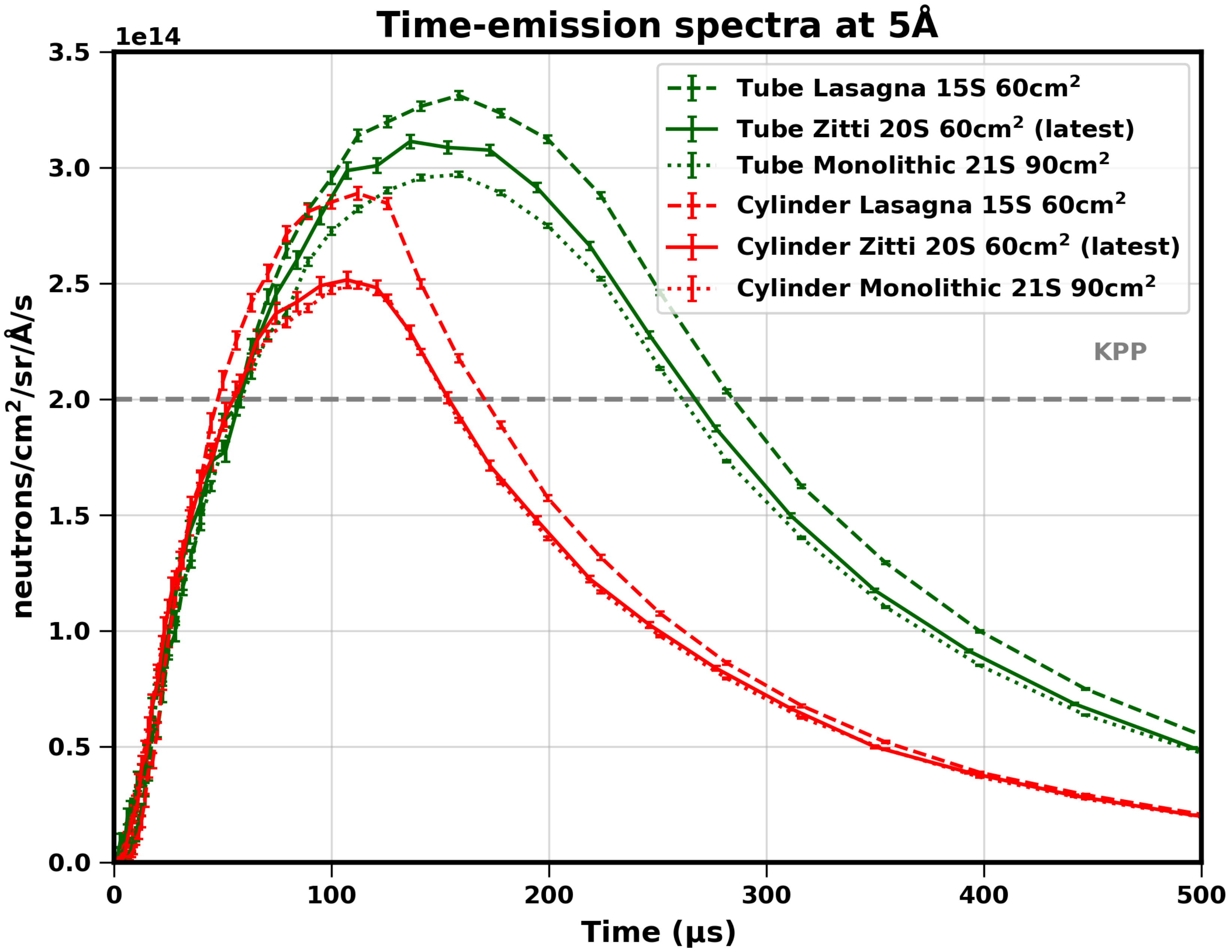
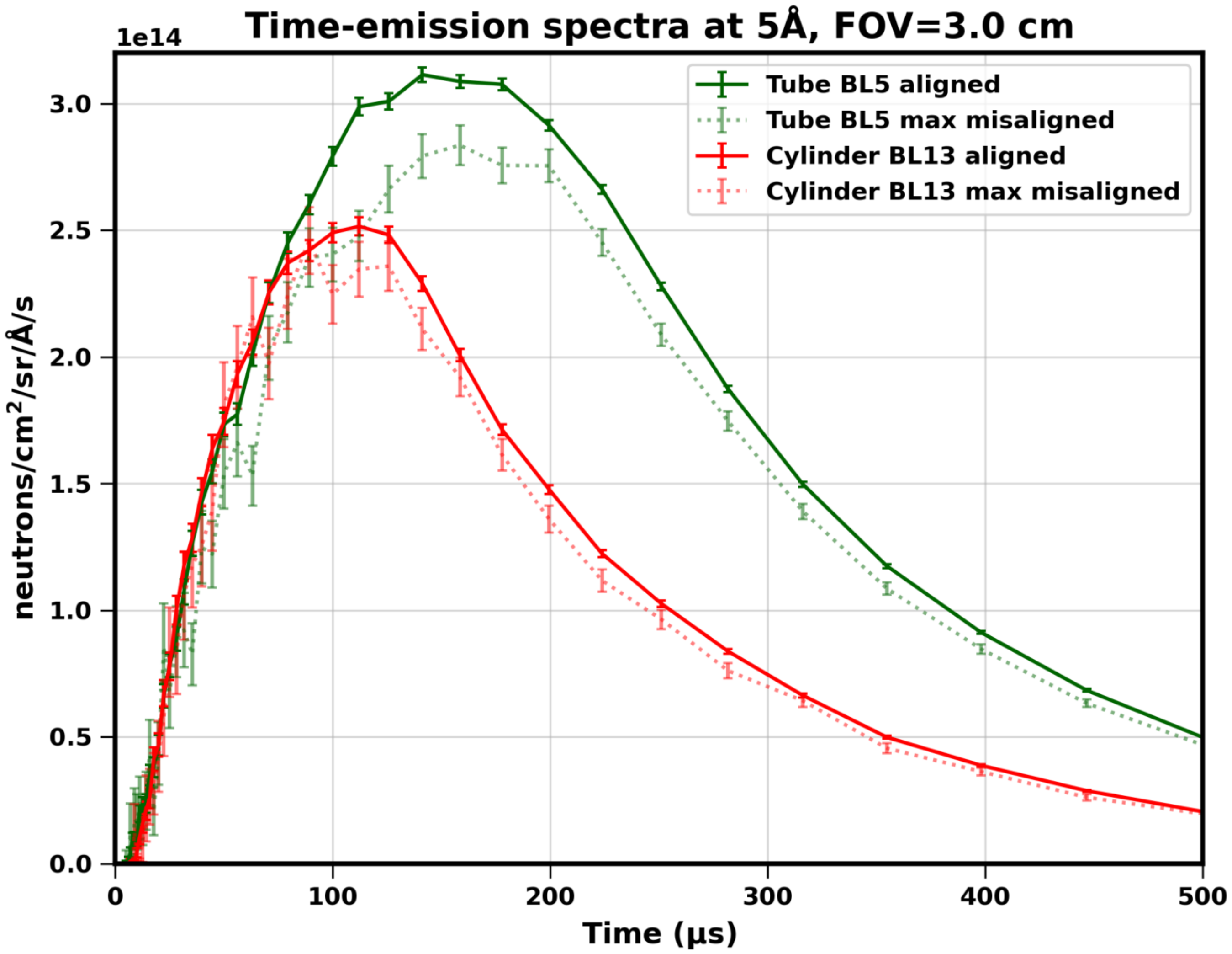
Tube moderator performance comparison



Moderator performance comparison

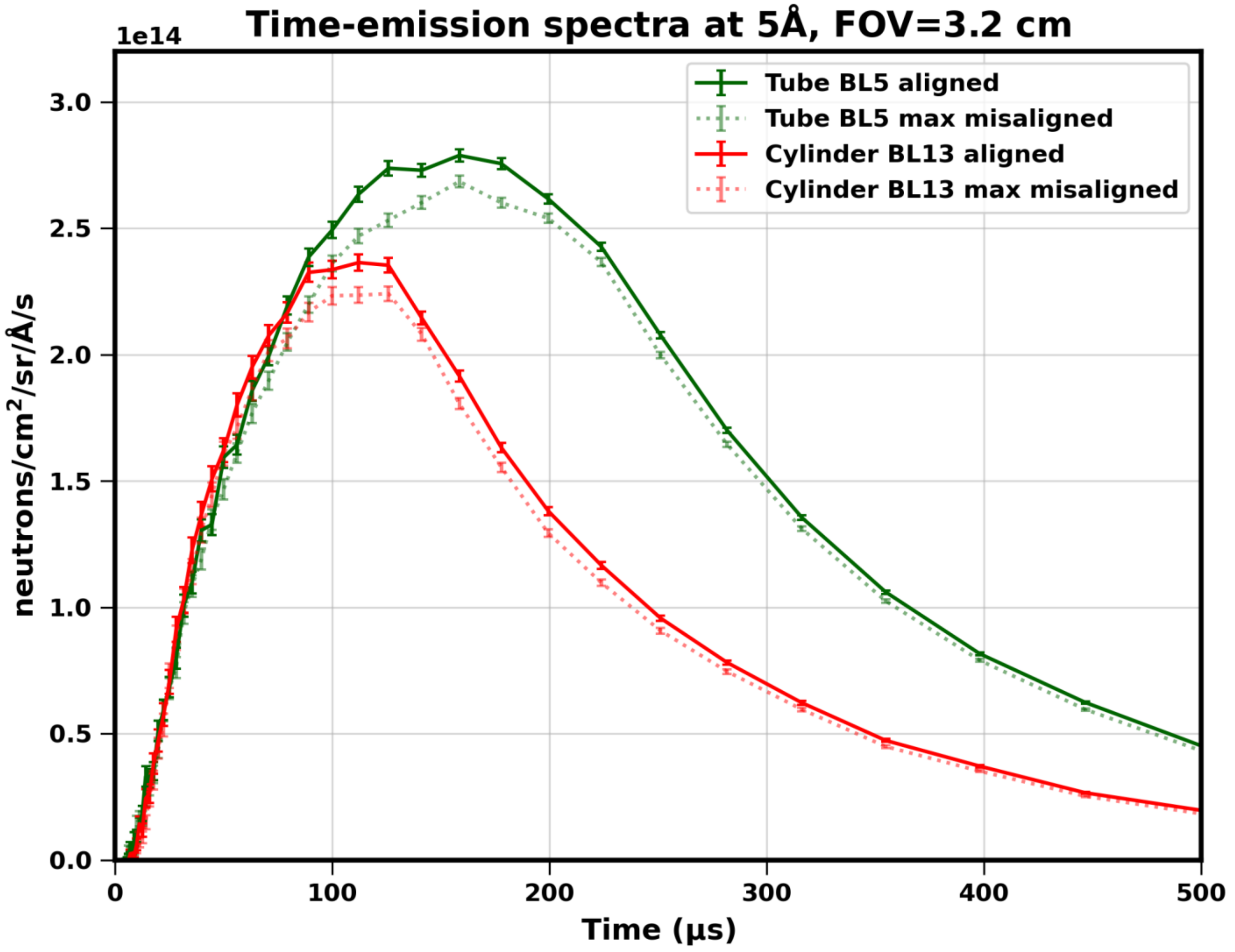


Misalignment: details



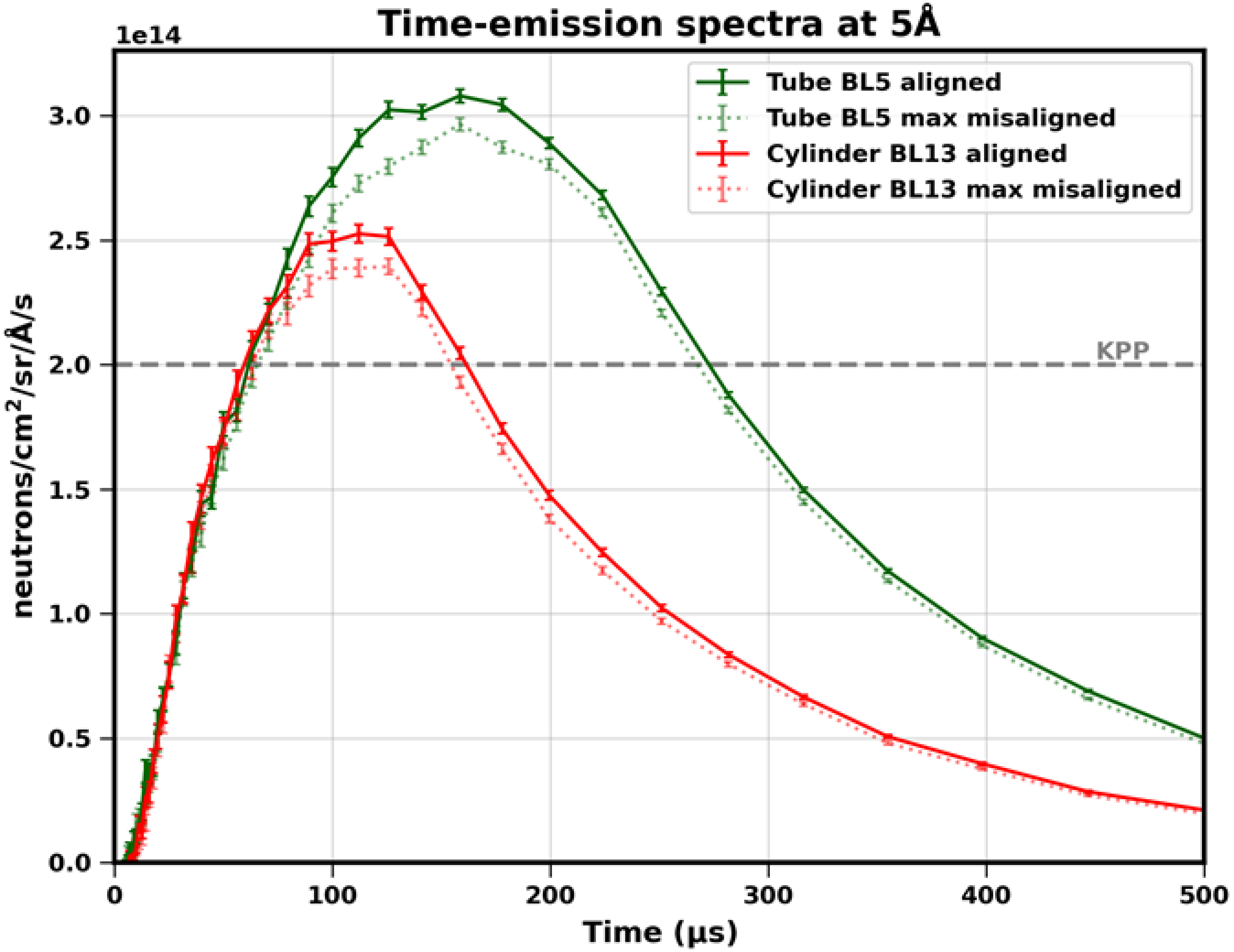
- This plot uses field of view (FOV) 3.0 cm for the misalignment study:
- Penalty is 8% for tube and 6% for cylinder. However, this is somewhat exaggerated because the tube and cylinder moves out of the field of view and FOV is partially obstructed by the Beryllium reflector.

Misalignment: details



- To reduce this effect and make the estimate of misalignment more realistic, the calculation was run with increased FOV 3.2 cm, as shown here:
- Penalty is about 5% for both moderators. However, you can notice a drop in brightness, because of the larger FOV.

Misalignment: details



- So more realistic estimate of the misalignment is the combination of both calculations, where the results for FOV 3.2 cm are scaled (by one factor for tube and another for cylinder) to match the peak of FOV 3.0 cm, as shown here:

Heavy water (HW) effect

- 6% gain due to HW as premoderator and backbone coolant