Oak Ridge National Laboratory

MRA Neutronics Optimization

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MRA PDR Review

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U.S. DEPARTMENT OF ENERGY

Outline

- Introduction
- Early optimization investigation
- Optimization with high fidelity models
- Preliminary Design Configuration
- Further work: simultaneous MRA/target/beam profile optimization
- Conclusion

Preliminary STS KPPs

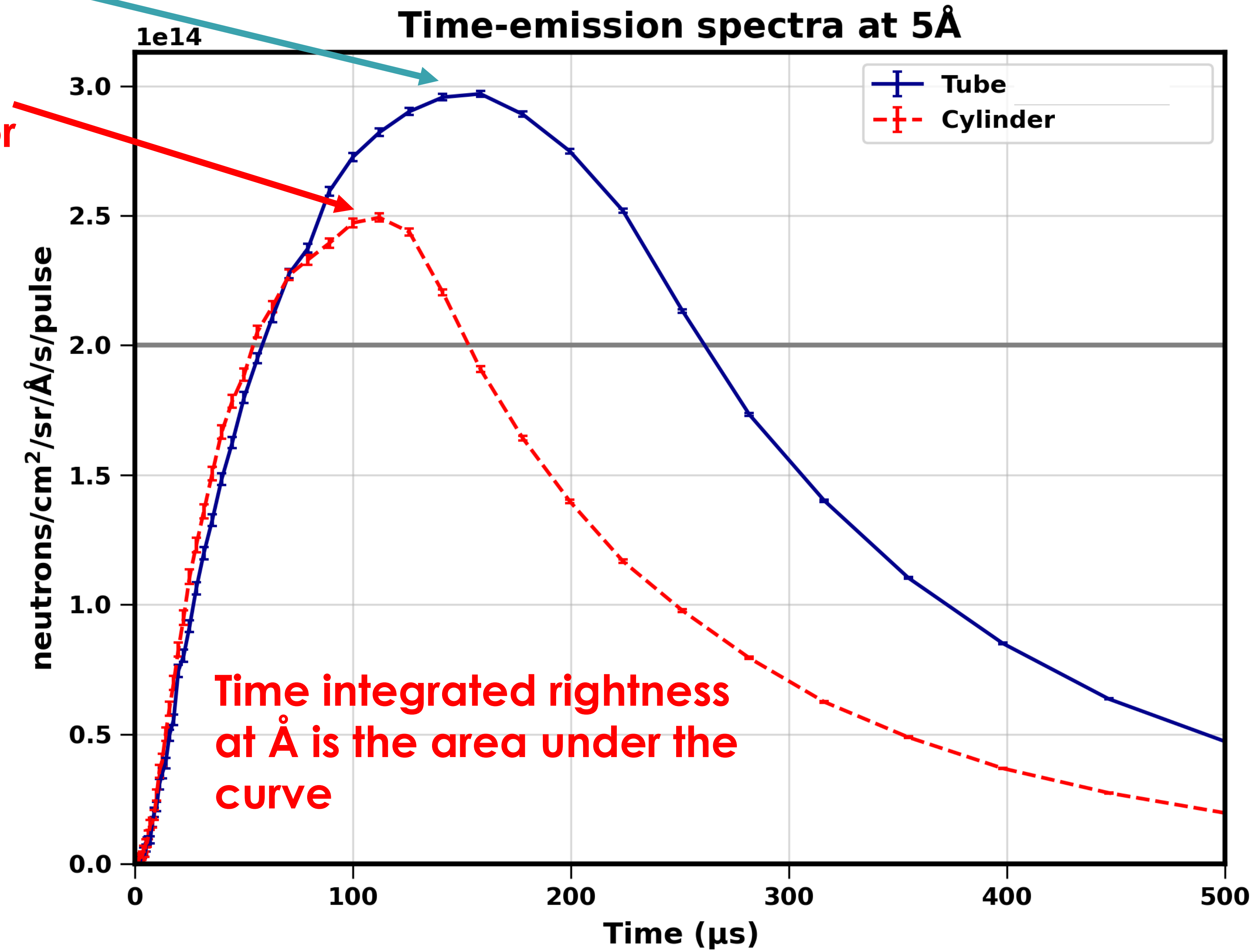
KPP	Thresholds	Objectives
Demonstrate independent control of the proton beam on the two target stations	Operate beam to FTS at 45 pulses/s, with no beam to STS Operate beam to STS at 15 Hz, with no beam to FTS Operate with beam to both target stations: 45 pulses/s at FTS and 15 Hz at STS	
Demonstrate proton beam on STS at 15 Hz	100 kW beam power	700 kW beam power
Measure STS neutron brightness	Peak brightness of 2×10^{13} n/cm^2/sr/Å/s at 5 Å	Peak brightness of 2×10^{14} n/cm^2/sr/Å/s at 5 Å
Beamlines transitioned to operations	Eight beamlines successfully passed the integrated functional testing per the TTOP acceptance criteria	$\geq$ Eight beamlines successfully passed the integrated functional testing per the TTOP acceptance criteria

TTOP = Transition to Operation Parameters.

Peak brightness

Peak Brightness, tube moderator

Peak Brightness, cylindrical moderator



Time integrated rightness at Å is the area under the curve

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The pathway to high brightness

To achieve high moderator brightness, we can:

- Create compact and intense neutron production zone in the target
  - Keep small proton beam footprint on the target
  - Use high density and high-Z target material
- Place moderators near the target (tight coupling)
- Reduce the size of the moderator viewed areas
- Use pure para hydrogen as moderator material
- Include H_2O premoderators in moderator design
- Surround moderators with good reflector material (beryllium enhances fast neutron reflection into moderators and neutron production by (n,2n) reactions; a standard at spallation neutron sources)

Moderator brightness could also be increased by:

- Increasing proton beam power (# protons/pulse; proton energy)
- Increase pulse repetition rate (increases time-averaged brightness)

Selected for STS: 1.3 GeV, 700 kW, 15 Hz

The pathway to high brightness… and limitations

High p-beam power (700 kW), short pulse operation, and small beam footprint delivers high amounts of energy in small volume of the target, resulting in high stresses

- Material properties limit the allowable stress and the acceptable energy density deposition
- Reducing stresses requires larger footprint which conflicts with the small footprint desired for neutronics performance

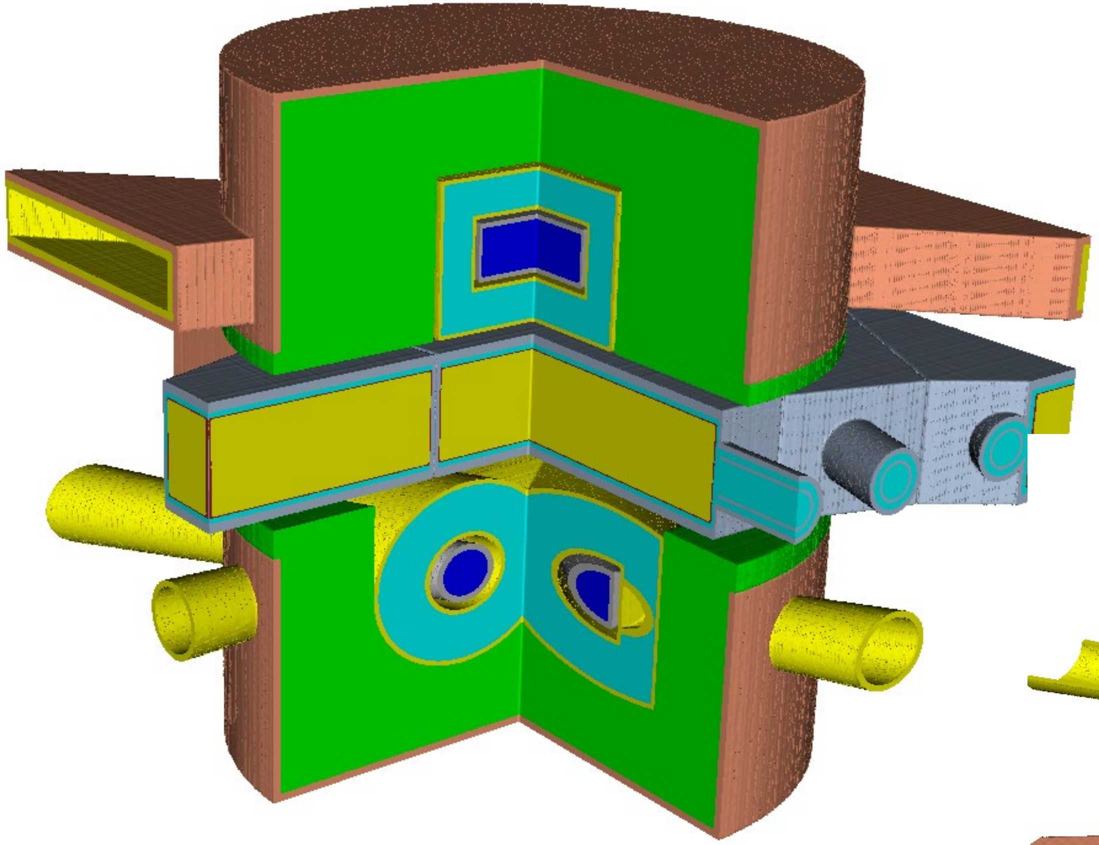
Reducing the size of the moderator viewed area increases the brightness but decreases the beam intensity – conflicting effects

- Previous analyses performed at SNS (Zhao et al, Rev Sci. Inst. 84, 2013) showed that neutron beam dimensions of ~ 3 cm provide good illumination of sample sizes up to ~1 cm
- For the STS moderator viewed areas of 3 cm × 3 cm, or diameter 3 cm were selected
  - Smaller viewed areas allow smaller moderator and tighter coupling to the neutron production area in the target
  - Significant increase in brightness can be achieved

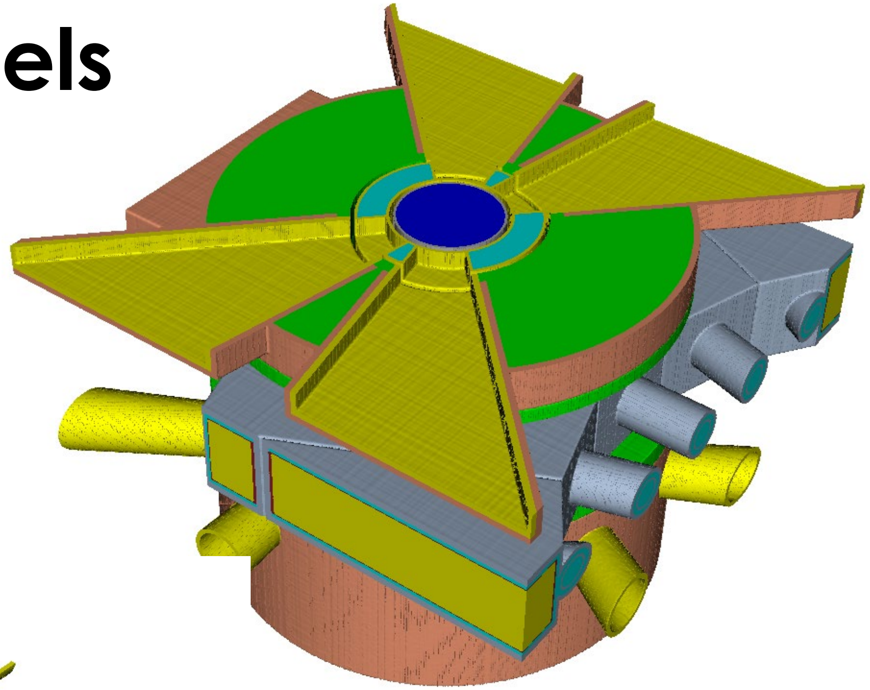
- **High neutron flux and high heating rates require use of liquid hydrogen for moderator (rules out hydrocarbon moderators even in liquid state)**
  - max. ~ 1.2 W/cc in H_2, ~8 W/cc in H_2O and Al
  - Required high brightness demands use of parahydrogen (and ortho-para converter)

Early optimization work

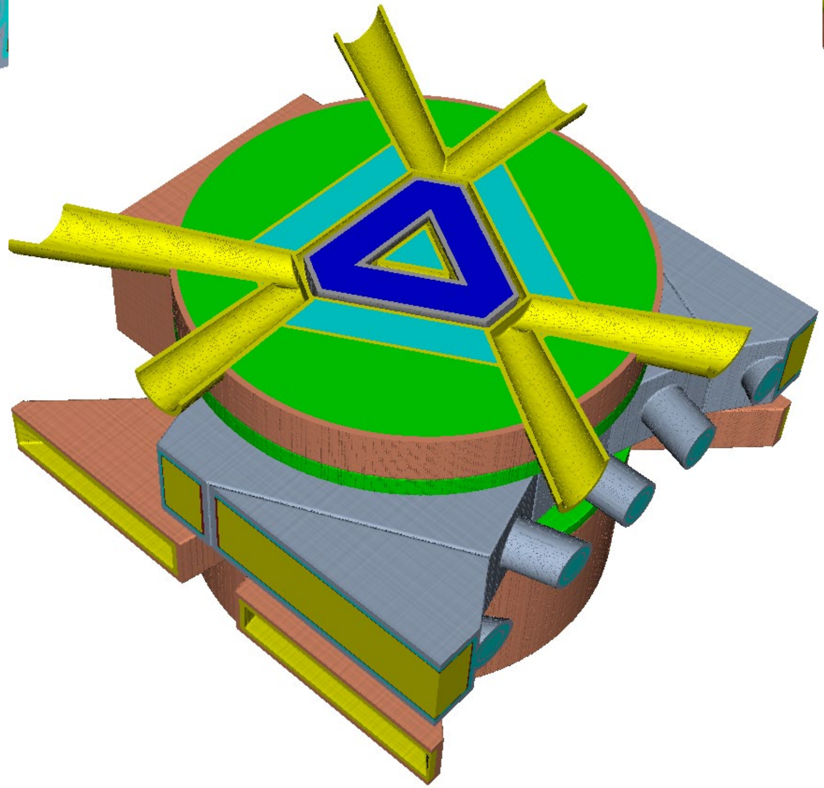
STS moderators: CSG “simple” models



Two moderators:
- Both coupled, para-H at 20ºK,
- H_2O pre-moderator



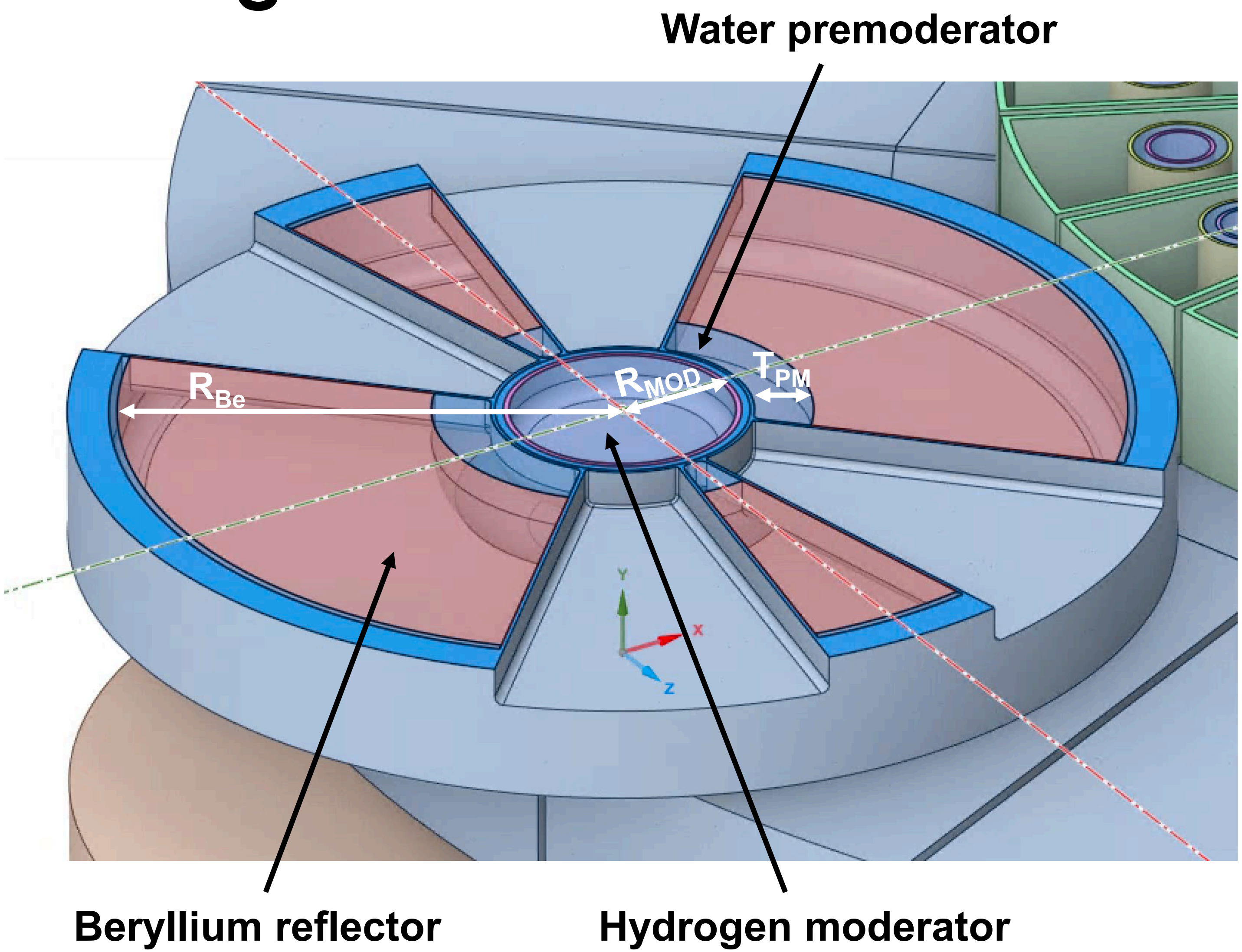
Top:
 cylindrical moderator



Bottom:
tube moderator

STS Cylindrical Moderator Design

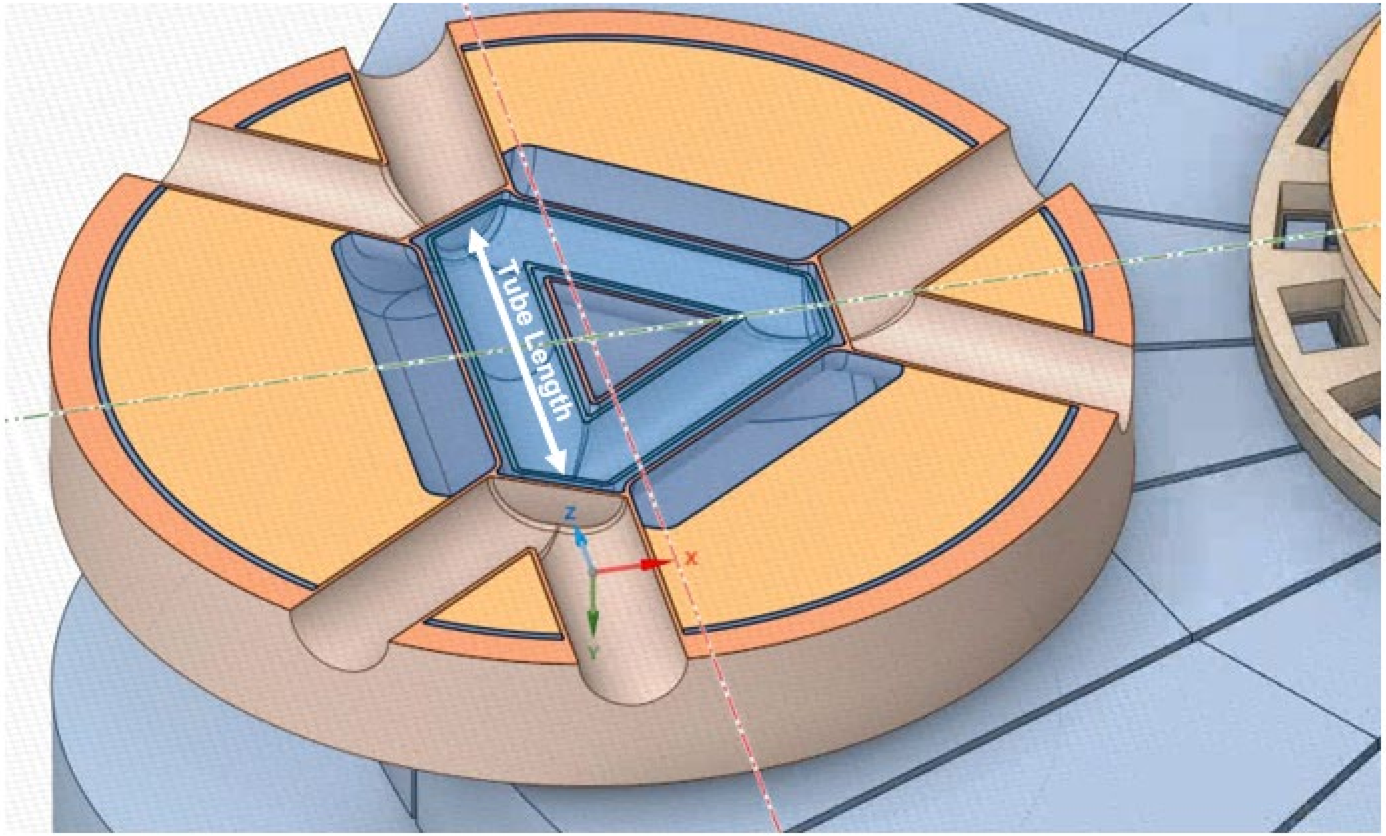
- **"2 dimensional"** moderator, small, vertical dimension minimized
- NOT a volume moderator (3D)
- 16 beam lines
- 3 x 3 cm^2 viewed area
- Key parameters:
  - Hydrogen radius
  - Premoderator radial thickness
  - Premoderator top/bottom thickness
  - Beryllium radius
  - Moderator position relative to target edge



Original plan: optimize for peak brightness

STS Tube Moderator Design

- **“1dimensional”** moderator
- 6 beam lines
- 3 cm diameter viewed areas
- Key parameters:
  - Tube length
  - Tube radius
  - Premoderator thickness
  - Beryllium radius
  - Moderator position

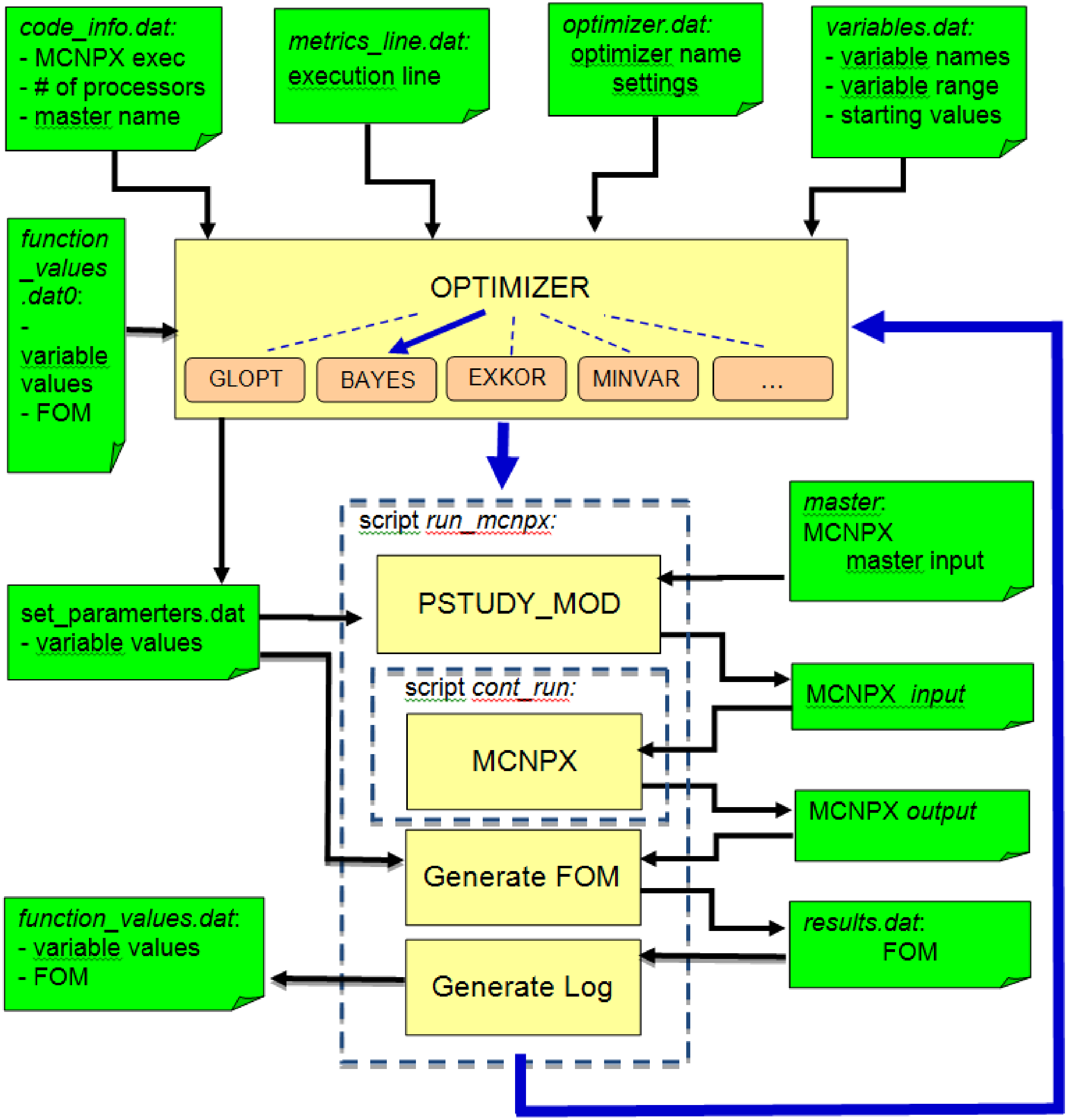


Original plan: optimize for time-integrated brightness

Original/Old moderator optimization procedure

Main components:

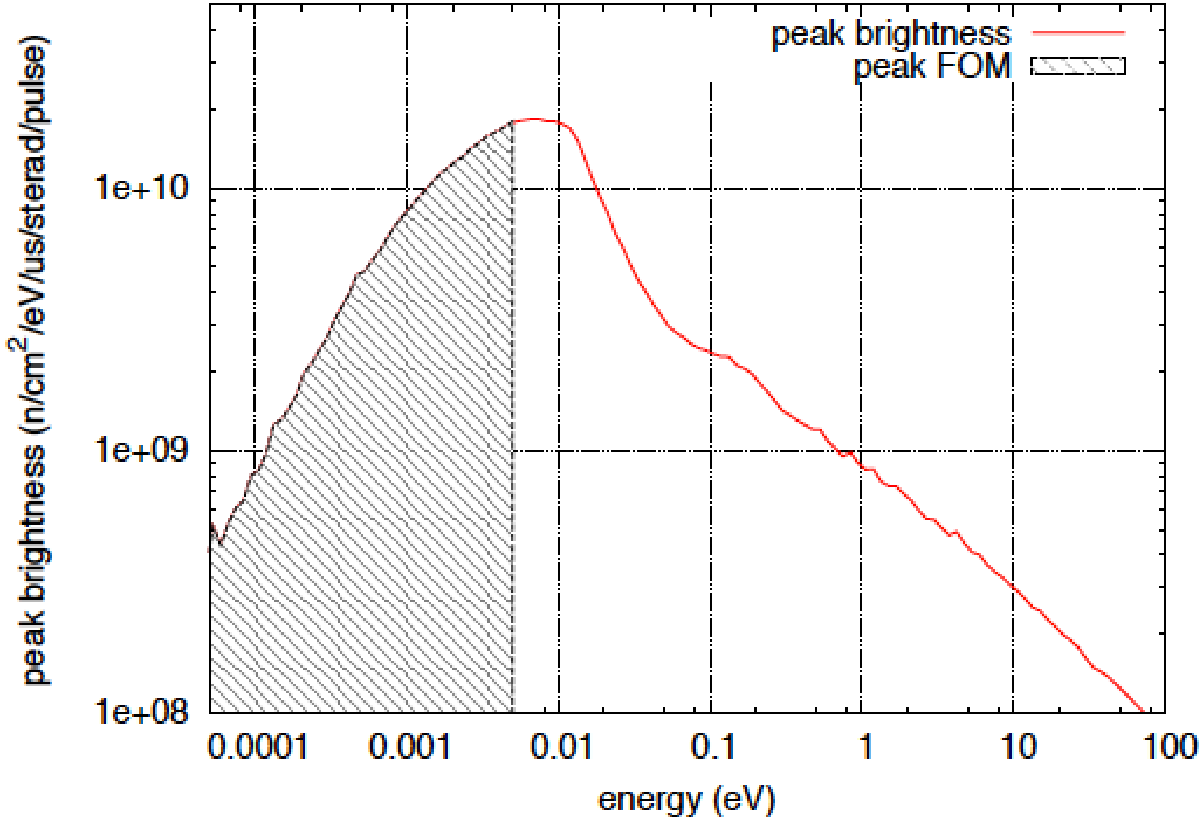
- **MCNPX**
- **Pstudy_mod**[1]
- **Run_mcnpx**
- **Optimizer**
- **Optimization routines** by Mockus[2]

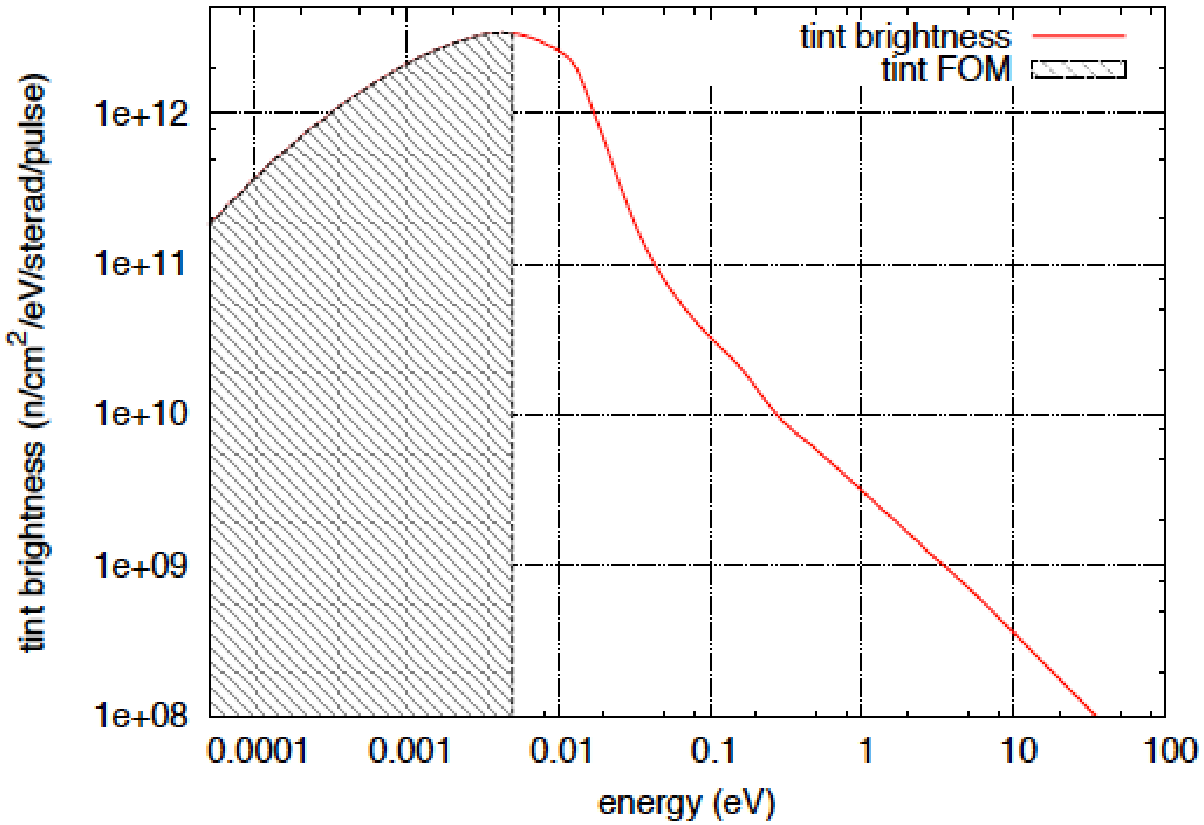


[1] F. B. Brown et al., Monte Carlo Parameter Studies and Uncertainty Analysis with MCNP5, PHYSOR-2004, *American Nuclear Society Reactor Physics Topical Meeting*, Chicago, IL, April 25-29 (2004)

[2] J. Mockus et al, *Bayesian Heuristic Approach to discrete and Global Optimization*, Kluwer Academic Publishers, Boston/London/Dordrecht (1996).

Moderator optimization: figures-of-merit





Peak-brightness integral up to E< 5 meV or 10 meV

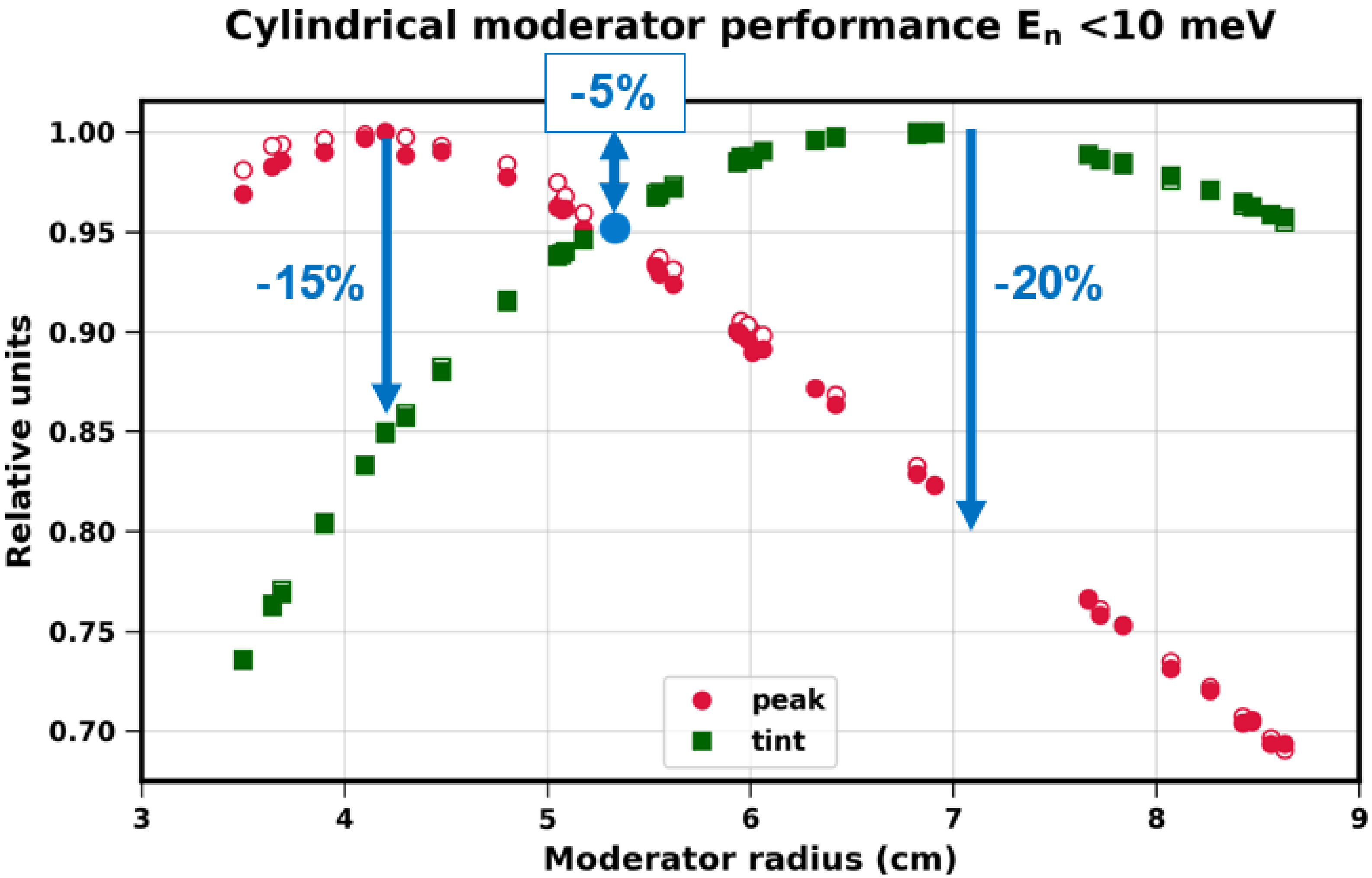
Time-integrated brightness integral up to E< 5 meV or 10 meV

Moderators peak versus time-averaged brightness

CYLINDRICAL MODERATOR					
		Pre-moderator Thickness			
Figure-of-Merit (Brightness)	H_2 Radius (cm)	Radial (cm)	Bottom (cm)	Top (cm)	Offset from W Edge (cm)
Time-averaged	8.500	2.000	2.992	2.000	8.7
Peak	4.341	2.000	2.607	2.000	8.7
Intermediate (Peak-Tint)	6.100	2.000	2.700	2.000	8.7

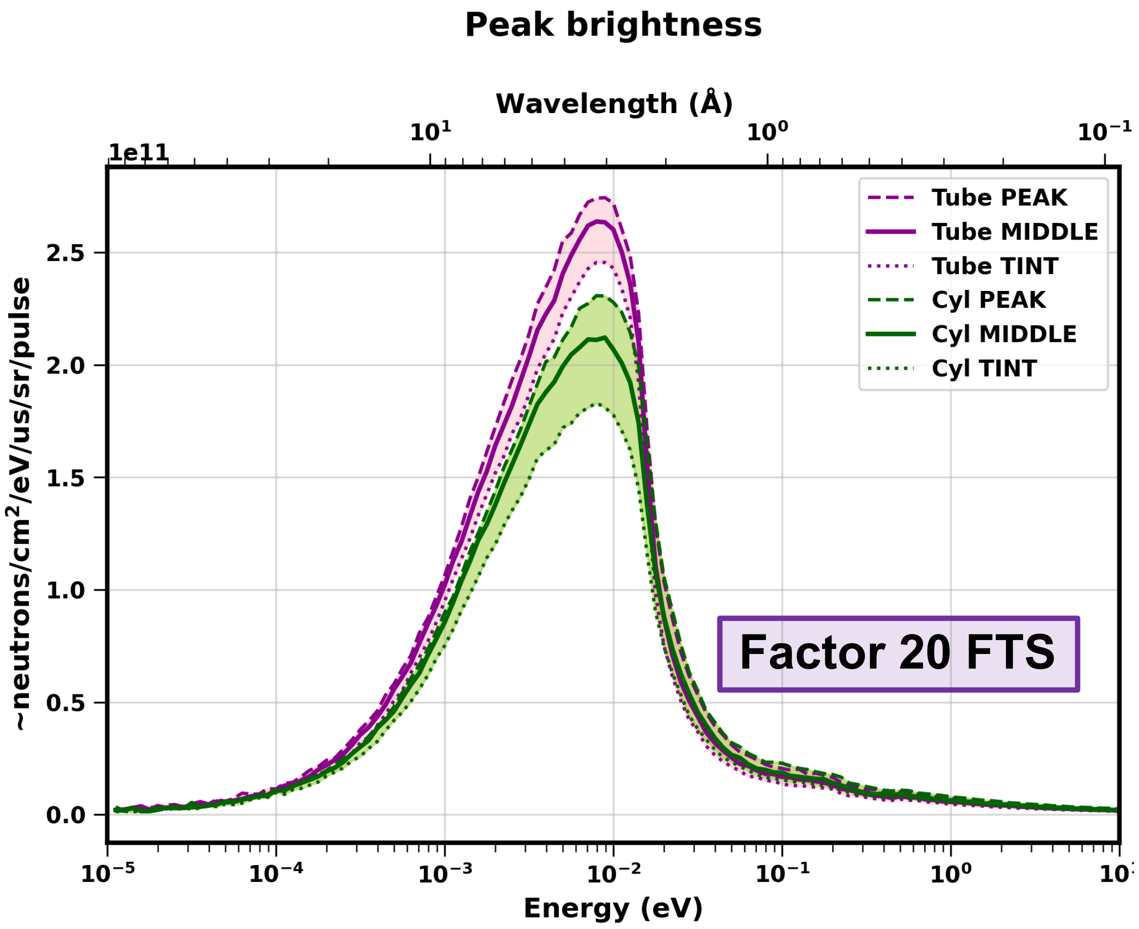
TUBE MODERATOR			
Figure-of-Merit (Brightness)	Tube length (cm)	Pre-mod. Thickness (cm)	Offset from W Edge (cm)
Time-averaged	19.820	2.727	8.7
Peak	10.330	2.727	8.7
Intermediate (Peak-Tint)	15.000	2.727	8.7

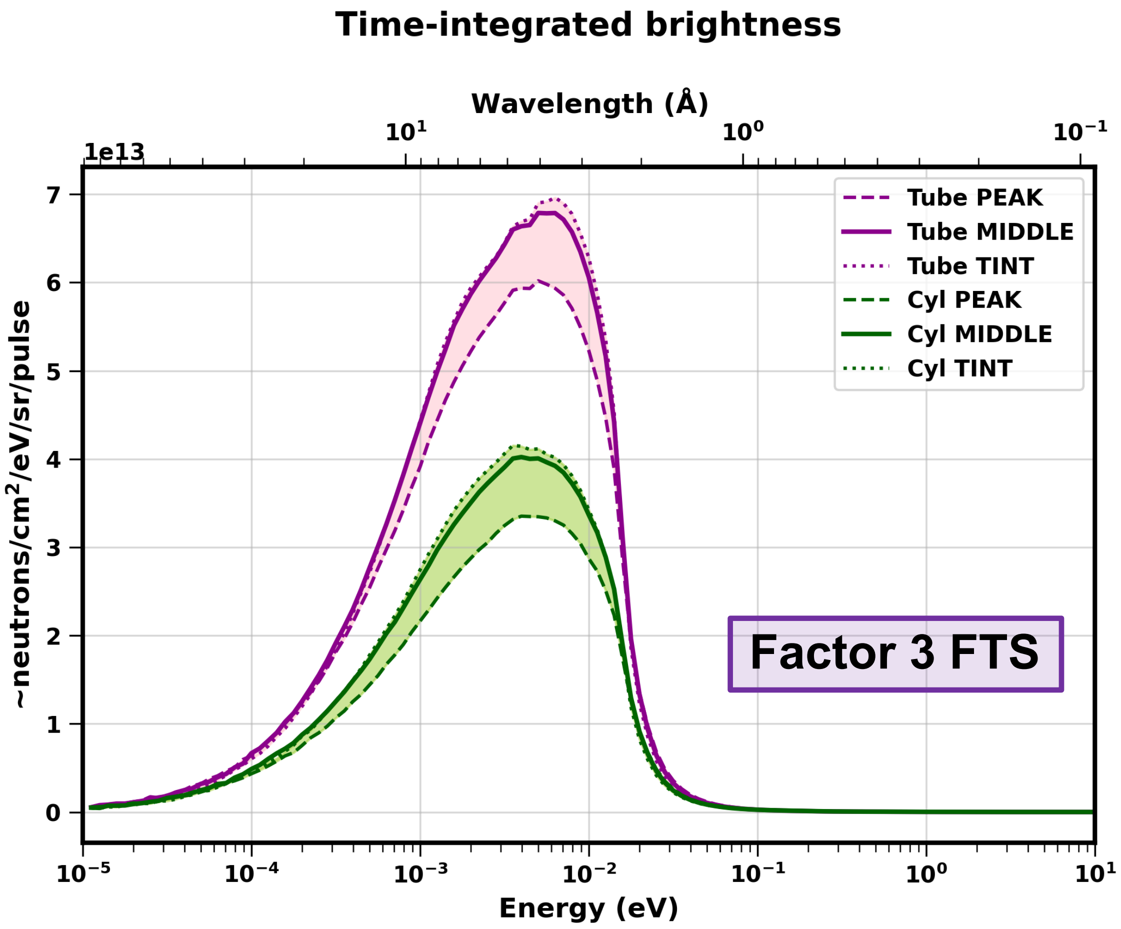
Moderator Optimization



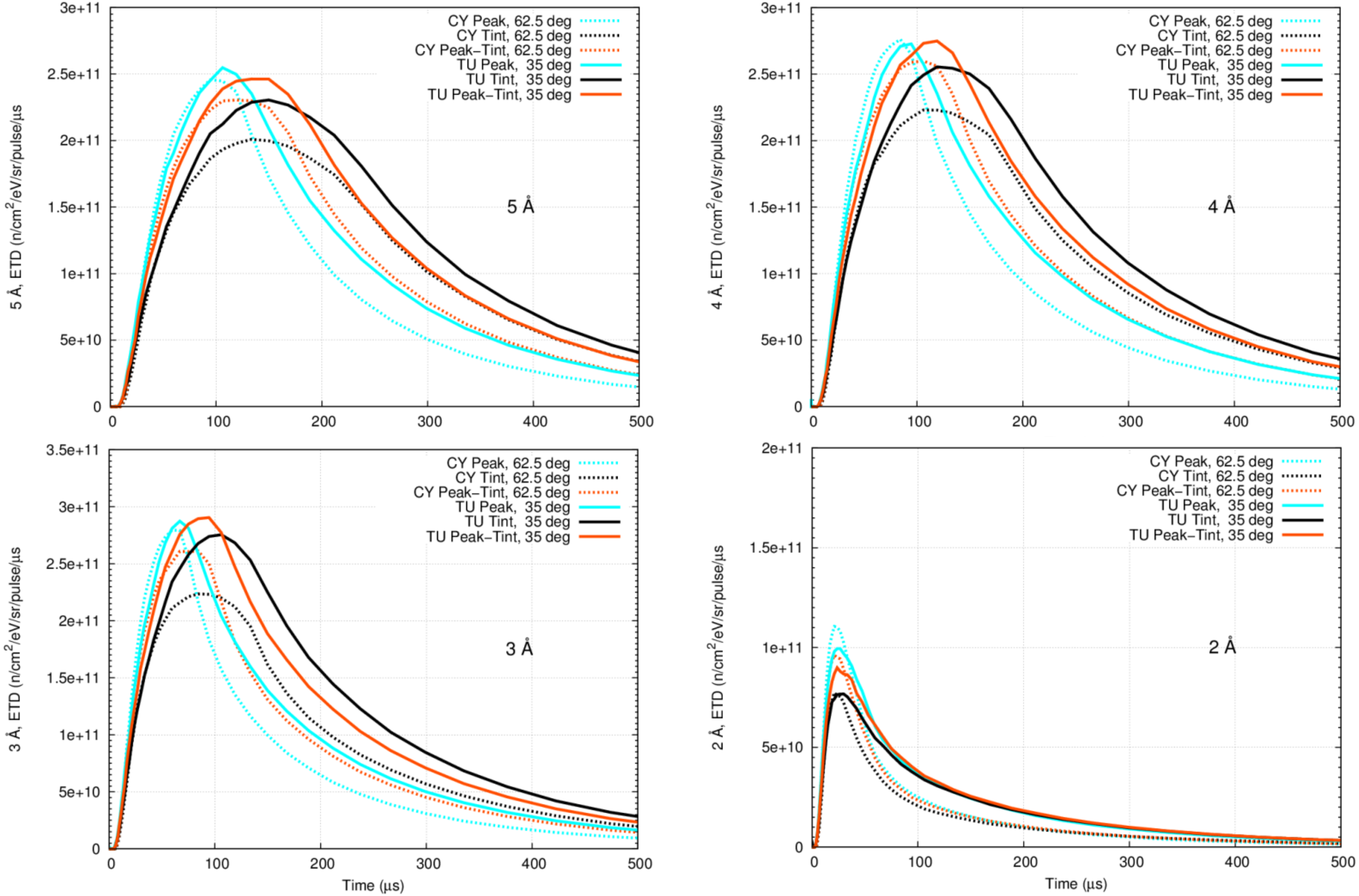
- Middle configuration between the peak and the time-integrated brightness is preferred
- 5% loss in peak and time-integrated brightness in comparison with 15% and 20% losses when optimized to resp. maxima

STS Moderator Performance



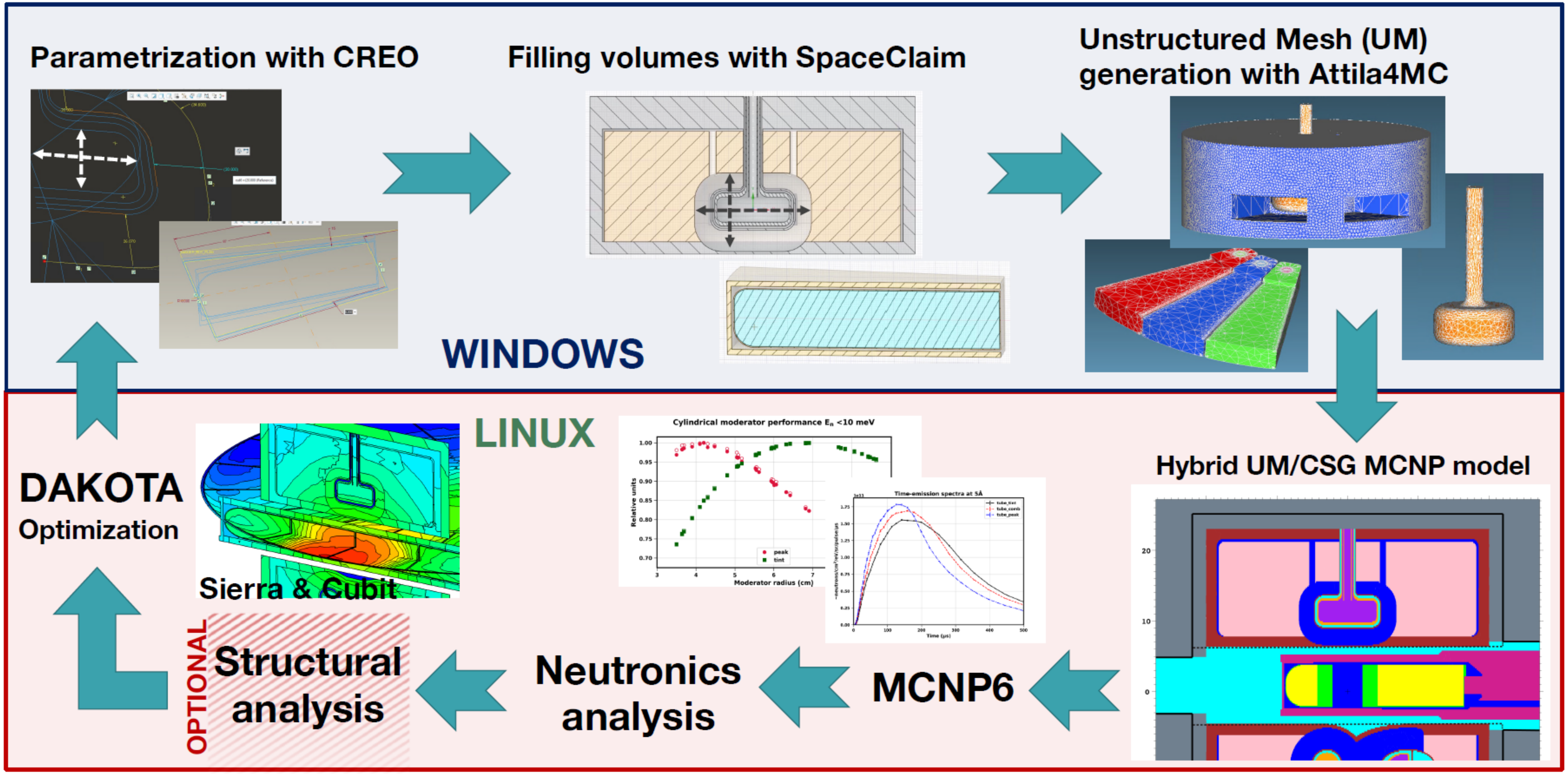


Pulse shapes for different configurations of cylindrical and tube moderators



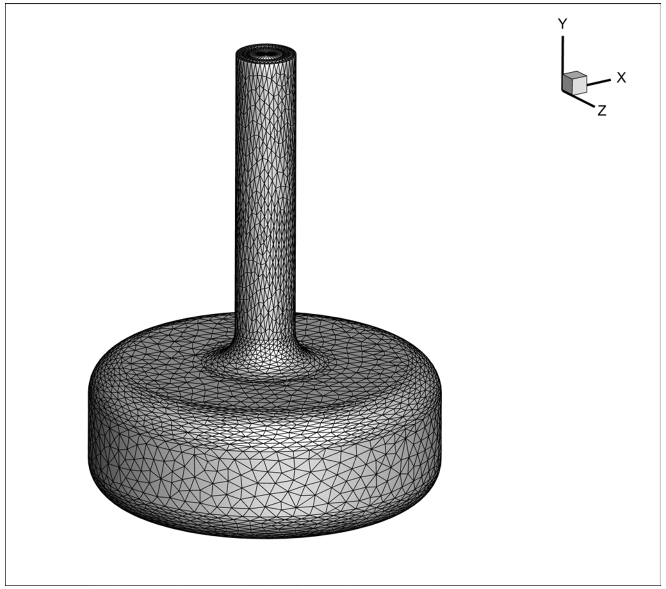
Optimization with high fidelity models

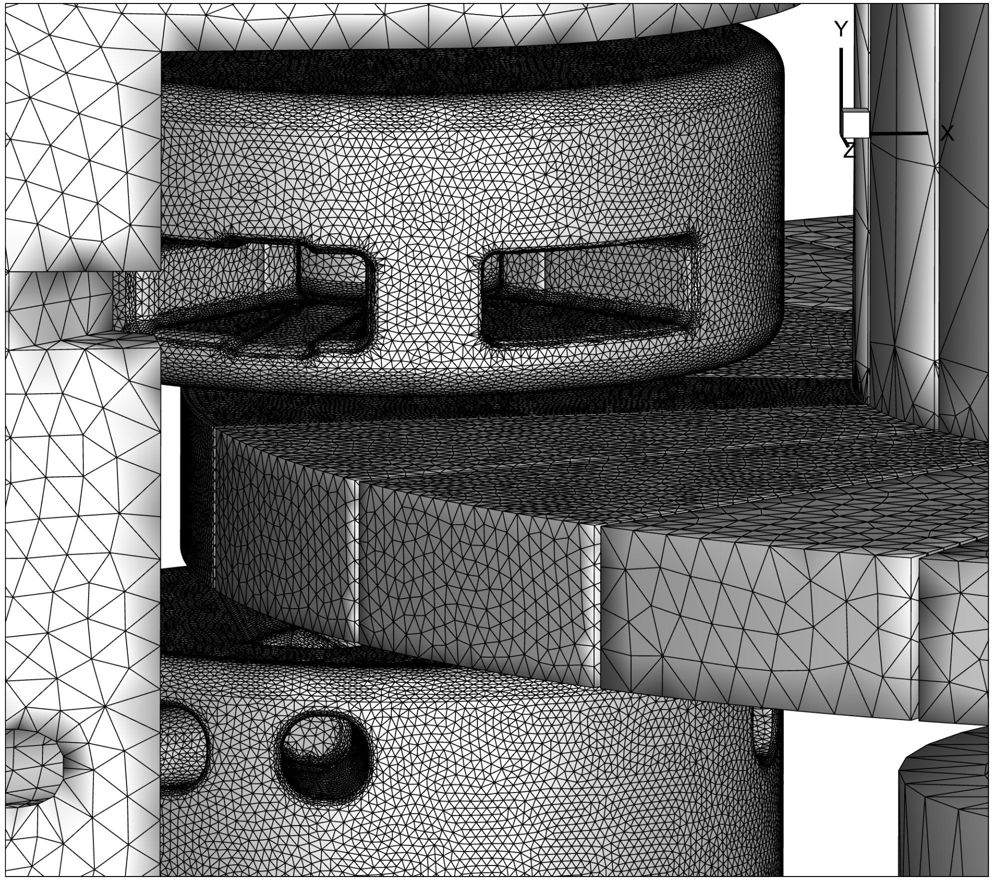
Simultaneous moderator and target (MT) optimization

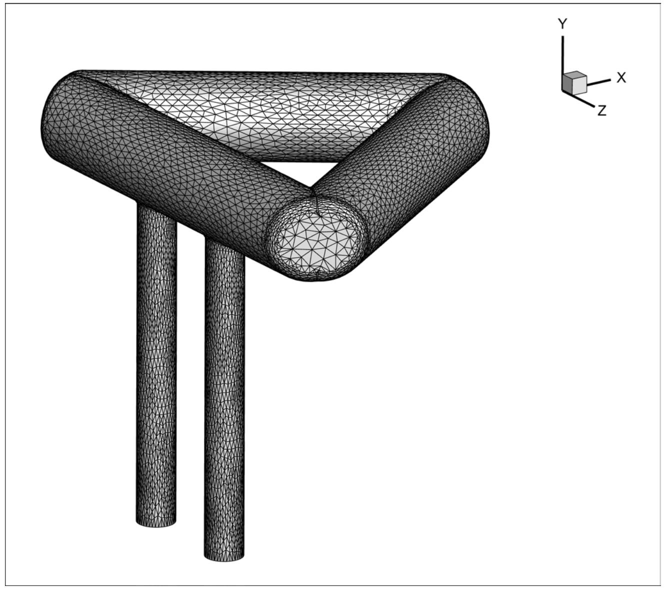


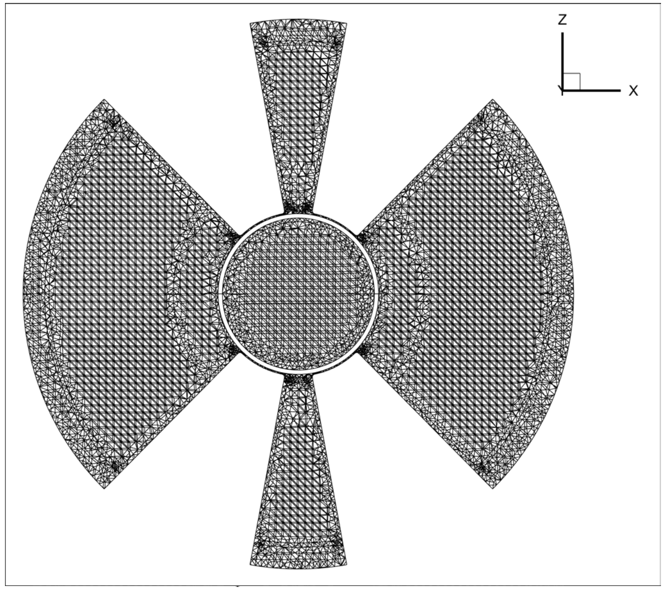
L. Zavorka et al., An unstructured mesh based neutronics optimization workflow, NIM A 1052 (2023) 168252.

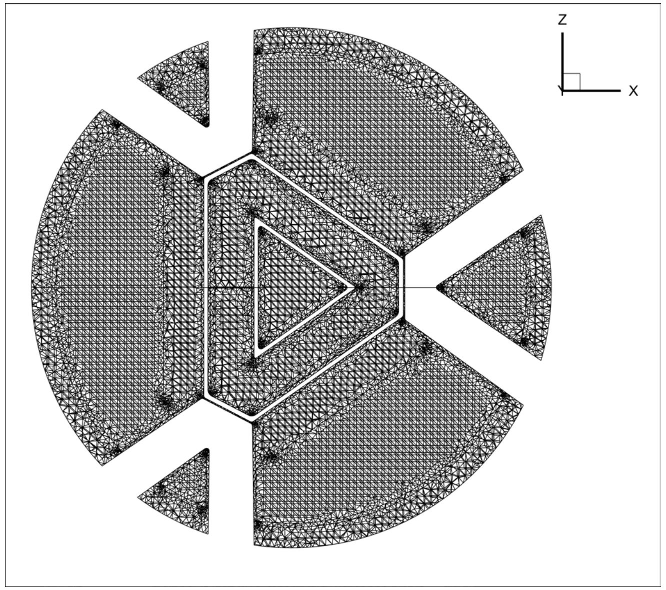
Moderator models with unstructured mesh



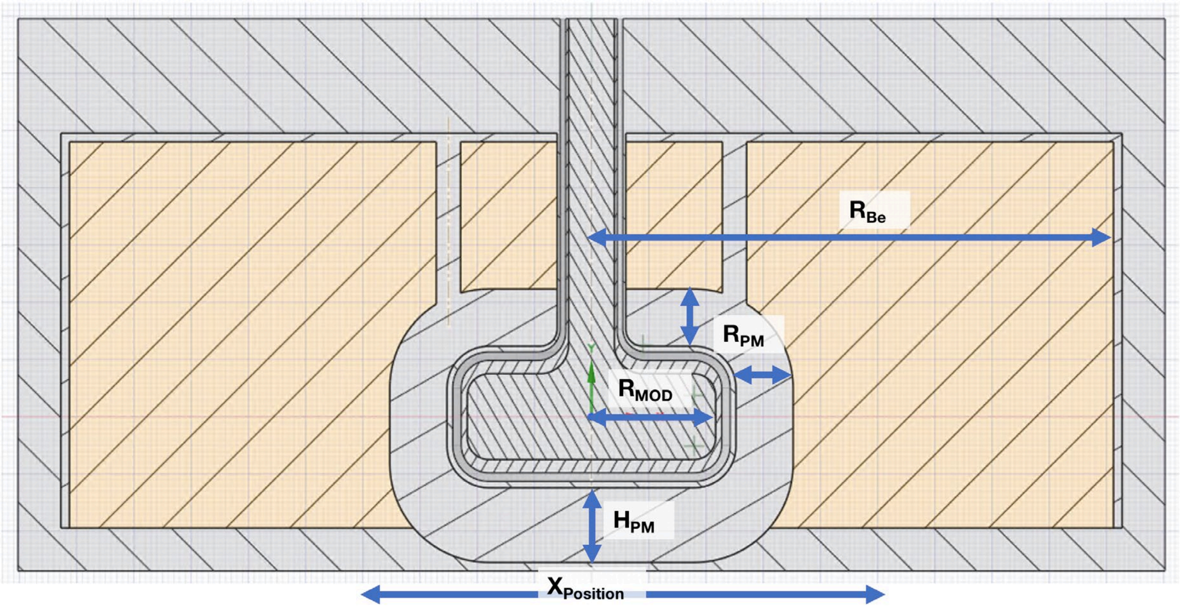








Optimization with Dakota, UM models, Pareto



Efficient global algorithm for 6 sets of weights to balance the two objectives:

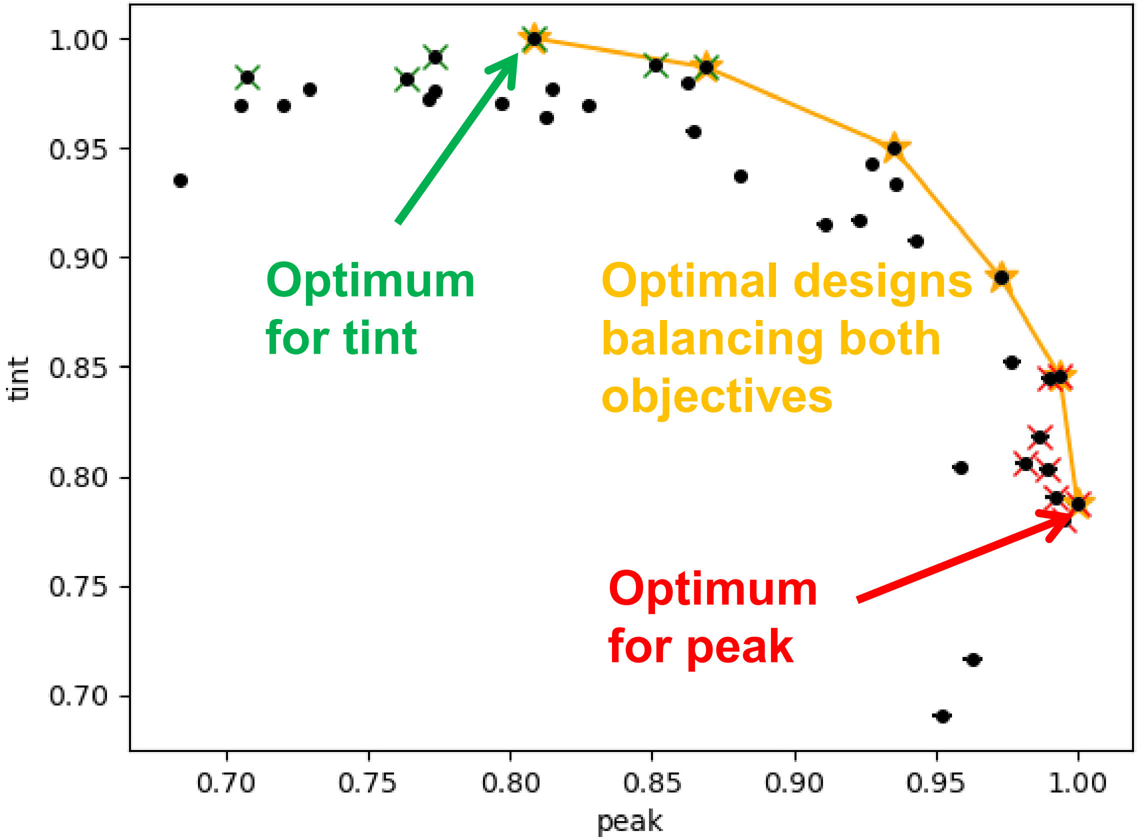
Objective = $\boldsymbol{w_1} \frac{peak}{1.519e{-}12} + \boldsymbol{w_2} \frac{tint}{2.7985e{-}8}$

Runs from previous sets are re-used for the next
→ total number of MCNP runs = 38 !!

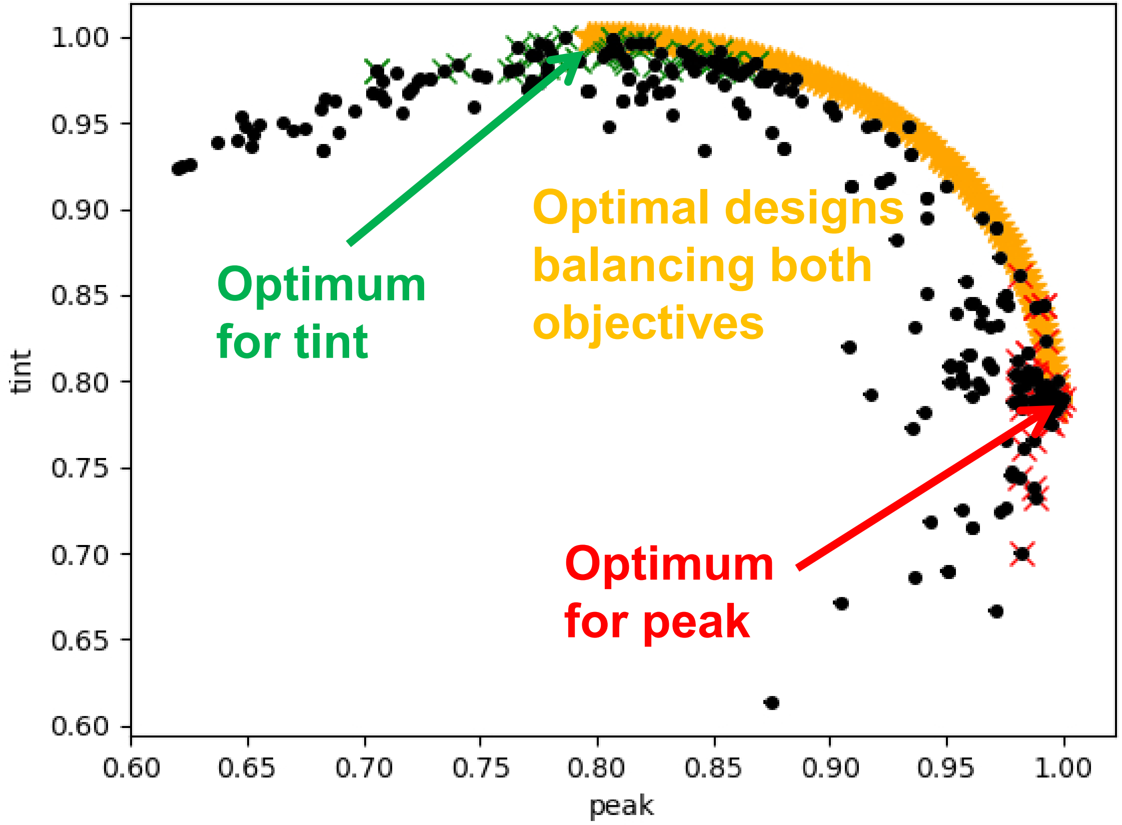
Set	Nr runs (new)	w_1	w_2 $(1 - w_1)$	R_{mod} [mm]	R_{pm} [mm]	H_{pm} [mm]	R_{Be} [mm]	X_{pos} [mm]	Peak [e-12]	Tint [e-8]
1	25 (24)	0	1	61.4	31.8	29.2	194	3.2	1.254 (81.5 %)	2.893 (100 %)
2	25 (2)	0.25	0.75	55.0	29.3	29.0	188	1.8	1.338 (86.9 %)	2.855 (98.7 %)
3	25 (2)	0.5	0.5	47.5	29.3	28.7	178	-0.2	1.439 (93.5 %)	2.750 (95.1 %)
4	25 (2)	0.7	0.3	40.9	29.5	29.1	181	1.4	1.497 (97.3 %)	2.577 (89.1 %)
5	27 (4)	0.85	0.15	38.8	26.0	29.5	159	2.7	1.530 (99.3 %)	2.446 (84.5 %)
6	27 (4)	1	0	35.7	24.6	29.0	150	4.0	1.539 (100 %)	2.279 (78.8 %)

Optimization with Dakota, UM models, Pareto

Pareto-front from Dakota run (38 MCNP runs)



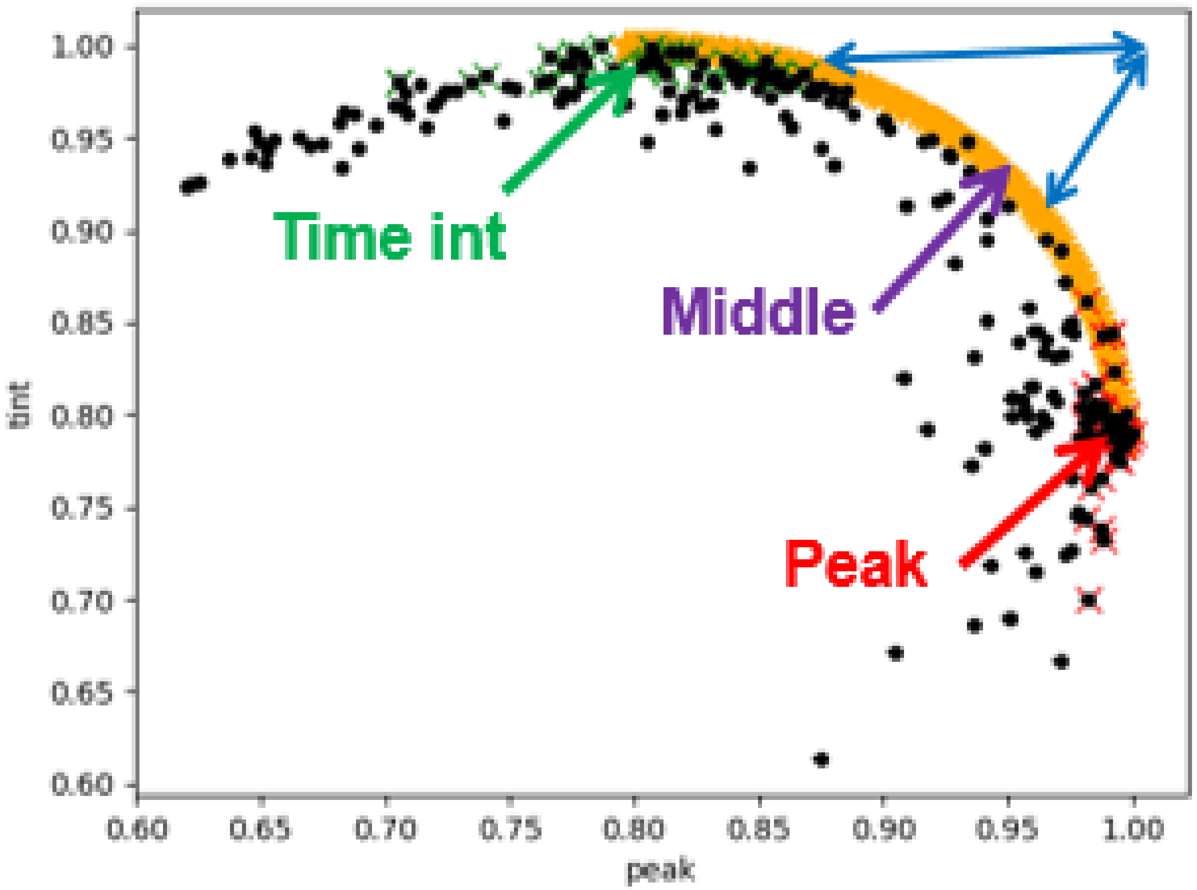
Pareto-front from surrogate model fitted to all 196 MCNP runs to smooth out noise



Black = 38 runs from pareto simulation
Orange = pareto front
Green/red = within 2% of maximal **tint**/**peak**

Black = all available runs
Orange = pareto front with surrogate model
Green/red = within 2% of maximal **tint**/**peak**

Cylindrical moderator parameters for three optimal designs



Point (1,1) = Ideal Peak & Tint

	R_{mod} [mm]	R_{pm} [mm]	H_{pm} [mm]	R_{Be} [mm]	X_{pos} [mm]	Peak Brightness [e-12]	Time-integrated brightness [e-8]
Time int	62	33	30	187	2	1.218 (80%)	2.899 (100%)
Middle	47	29	29	173	1	1.435 (94%)	2.734 (94%)
Peak	35	26	28	165	1	1.524 (100%)	2.276 (79%)

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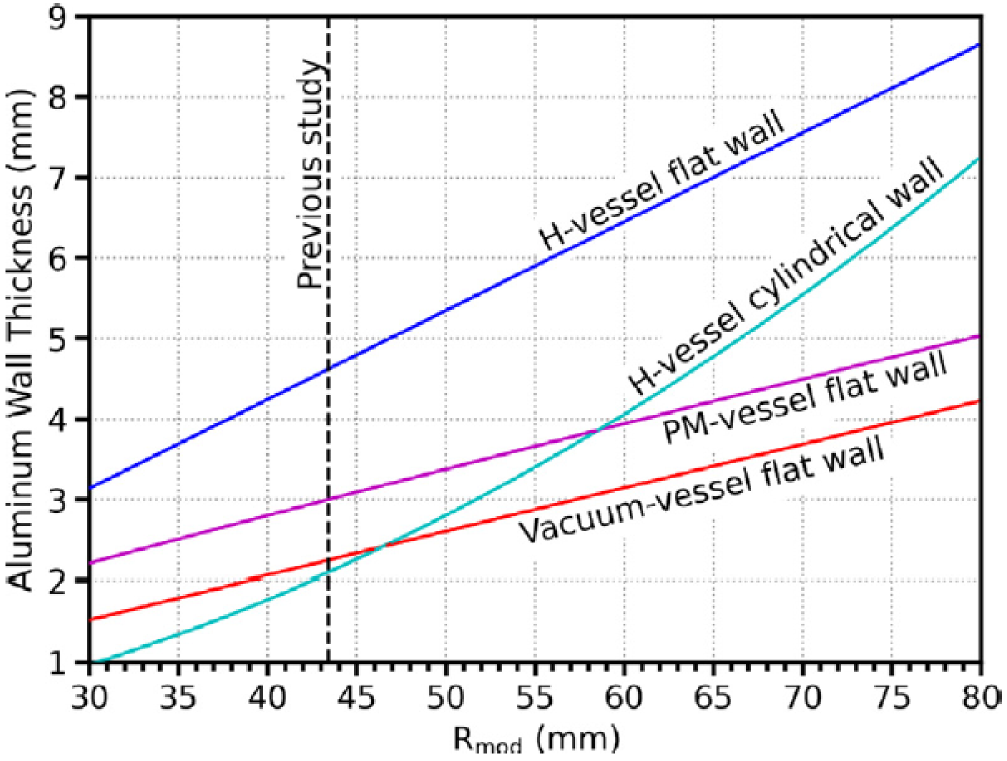
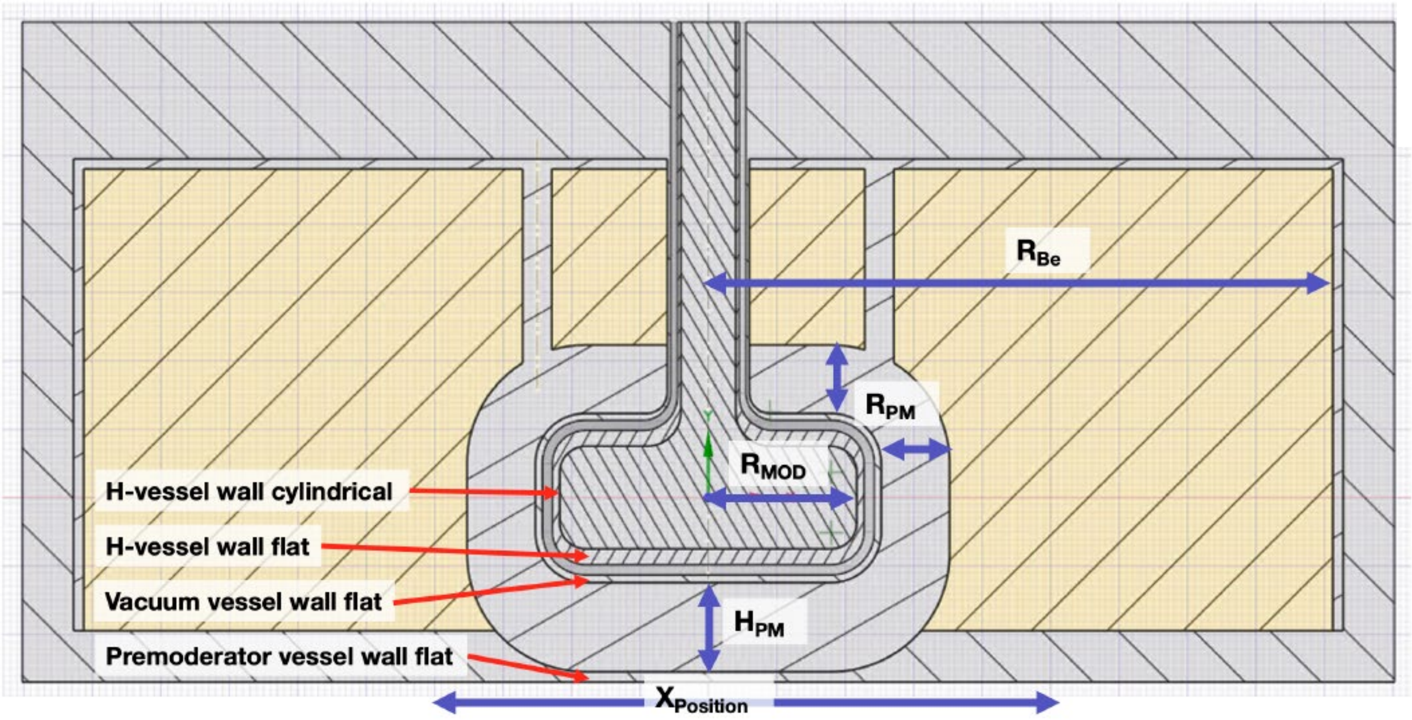
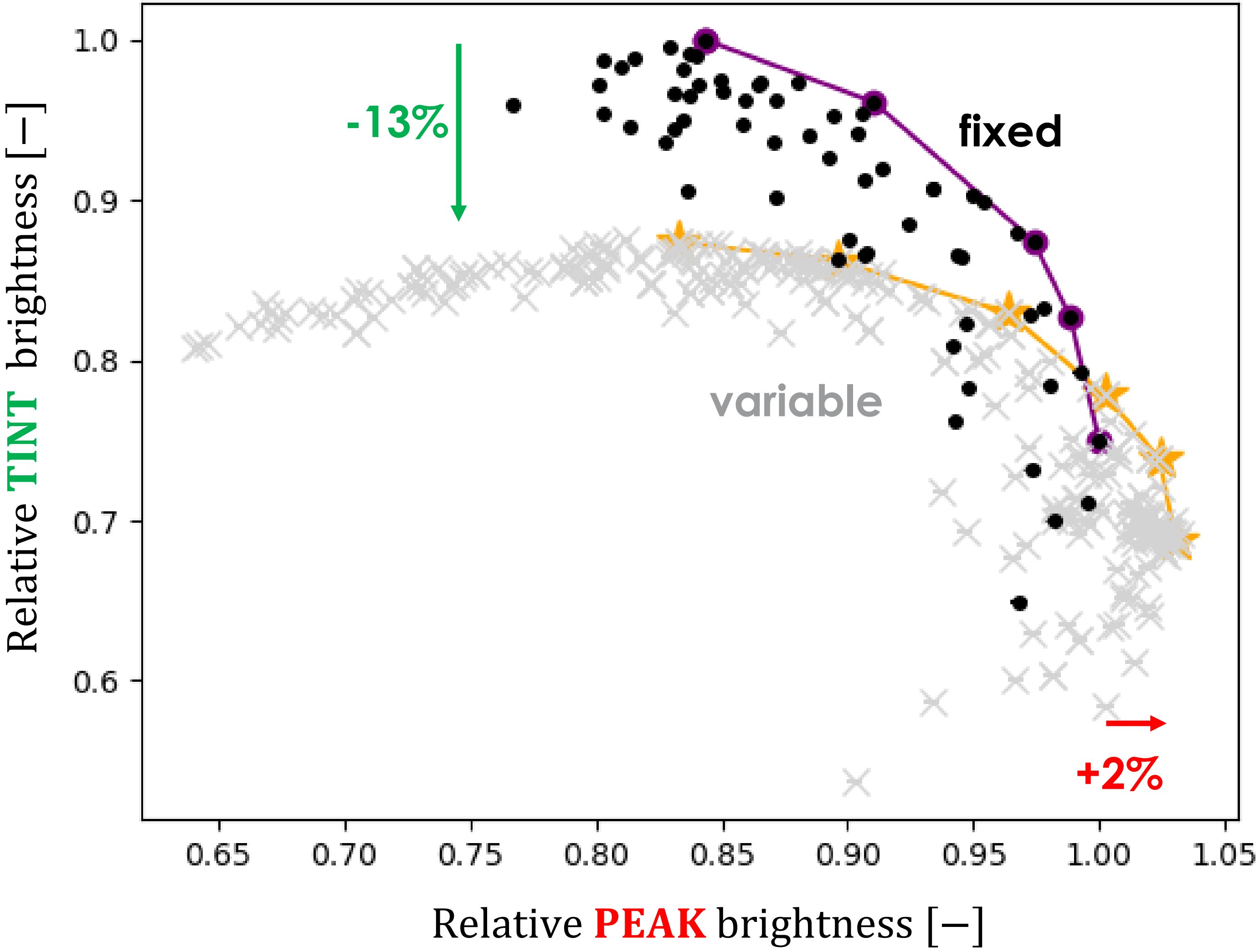
Variable moderator wall thicknesses





Variable Al-vessel thickness has significant effect



Black = fixed
Purple = pareto-front fixed

Grey = variable
Orange = pareto-front variable

From fixed to variable thickness:

- 13% tint
+ 2% peak

Fixed & variable Al-vessel thickness: summary

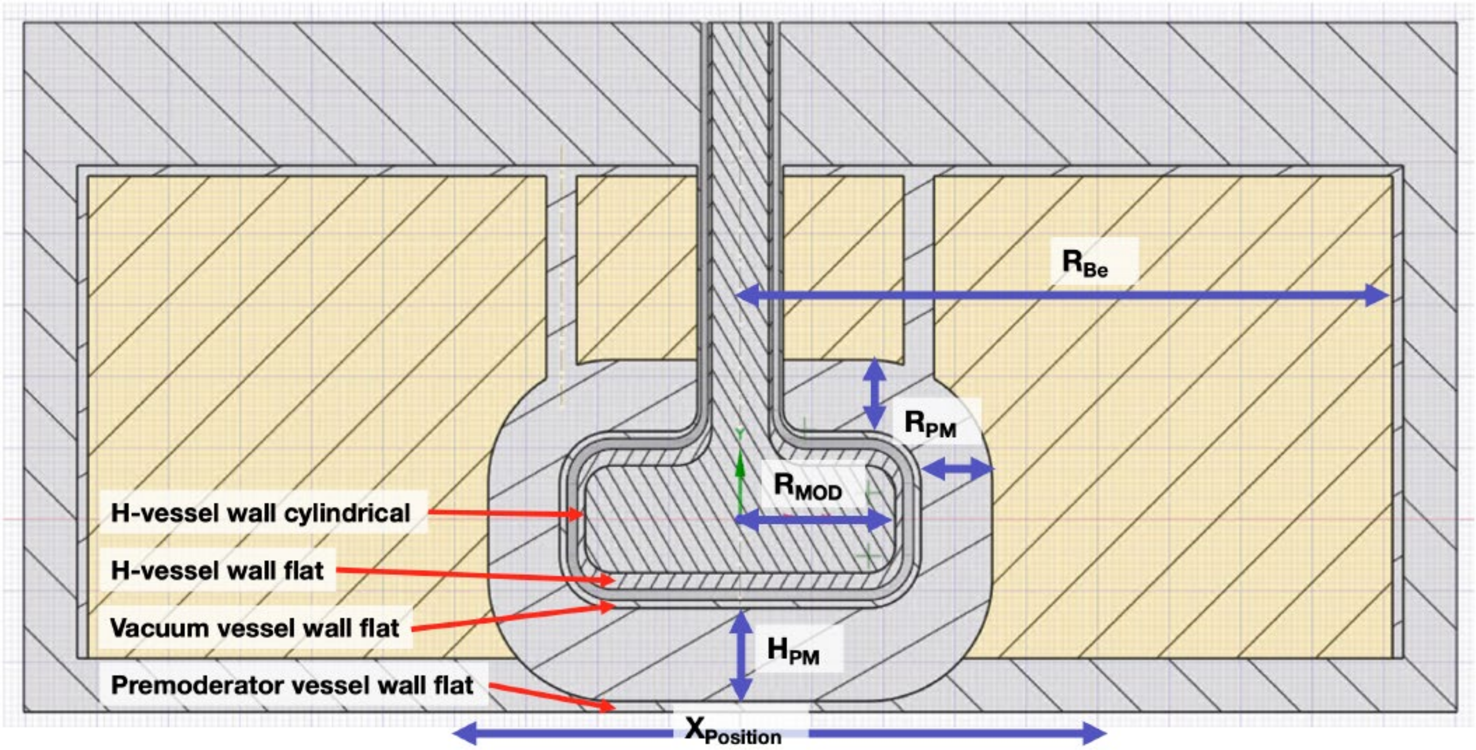
Peak optimized	R_{mod} [mm]	R_{pm} [mm]	H_{pm} [mm]	R_{Be} [mm]	X_{pos} [mm]	Peak Brightness FOM [e-12]	Time-integrated brightness FOM [e-8]
Peak optimized design							
Fixed	40	27	29	200	4	1.494	2.484
Variable	35	26	28	165	1	1.524 (+2%)	2.276 (-9%)
Tint optimized design							
Fixed	80	26	28	200	1	1.260	3.312
Variable	62	33	30	187	2	1.218 (-4%)	2.899 (-13%)

Cylindrical moderator: sensitivity to parameters

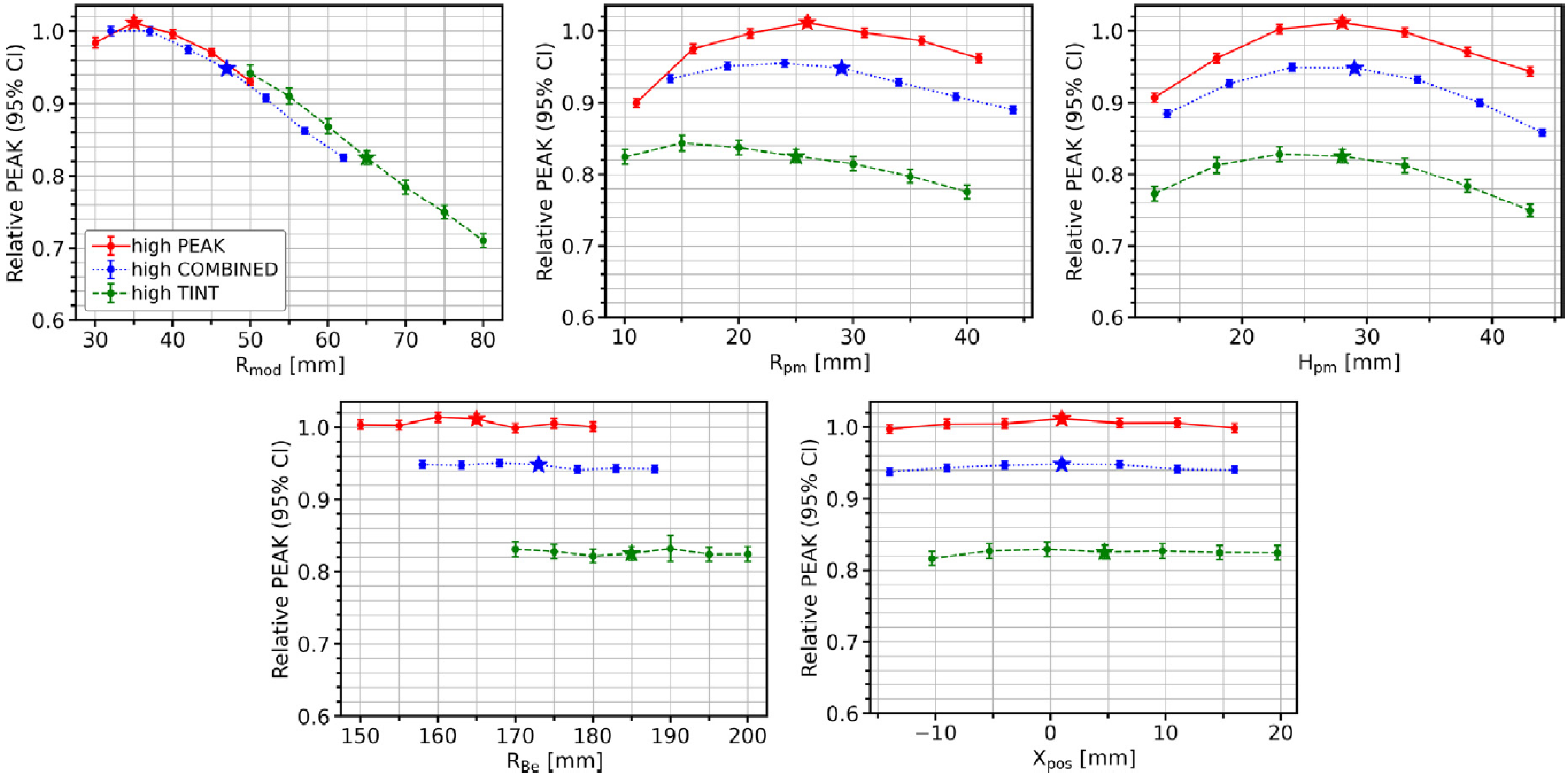
Parameters:

- Radius of the hydrogen vessel
  R_{mod} **(range: 32 to 80 mm)**
- Thickness of the water premoderator radially and above
  R_{pm} **(range: 18 to 35 mm)**
- Thickness of the water premoderator below the moderator
  H_{pm} **(range: 25 to 40 mm)**
- Radius of the beryllium vessel
  R_{Be} **(range: 150 to 200 mm)**
- Position of the moderator axis in the direction of the proton beam
  X_{pos} **(range: −20 to 20 mm)**

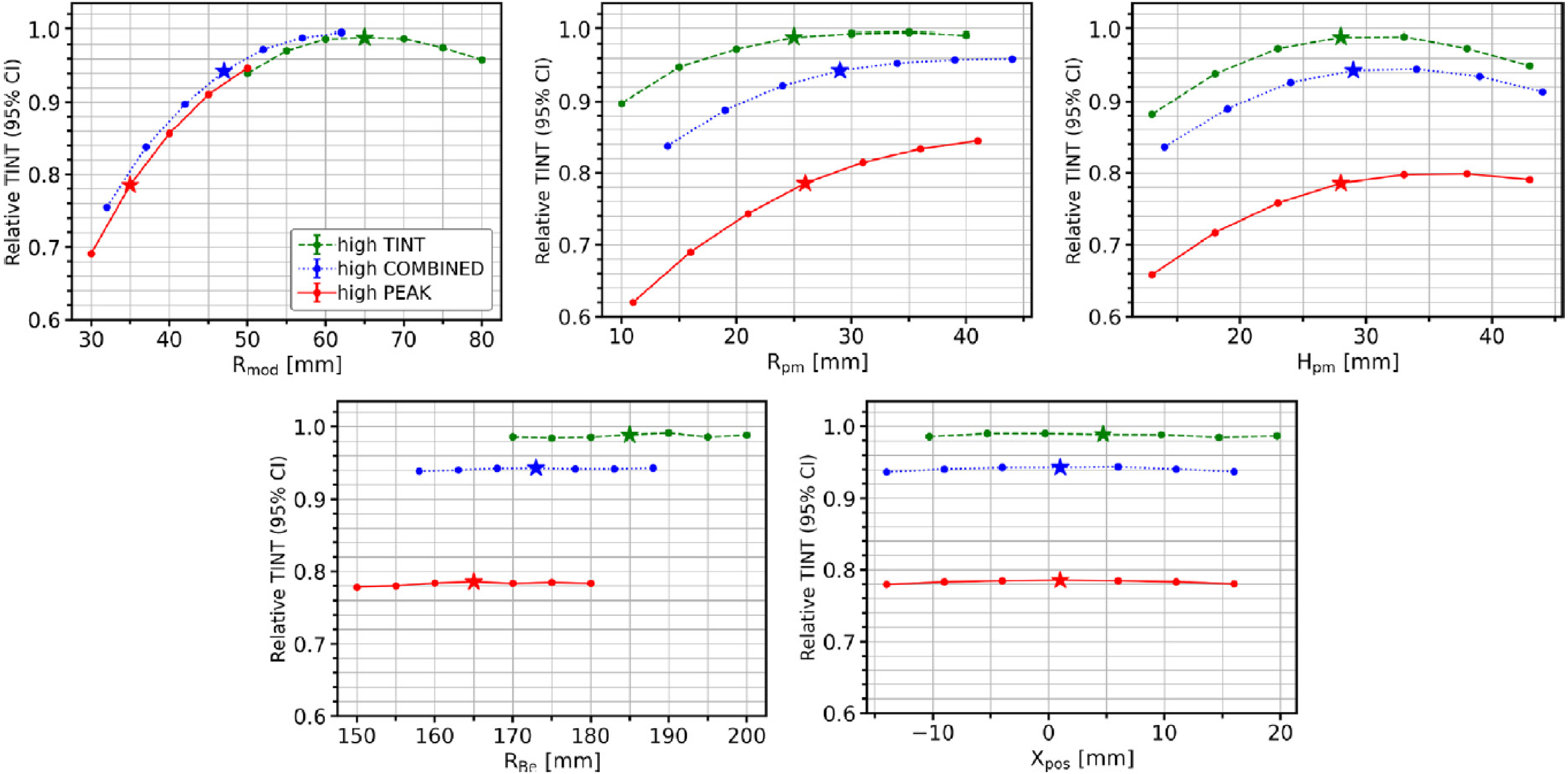
- **2-dimensional moderator configuration**
- 12 beam lines
- 30 mm × 30 mm viewed areas



Cylindrical moderator peak brightness sensitivities



Cylindrical moderator time-integrated brightness sensitivities

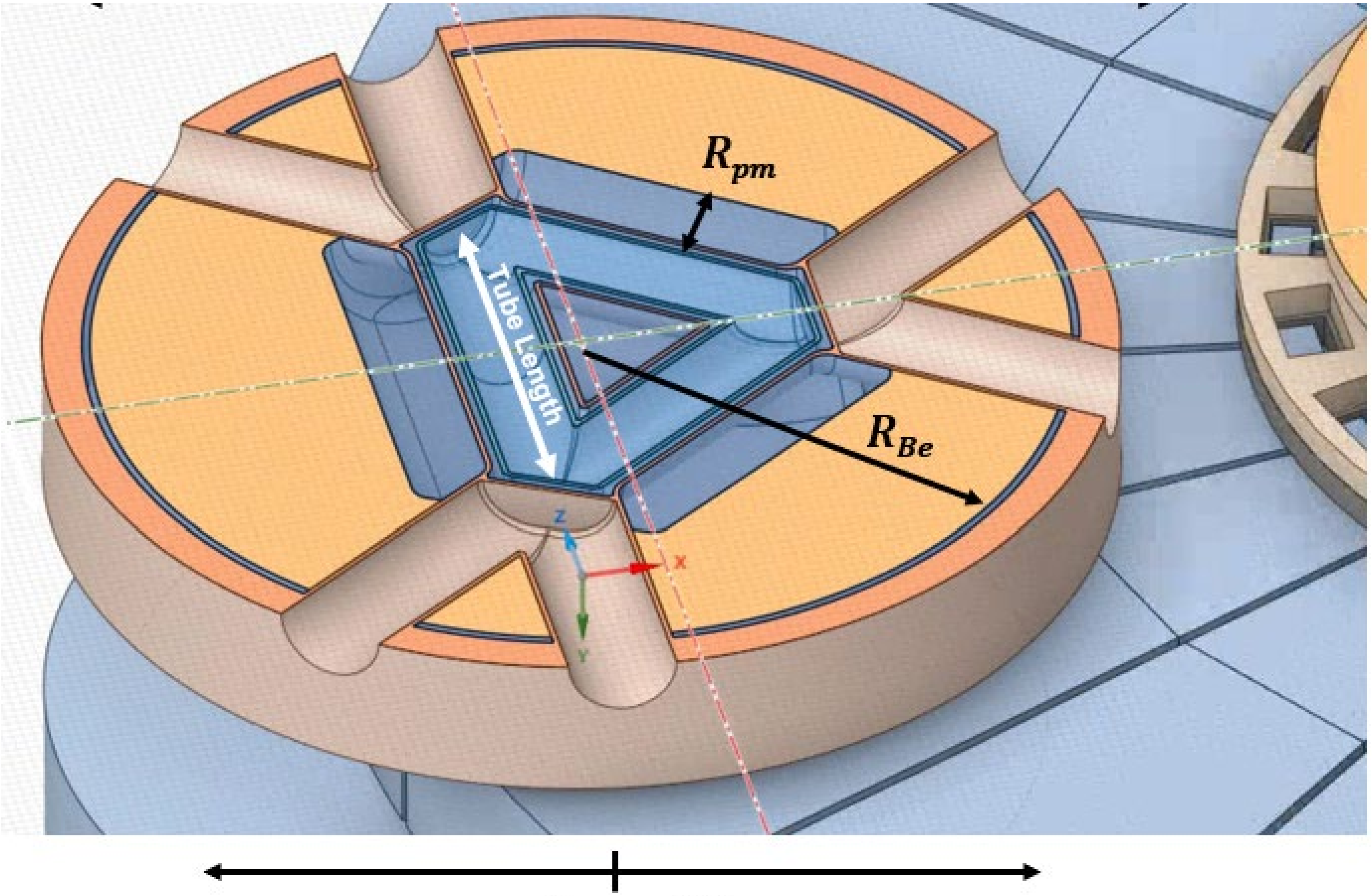


Tube Moderator: sensitivity to parameters

- **1dimensional moderator configuration**
- 6 beam lines
- 30 mm diameter viewed areas

Parameters:

- the hydrogen tube length T_{len} **(range: 120 to 230 mm)**,
- the annular thickness of the water premoderator R_{pm} **(range: 25 to 29.2 mm)**,
- the radius of the beryllium vessel R_{Be} **(range: 180 to 220 mm)**,
- the position of the moderator in the direction of the proton beam X_{pos} **(range: -20 to 20 mm)**.



X_{pos} = 0.0
at 87 mm from the edge of the target

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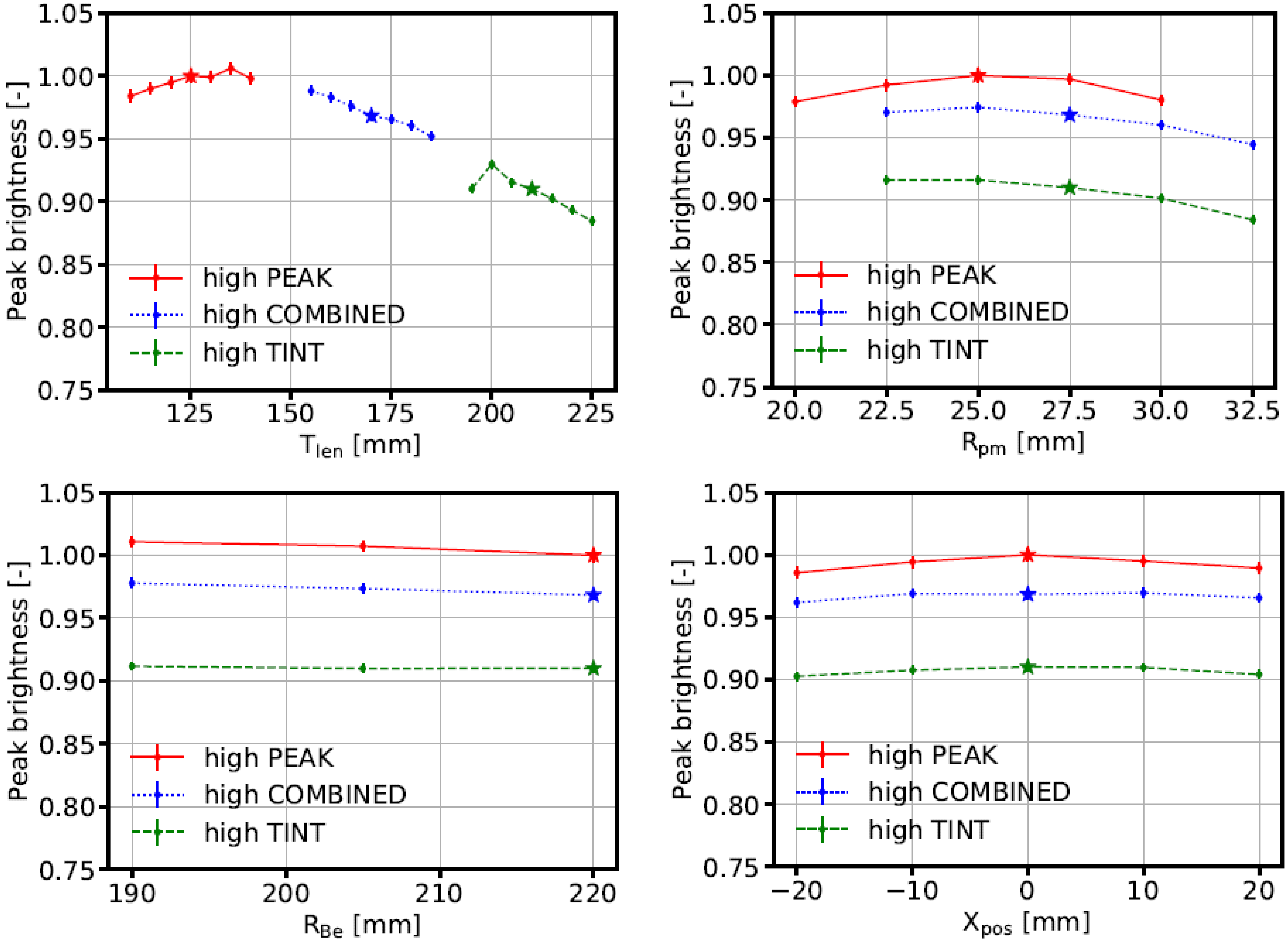
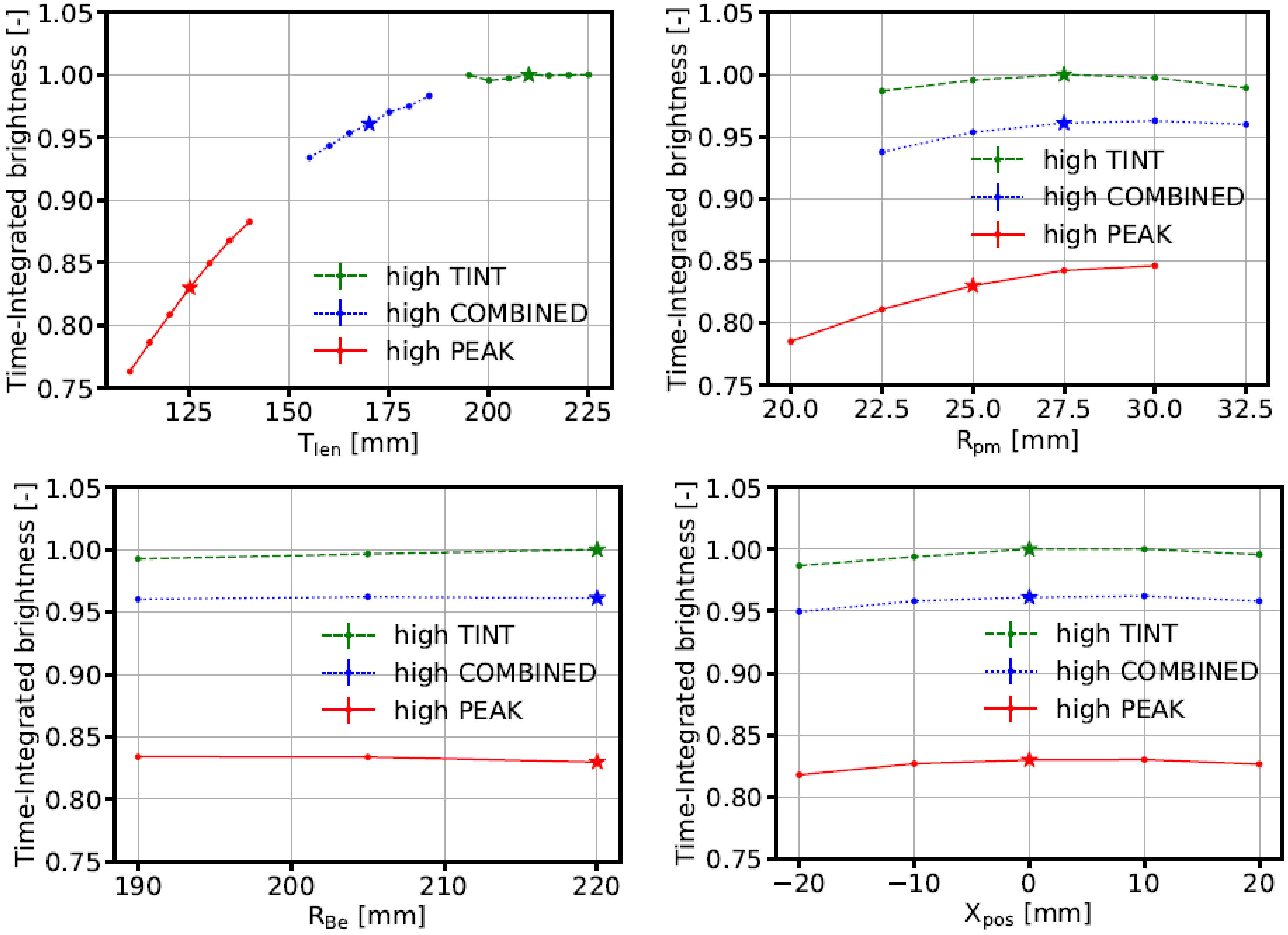
Tube moderator peak brightness sensitivity



Tube moderator time-averaged brightness sensitivity



Preliminary design: cylindrical moderator parameters

Optimized for	Para-H Radius (mm)	Lower Premod. (mm)	Radial Premod. (mm)	Top Premod. (mm)	Be Radius (mm)	Offset[1] (mm)
	UM	UM	UM	UM	UM	UM
Peak	40	27.5	20	20	162.5	87
Mid	**50**	**30**	**29**	**29**	**172.5**	**87**
Tave	62	30	33	33	182.5	87

[1]Offset is the distance from the front edge of tungsten plate to the vertical axis of the cylindrical moderator.

Based on this information the Instrument Systems decided that the middle configuration is the best and should be used for both moderators.

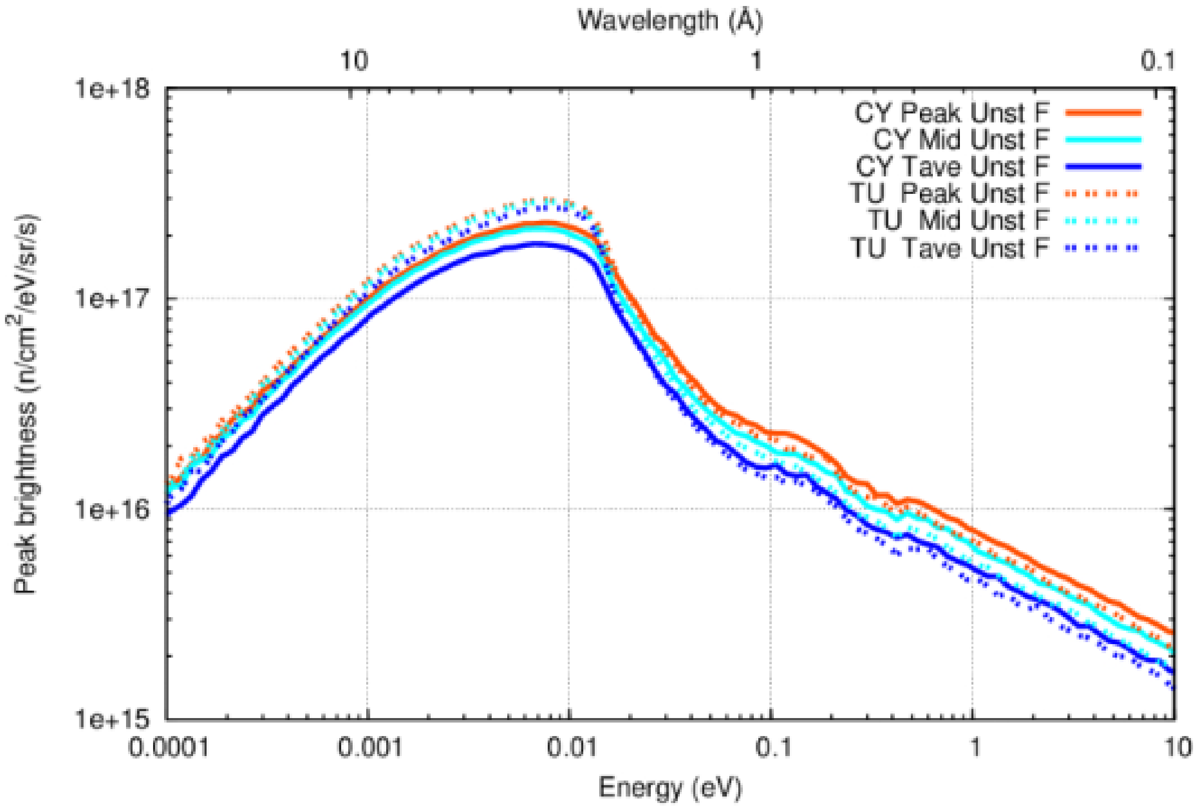
Preliminary design: tube moderator parameters

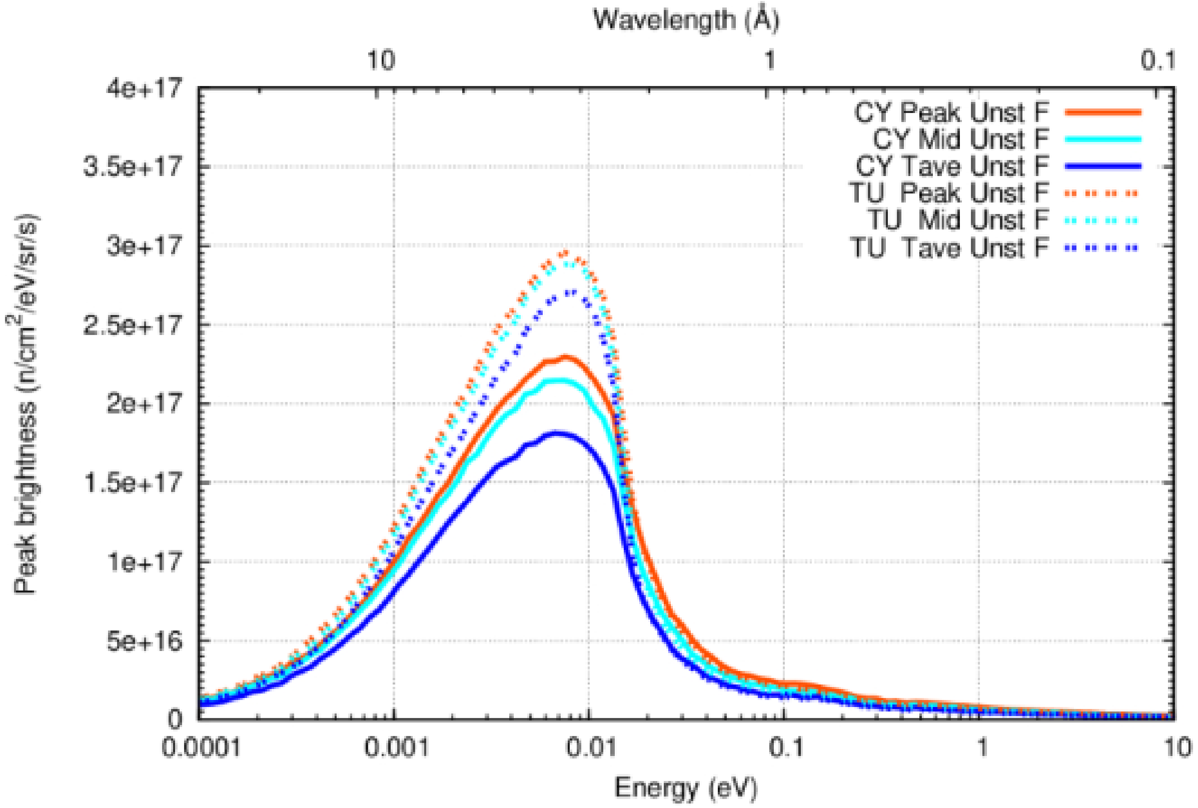
Optimized for	Para-H Tube Diameter (mm)	Para-H Tube length[1] (mm)	Premod. Thickness (mm)	Be Radius (mm)	Offset[2] (mm)
Peak	30	125	25	182.5	87
Mid	**30**	**170**	**27.5**	**182.5**	**87**
Tave	30	210	27.5	182.5	87

[1]The length of the tube perpendicular to the proton beam

[2]Offset is the distance from the front edge of the tungsten plate to the point defined by the intersection of angular bisectors of the tube moderator.

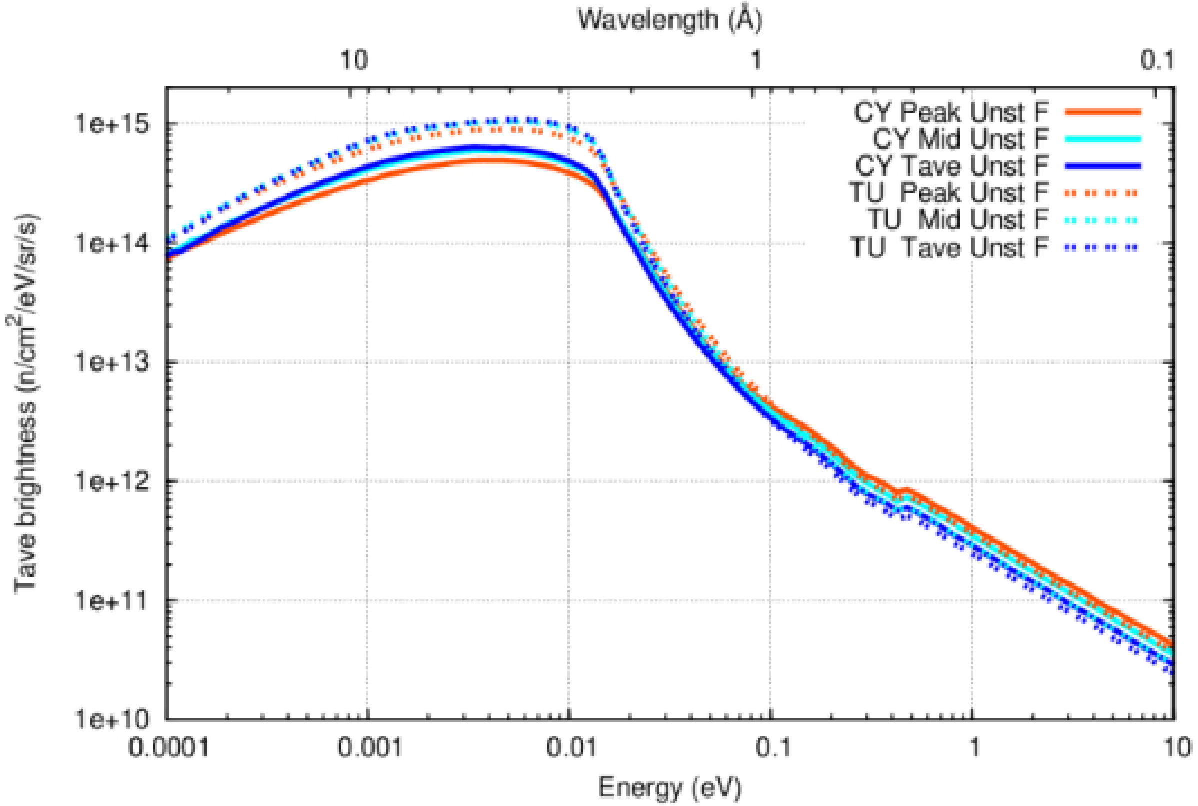
Peak brightness: Cylindrical and Tube moderator

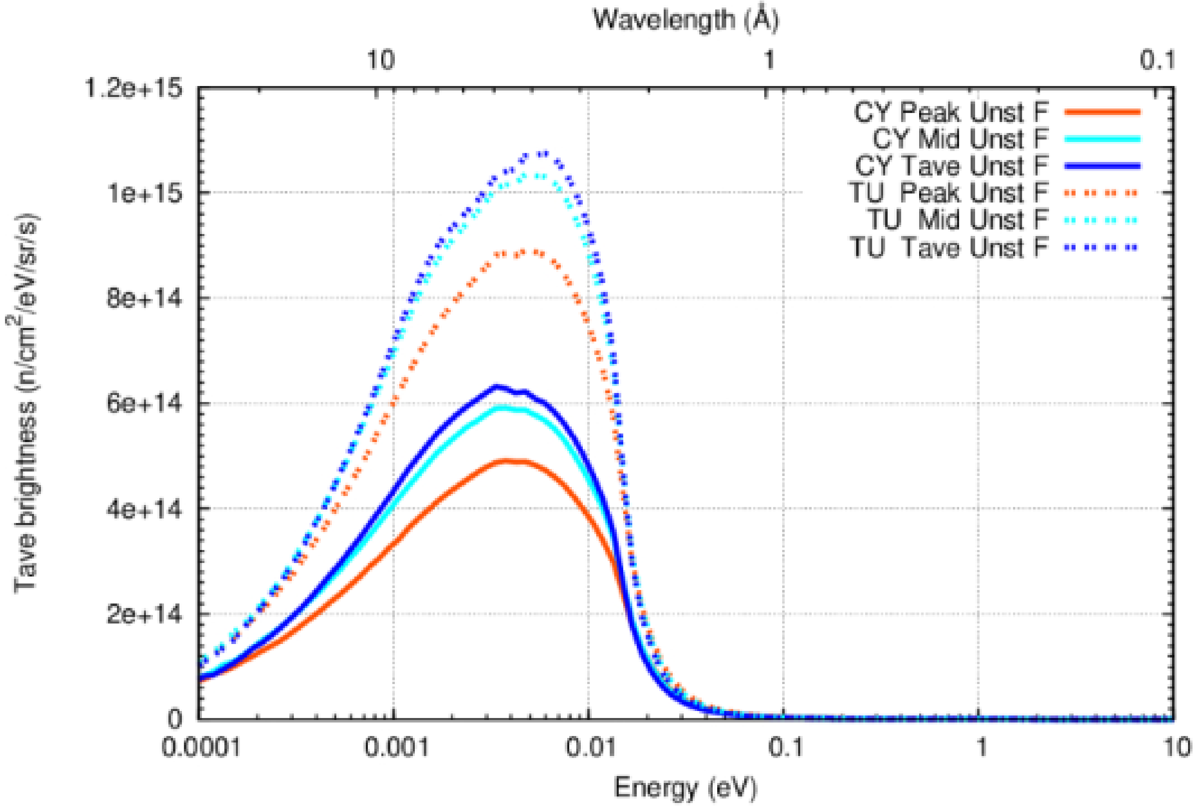




Based on this analysis and additional investigation by the Instrument Systems it was decided that the middle configuration is the best and should be used for both moderators.

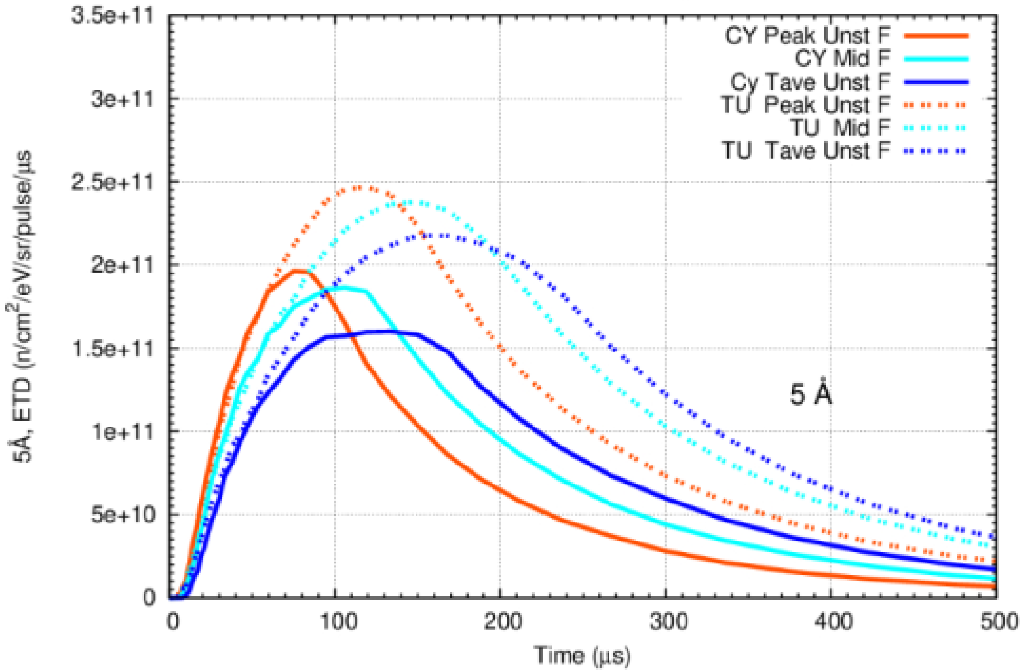
Tave brightness: Cylindrical and Tube moderator

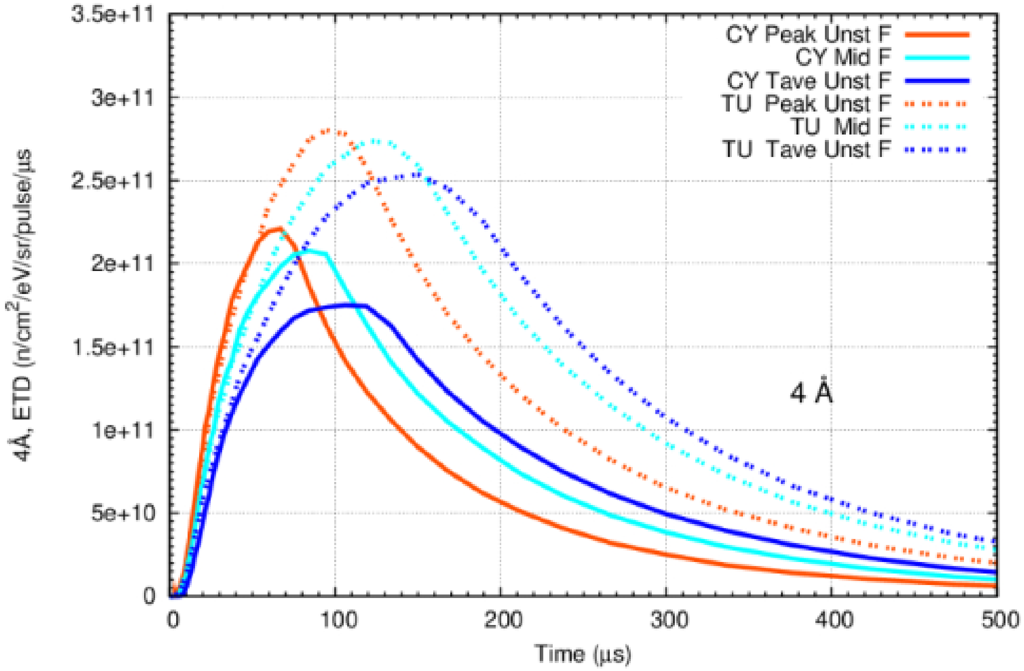


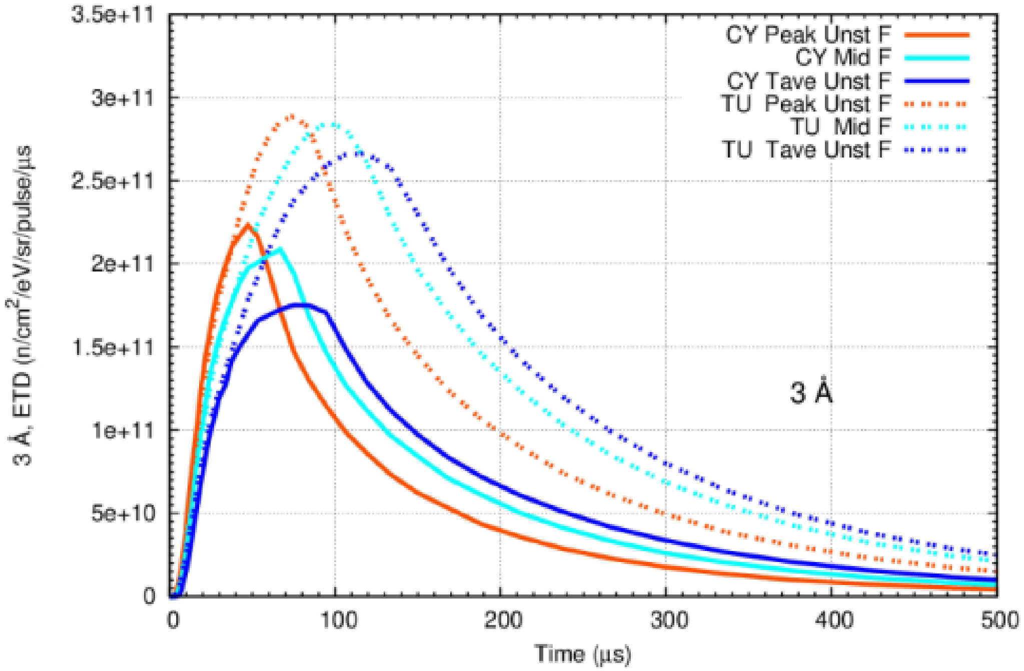


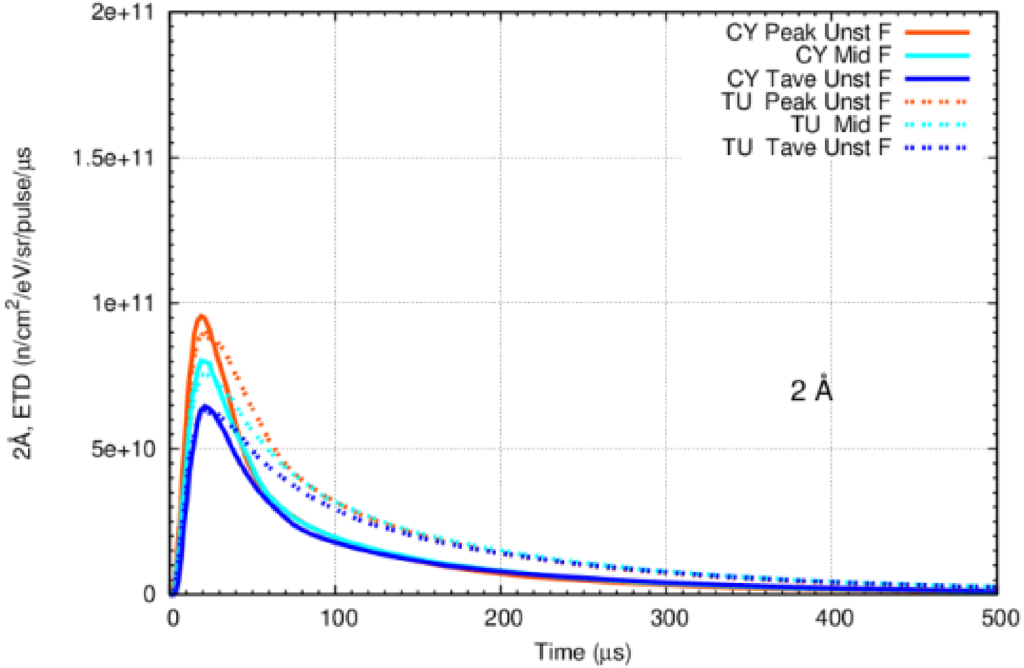
Based on this analysis and additional investigation by the Instrument Systems it was decided that the middle configuration is the best and should be used for both moderators.

Pulse shapes for different configurations of cylindrical and tube moderators



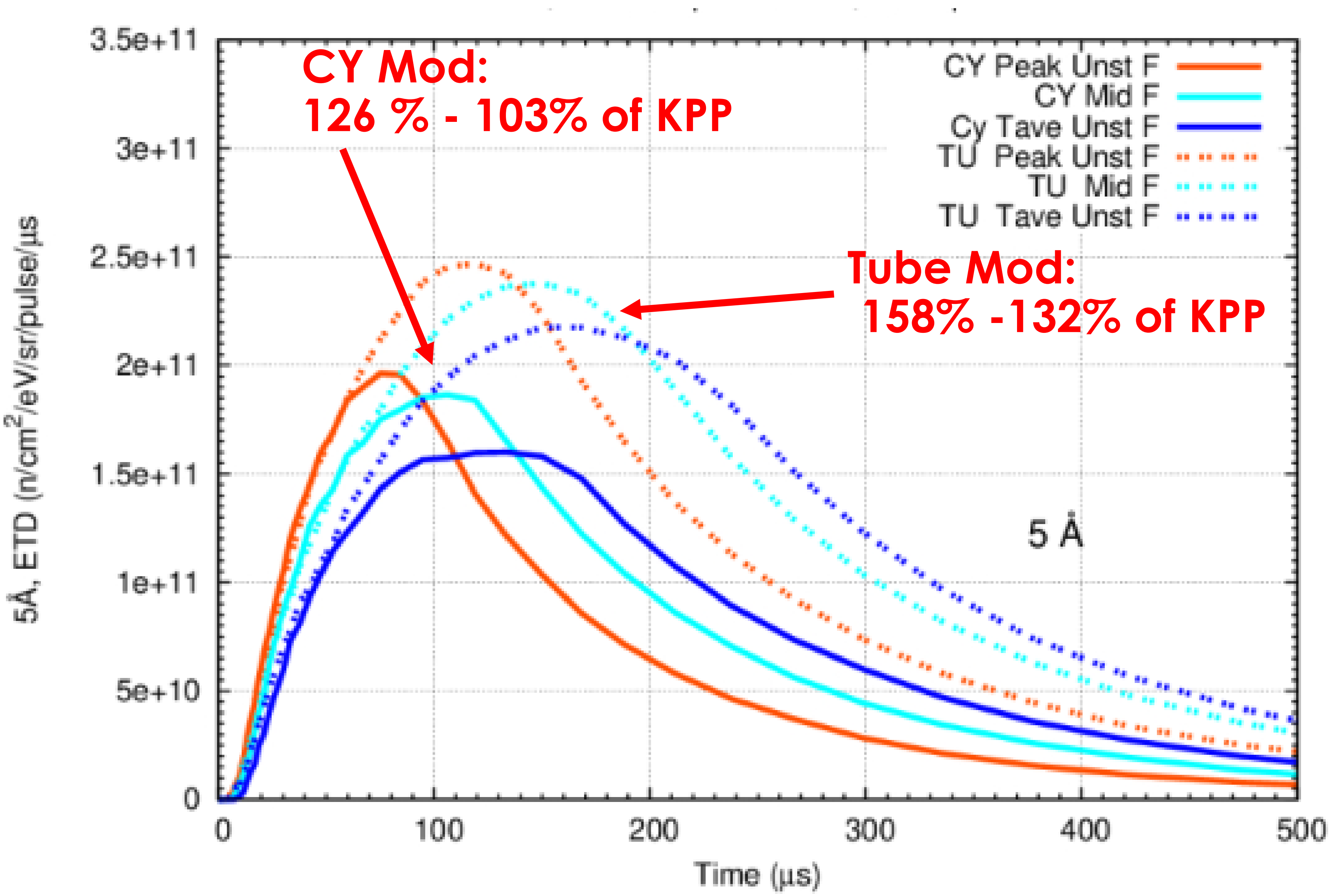






Cylindrical moderator, pulse shapes, 5 Å

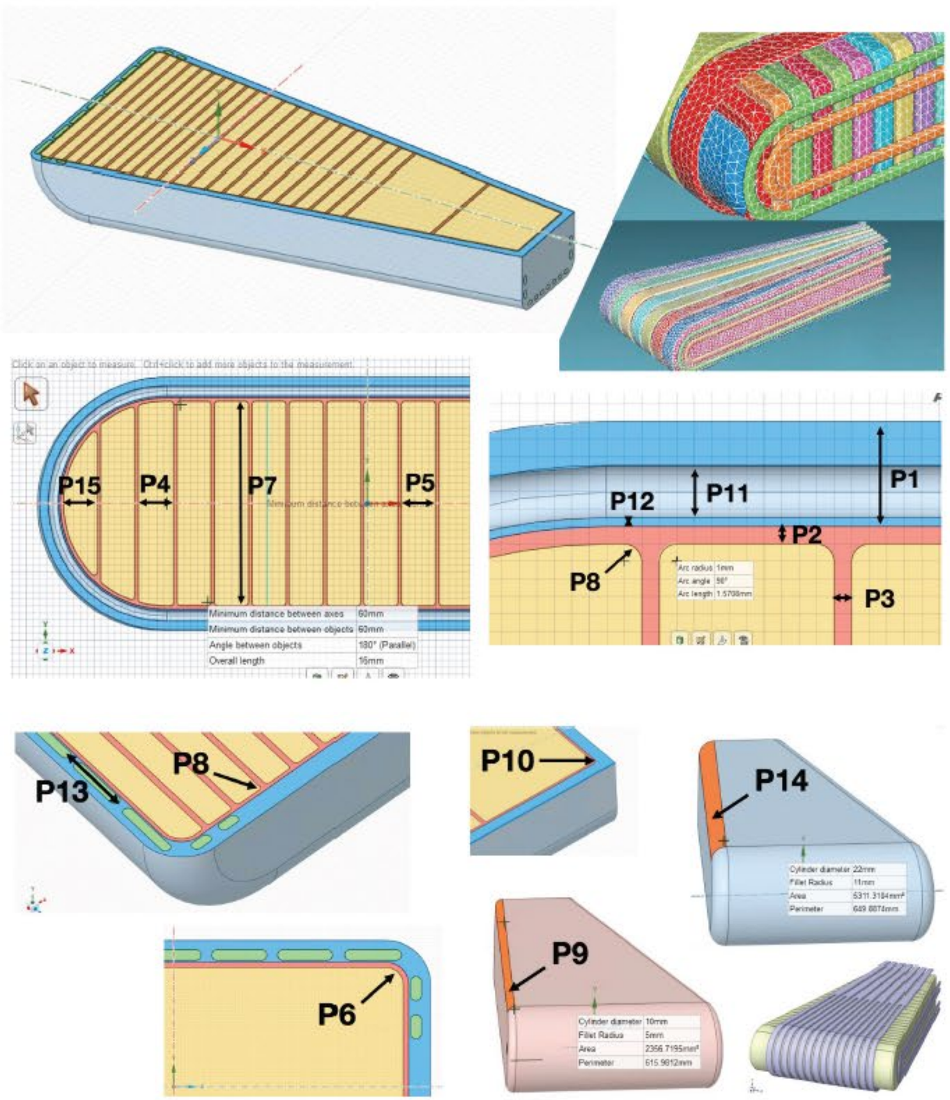
KPP:
2.0E+14
n/cm²/Å/sr/s

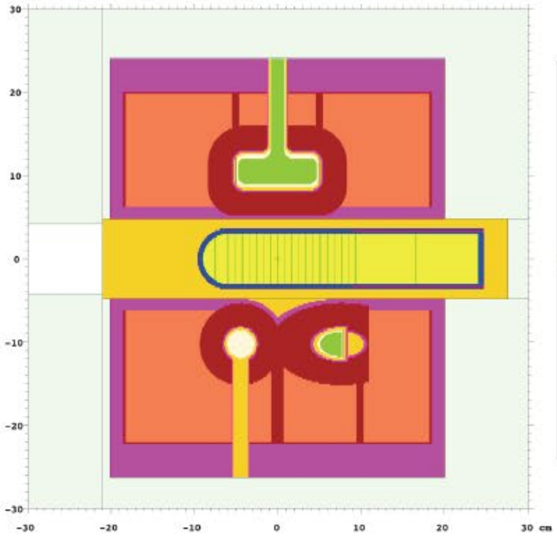


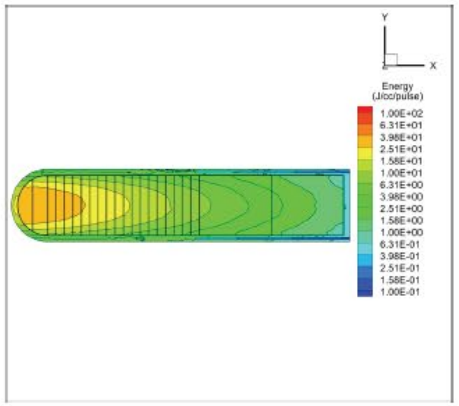
Further work: simultaneous MRA/target/beam profile optimization

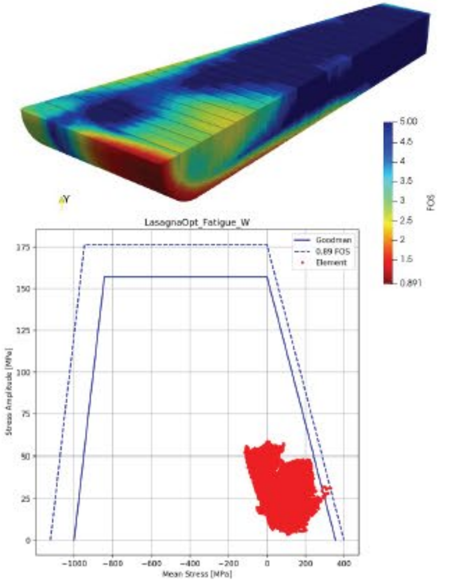
Simultaneous moderator and target optimization

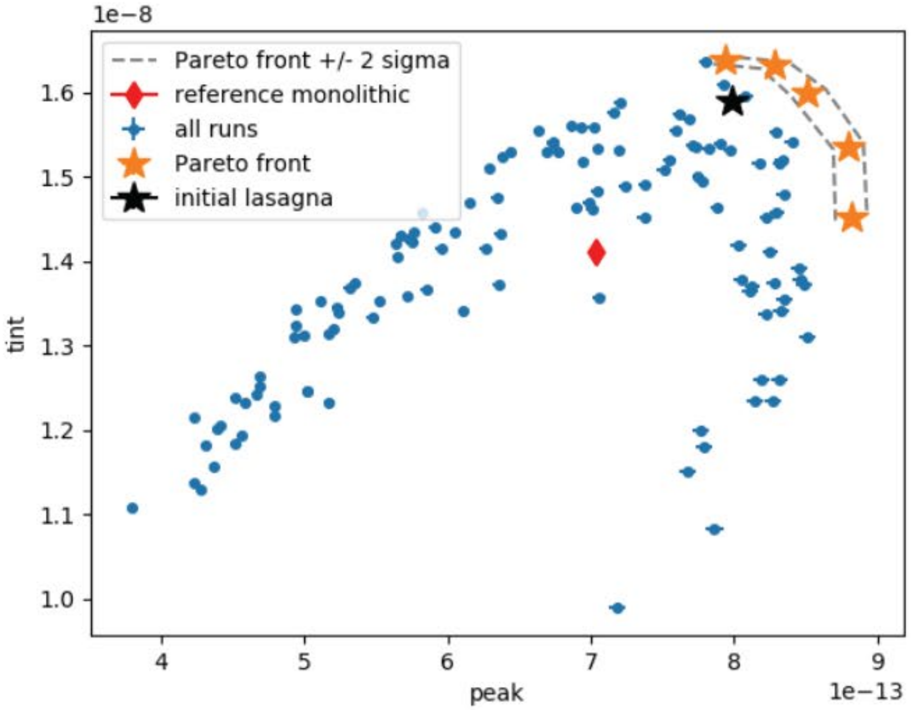
- **Lasagna target design**

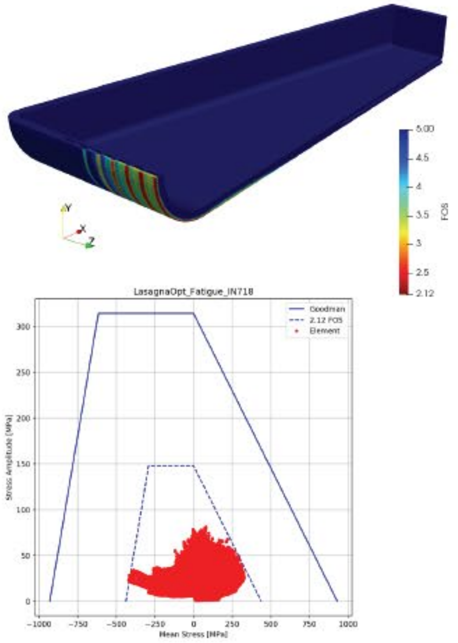






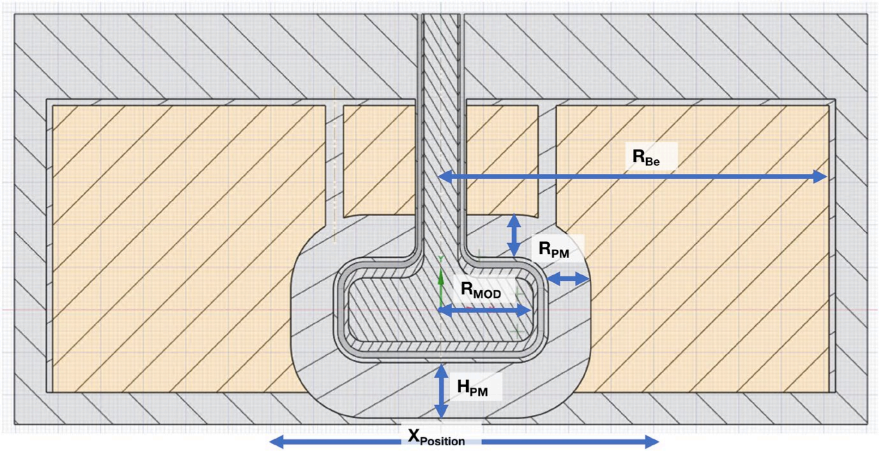




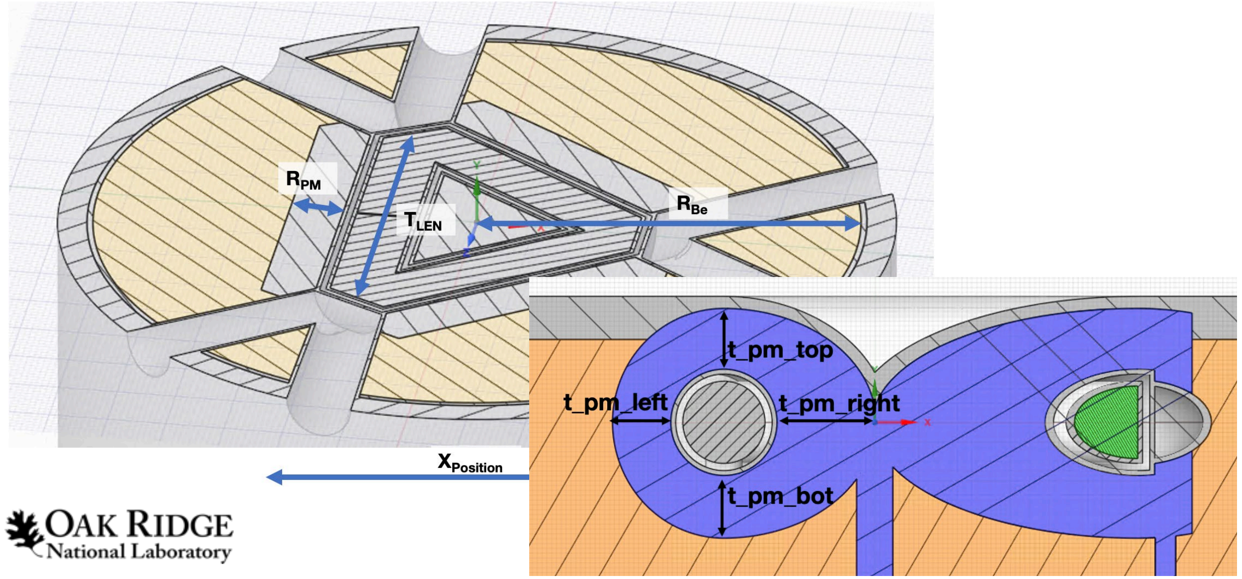


Simultaneous moderator-target-beam optimization

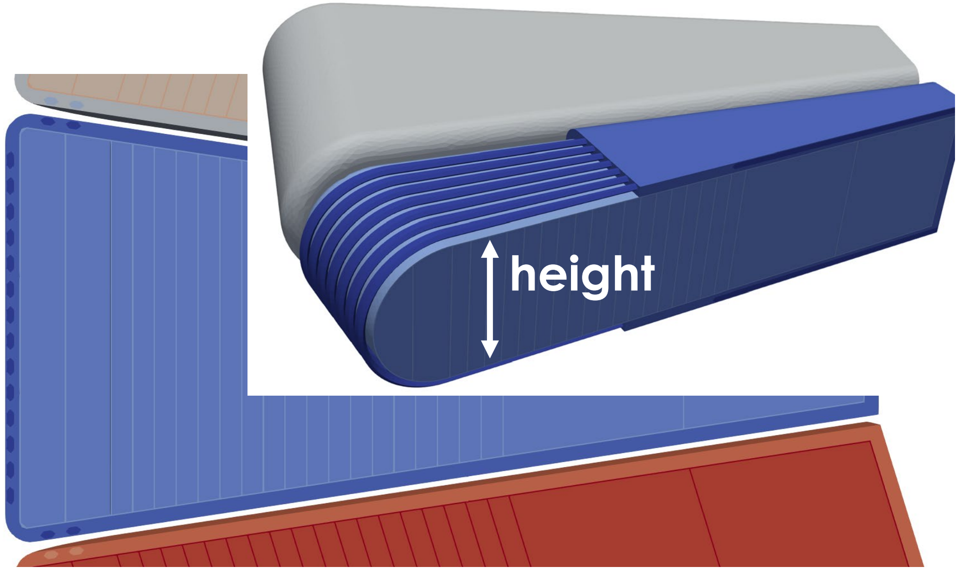
Cylindrical moderator: 6 parameters



Tube moderator: 7 parameters

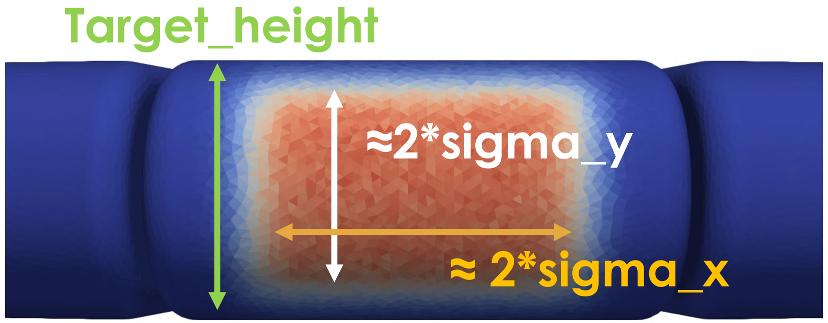


Target: only tungsten height varied



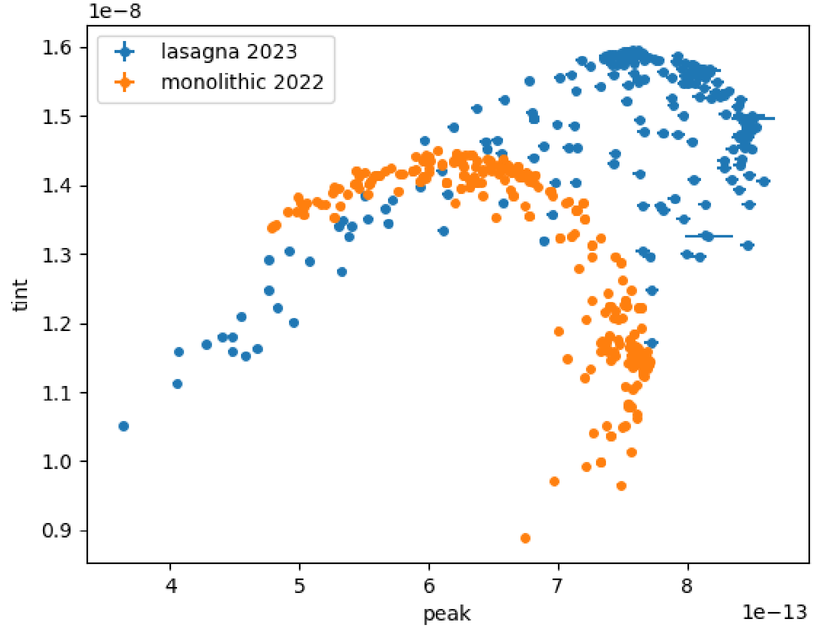
Proton beam : keep footprint 62 cm2 (nx=10)
Parameter c varied

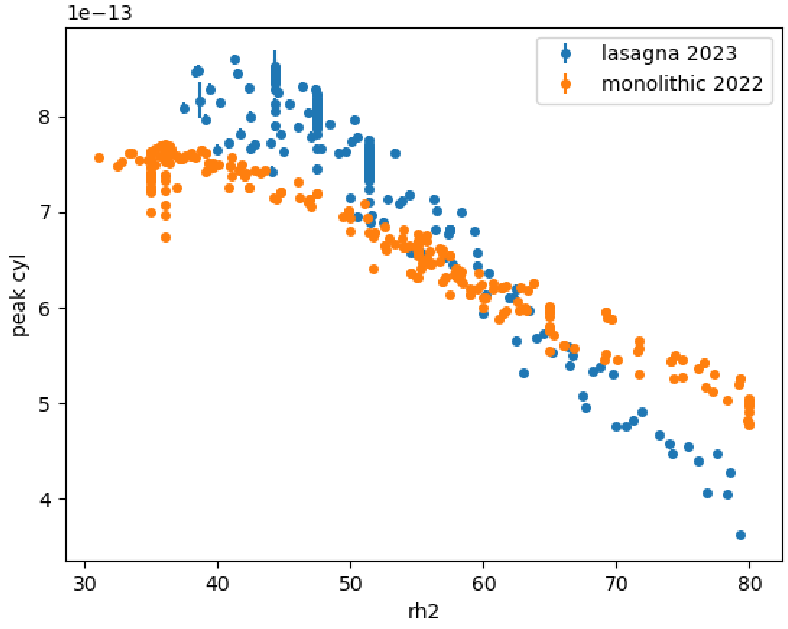
c=target_height / sigma_y

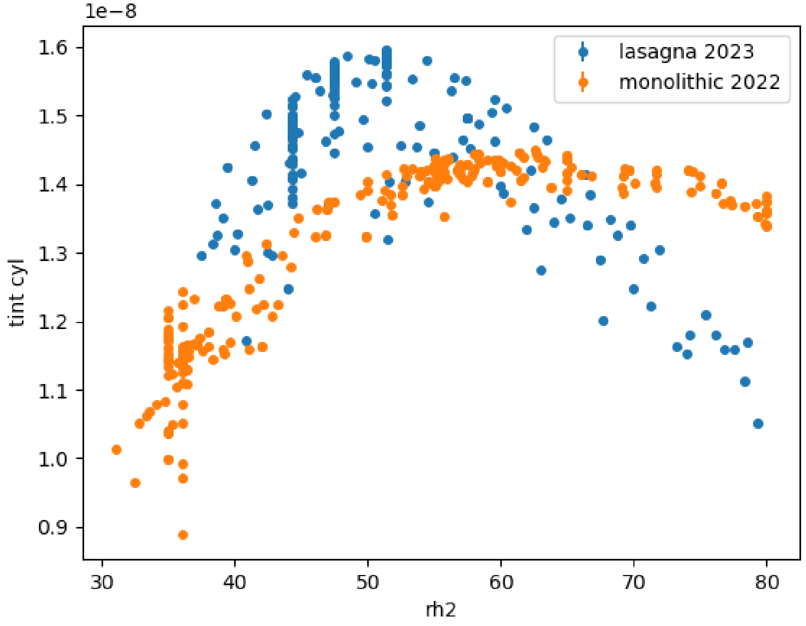


Cylindrical moderator: MTB optimization

Preliminary comparison CYLINDRICAL	Rh2 (mm)	t_pm_side (mm)	t_pm_bot (mm)	t_pm_top (mm)	r_be (mm)	x_shift (mm)	t_height (mm)	c	Sigma_x (mm)	nx	Sigma_y (mm)	ny	Peak	tint
Tint 2023	**51.39**	**37.89**	**31.41**	**29.81**	**183.80**	**6.58**	**69.97**	**2.38**	**51.00**	**10**	**29.79**	**10**	**7.5103e-13**	**1.5911e-8**
Tint 2022	62	33	30	33	182.5	0	58	-	51.7	3.9	19.8	4	6.06e-13	1.45e-8
Middle 2023	**47.50**	**31.62**	**29.97**	**28.70**	**183.38**	**6.58**	**69.97**	**2.31**	**49.4**	**10**	**30.74**	**10**	**8.0745e-13**	**1.566e-8**
Middle 2022	50	29	30	29	172.5	0	58	-	51.7	3.9	19.8	4	7.04e-13	1.41e-8
Peak 2023	**41.3**	**25.0**	**29.0**	**26.0**	**175.0**	**20.0**	**75.0**	**2.26**	**45.2**	**10**	**33.63**	**10**	**8.59E-13**	**1.41E-08**
Peak 2022	40	20	27.5	20	162.5	0	58	-	51.7	3.9	19.8	4	7.54e-13	1.18e-8

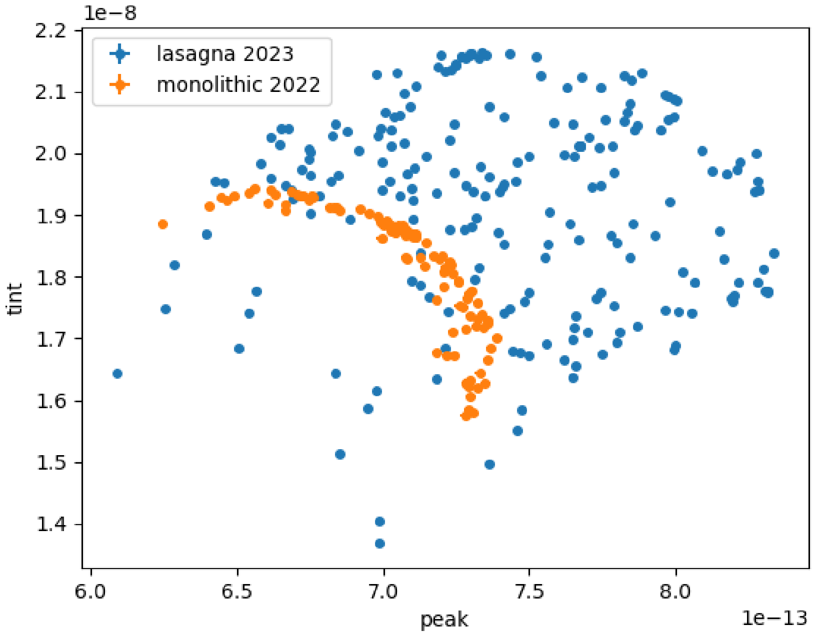


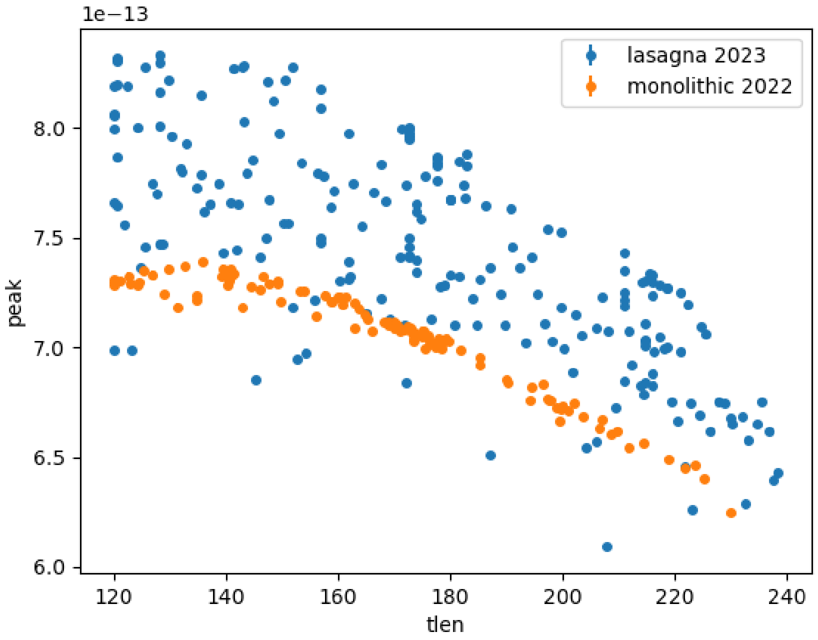


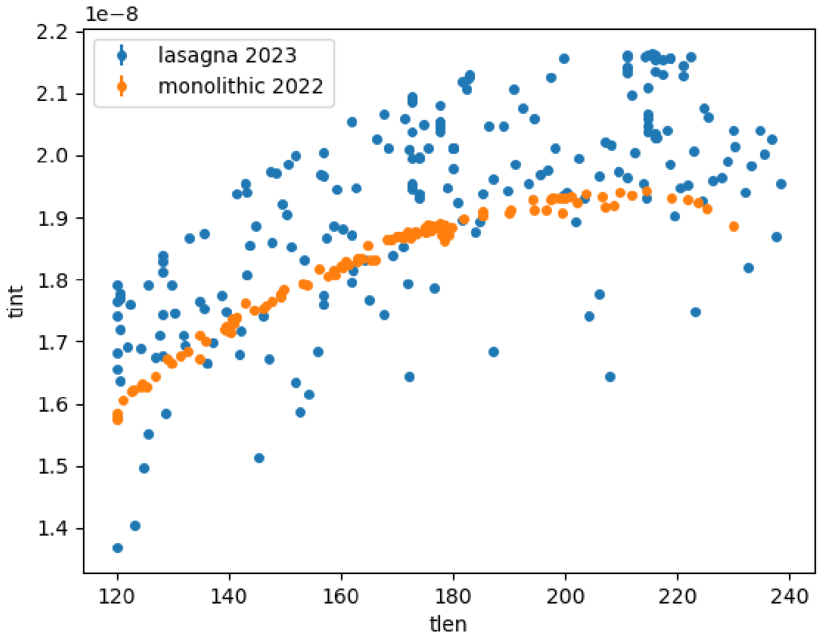


Tube moderator: MTB optimization

Preliminary comparison TUBE	T_len (mm)	t_pm_top (mm)	t_pm_right (mm)	t_pm_bot (mm)	t_pm_left (mm)	r_be_t (mm)	t_height (mm)	c	sigma_x (mm)	nx	sigma_y (mm)	ny	Peak	tint
Tint 2023	**211.1**	**27.75**	**41.00**	**18.49**	**31.45**	**200.0**	**74.91**	**2.60**	**52.00**	**10**	**29.14**	**10**	**7.433E-13**	**2.162E-08**
Tint 2022	210	27.5	27.5	27.5	27.5	220	58	-	51.7	3.9	19.8	4	7.0511e-13	1.6703e-8
Middle 2023	**172.6**	**25.59**	**31.24**	**18.80**	**30.22**	**191.5**	**74.91**	**2.68**	**53.60**	**10**	**28.33**	**10**	**8.003E-13**	**2.086E-08**
Middle 2022	170	27.5	27.5	27.5	27.5	220	58	-	51.7	3.9	19.8	4	6.7347e-13	1.8957e-8
Peak 2023	**120.7**	**25.90**	**31.61**	**18.49**	**25.59**	**182.6**	**69.91**	**2.53**	**54.20**	**10**	**28.02**	**10**	**8.314E-13**	**1.777E-08**
Peak 2022	125	25.0	25.0	25.0	25.0	220	58	-	51.7	3.9	19.8	4	6.2457e-13	1.9326e-8







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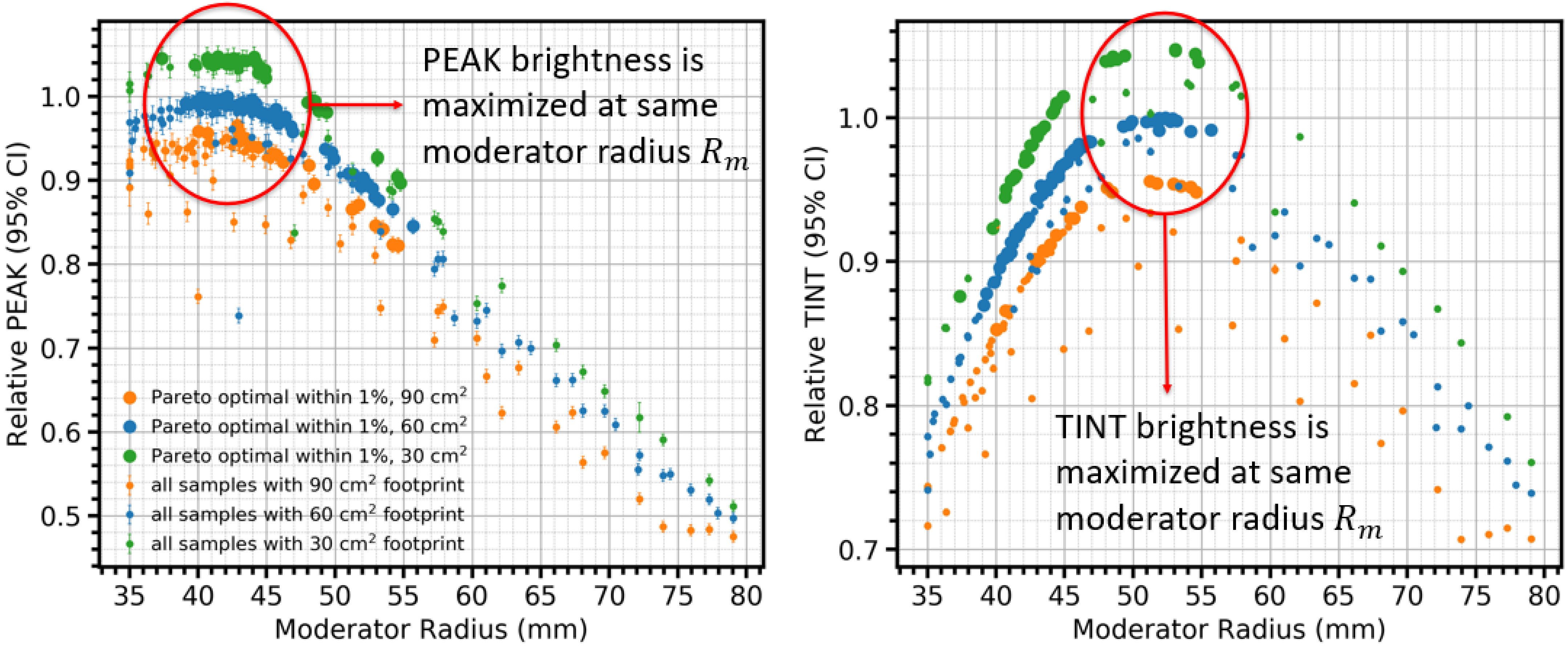
Effect of proton beam footprint (cylindrical moderator)



Optimized R_m, H_t, σ_y for footprints: 30 cm2, 60 cm2, 90 cm2

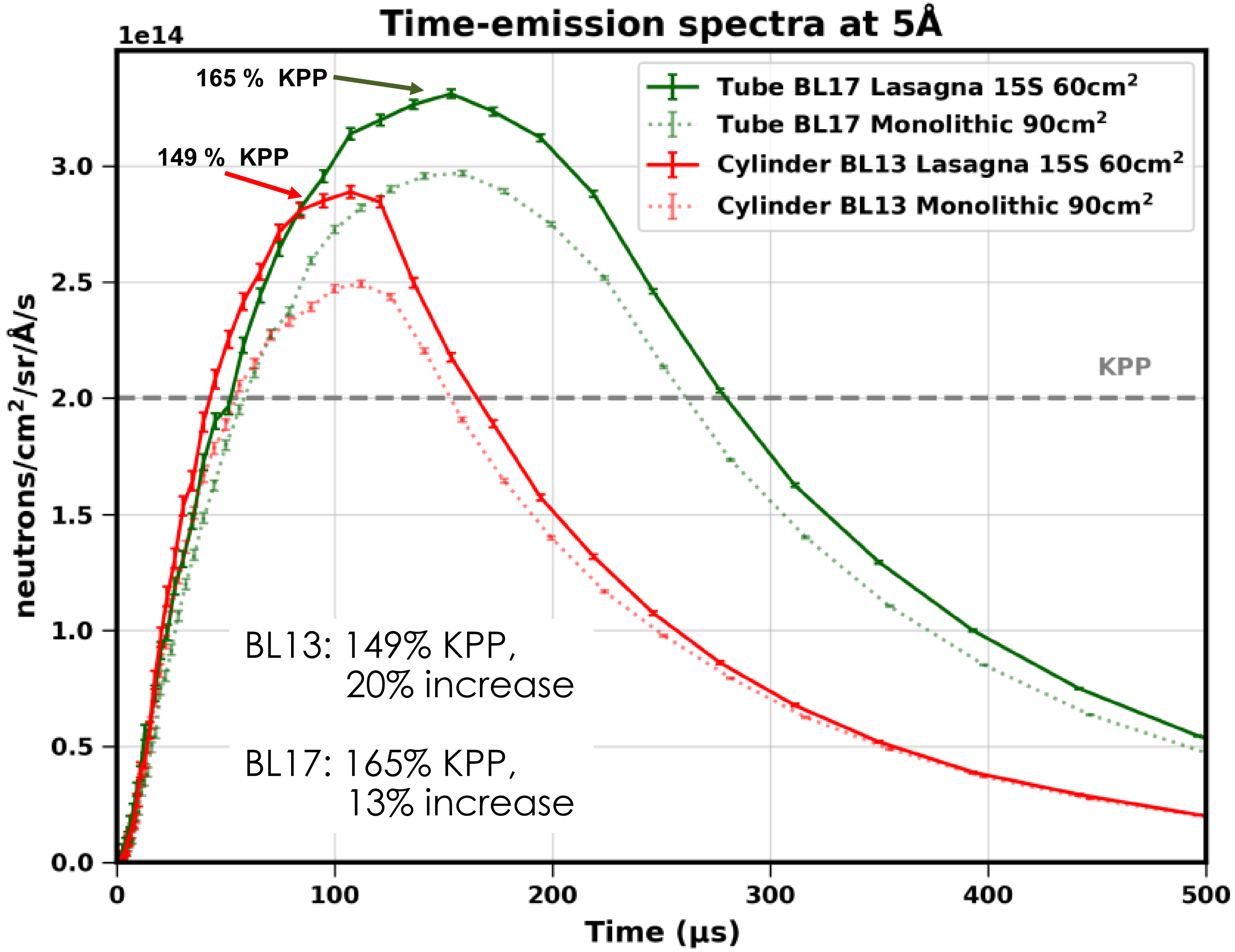
Optimal radius of the hydrogen does not depend on beam footprint

Simultaneous target and moderator optimization preliminary results

Monolithic target:
- 21-segment,
- SuperGaussian beam profile ~90 cm^2

Lasagna target:
- 66 mm tall,
- 15-segment,
- SuperGaussian beam profile ~60 cm^2

Improved brightness is due to:
- narrower beam (~+6%),
- 15-segment configuration (~+5%),
- taller target (~+4%)



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Conclusion

- The current stage in the preliminary neutronics design provides neutron beamlines with exceptional brightness at long neutron wavelengths, as required in the STS mission statement.
- The moderators exceed the preliminary KPP requirement for brightness at 5 Å by 25 % to 55% margin.
- Application of advanced techniques allows us to perform neutronics analyses at the high-fidelity level typically used only in more advanced project stage.
- Advance optimization workflow with high fidelity models was developed and is available for future work.
- Neutronics analyses performed to date provide solid foundation for successful preliminary design completion and clear path forward to support the CD-2, CD-3, and final MRA design.

Thank you for your attention!

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Additional Slides

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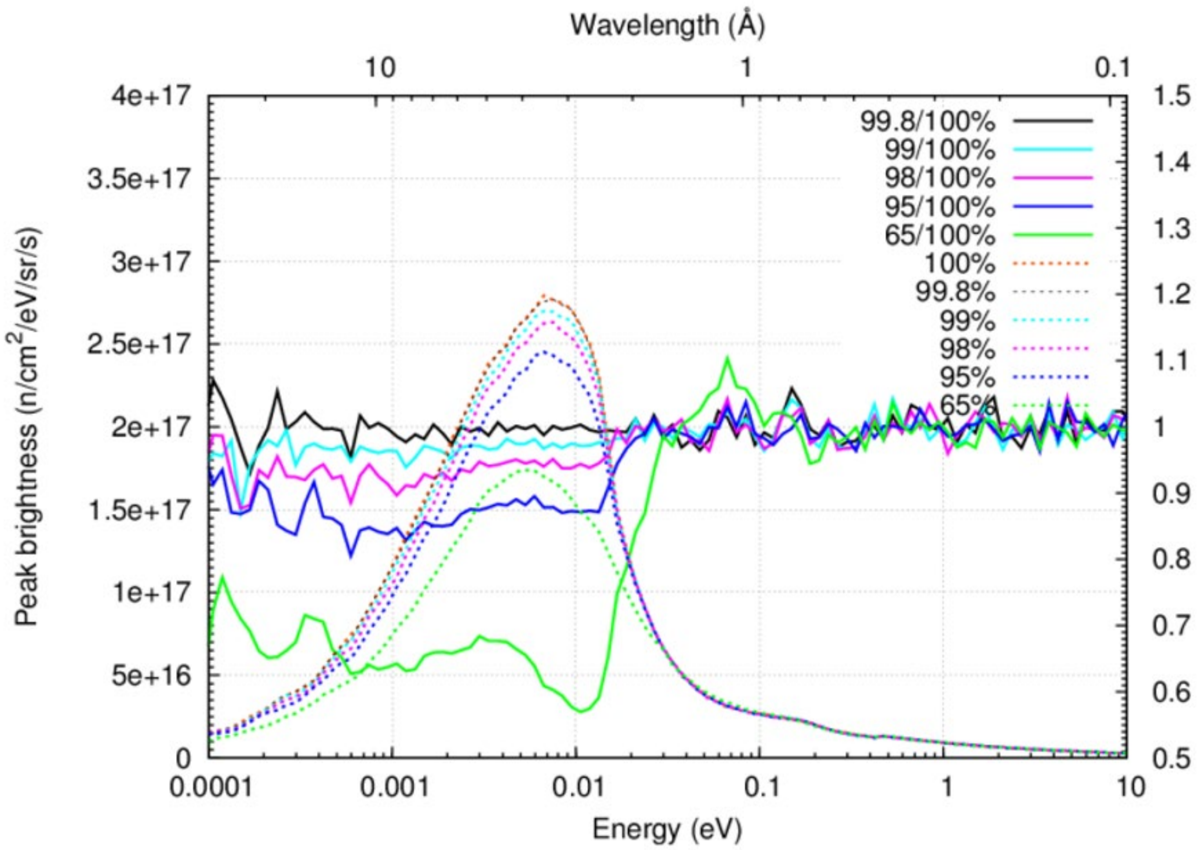
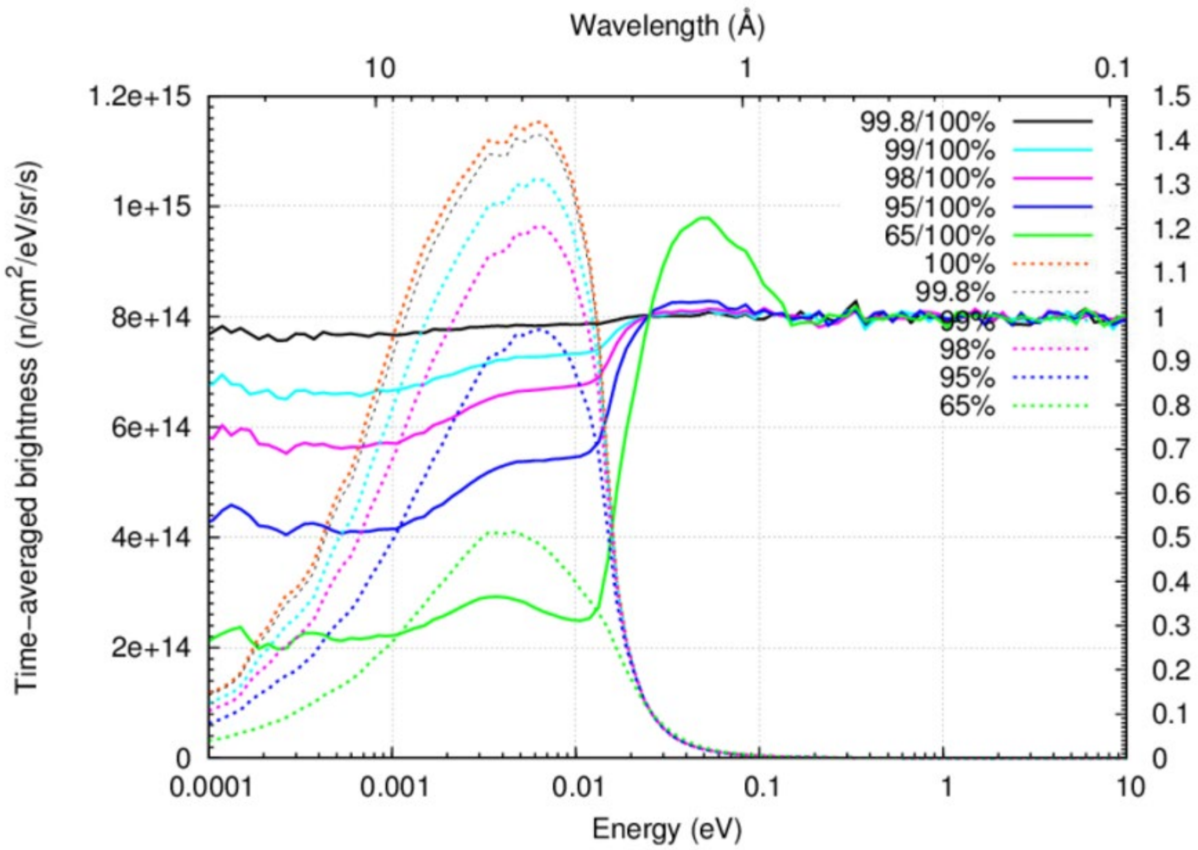
Effect of Para-H / Ortho-H Content

Para-H / Ortho-H effect

Cylindrical moderator, Peak brightness



Tube moderator, Tave brightness



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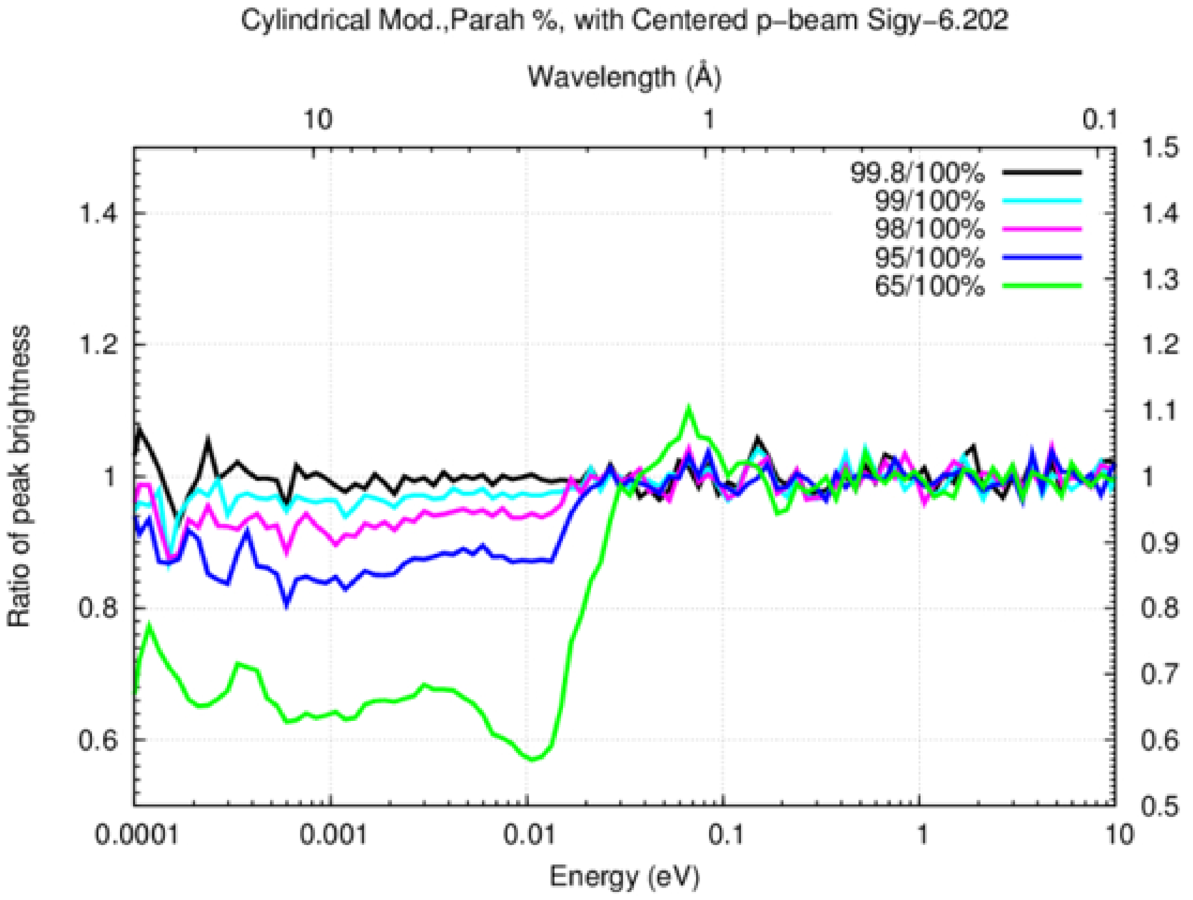
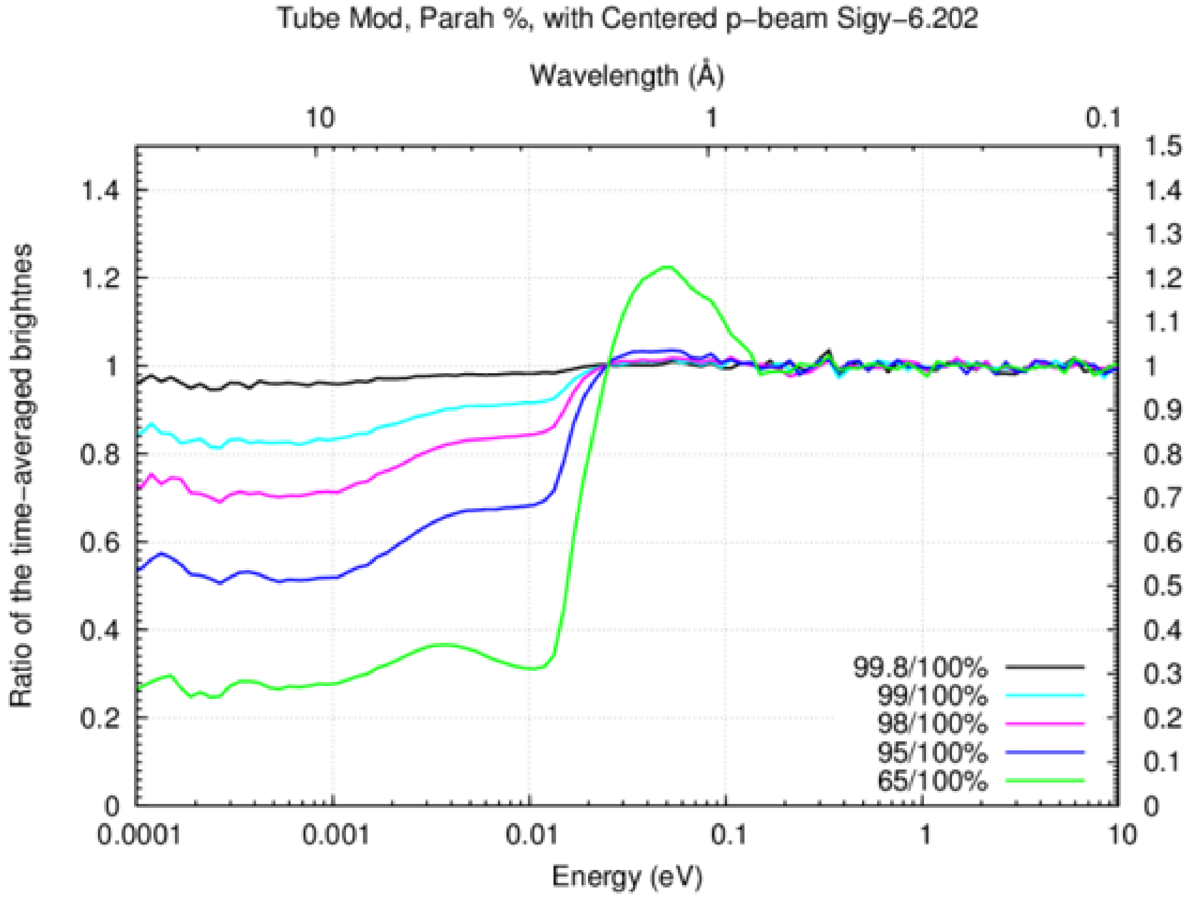
Para-H / Ortho-H effect

Cylindrical moderator, Peak brightness



Tube moderator, Tave brightness



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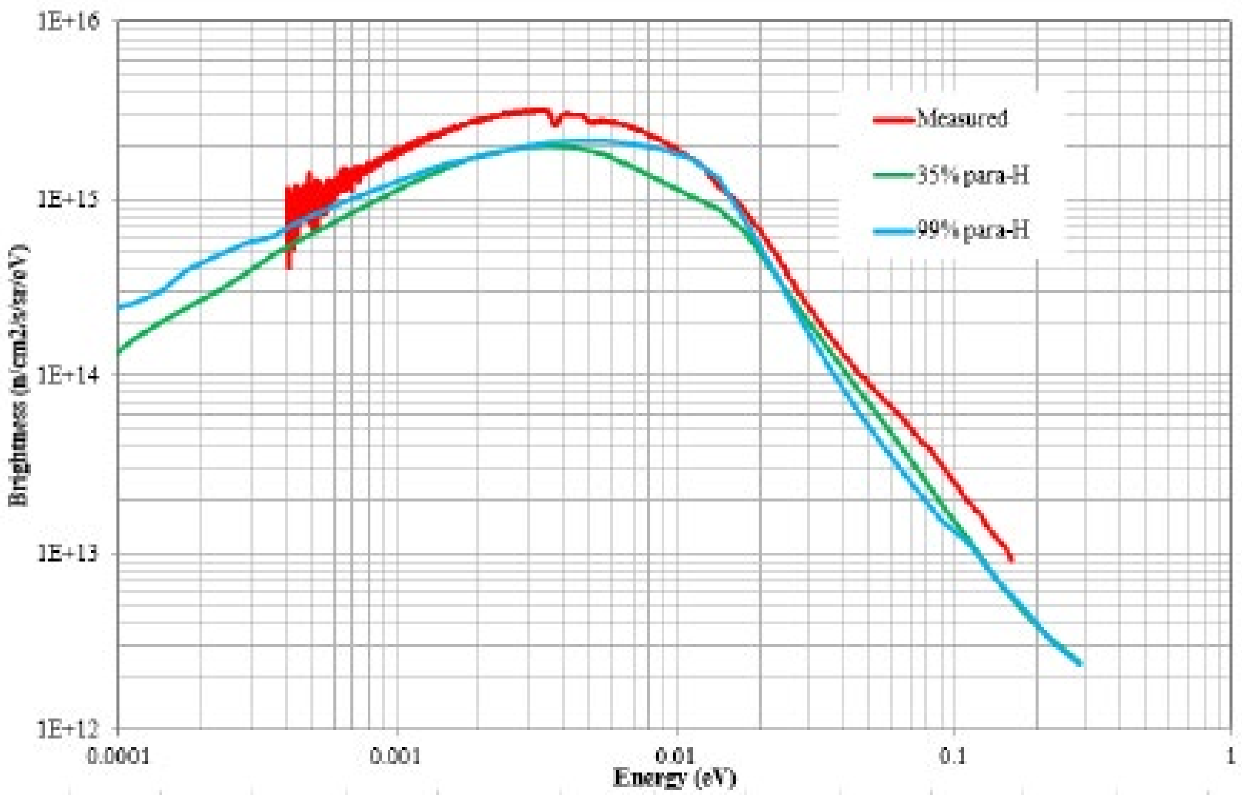
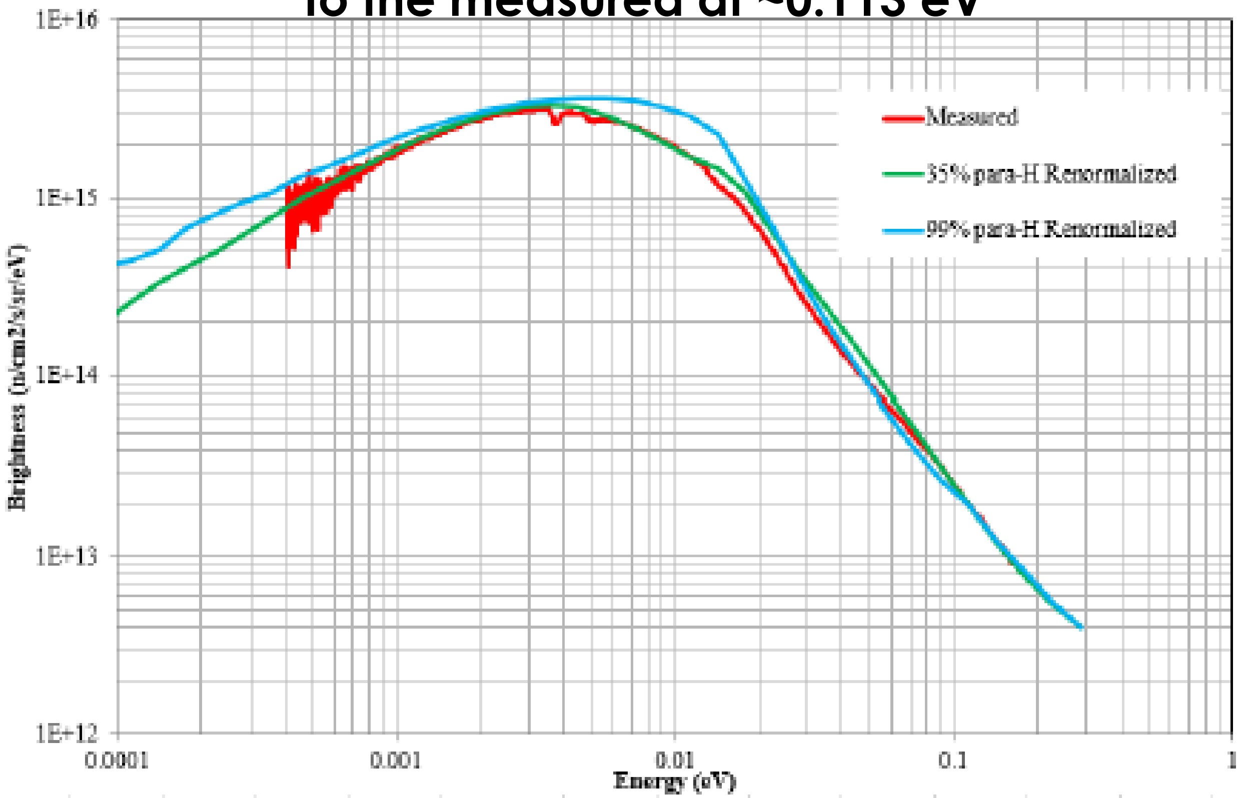
Open slide master to edit

Comparison: experiment – simulation for HFIR Cold source



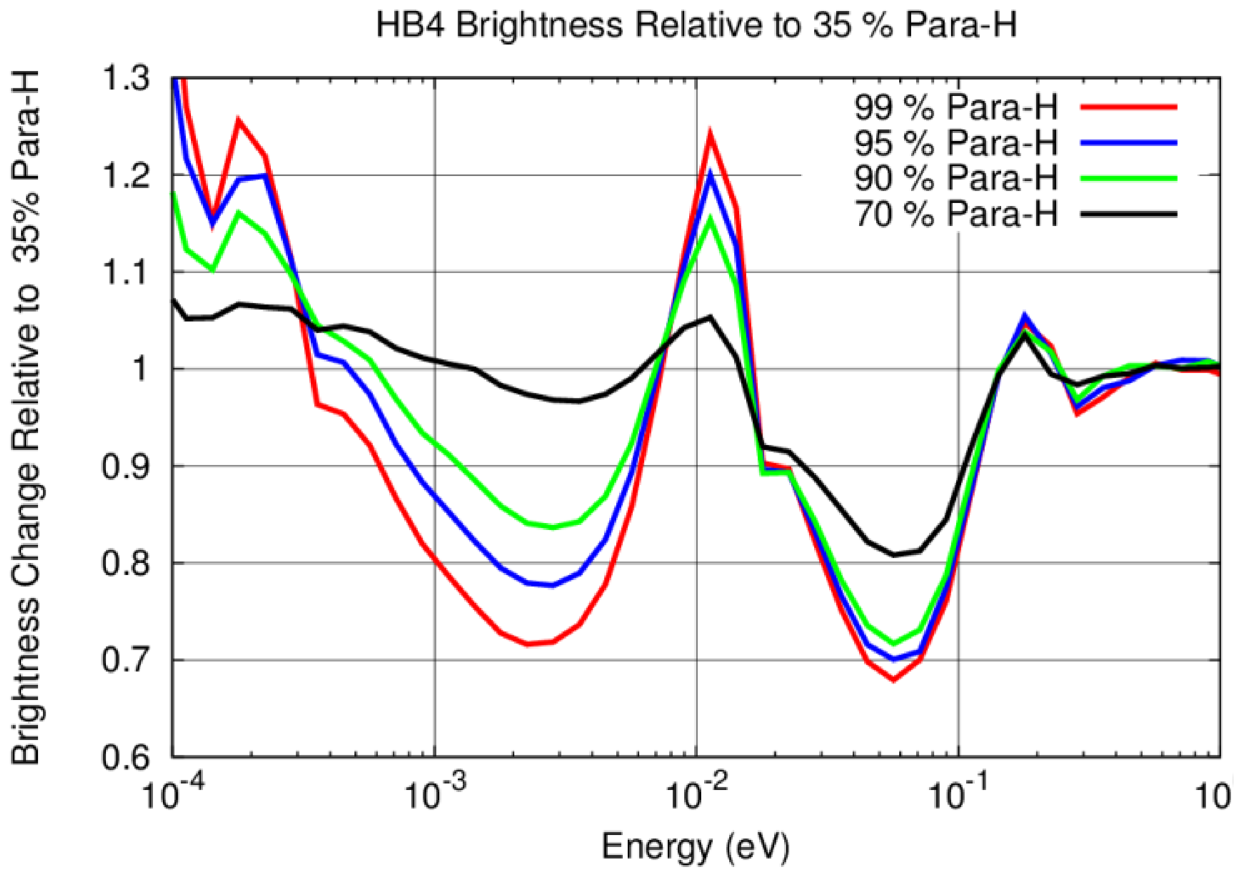
Calculated brightness normalized to the measured at ~0.113 eV



Experiment: J. L. Robertson and E. B. Iverson, Measurement of the Neutron Spectrum of the HB-4 Cold Sour at The HFIR, Reactor Dosimetry State of the Art 2008, Proc. Of the 13th Int. Symp., ISBM-13 978-981-4271-10-3, pp.85-93 (2008).

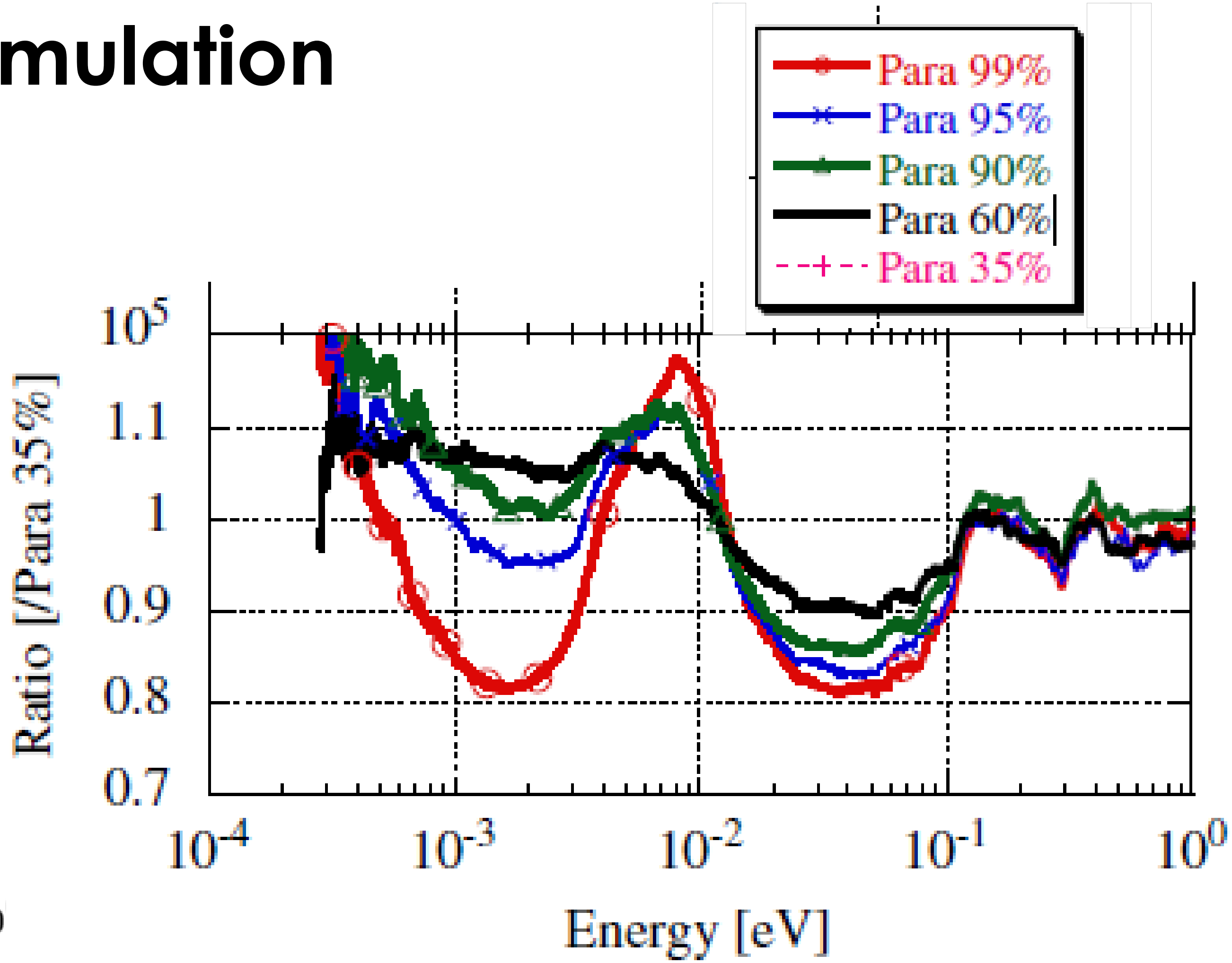
Simulation: I. Remec, F. Gallmeier, HFIR Cold Source Upgrade Options, ORNL/TM-2018/820 SNS-106100200-TR0235-R00

Comparison: experiment - simulation



MCNPX simulations, existing HFIR CS brightness change relative to 35 % para-H,

I. Remec, F. Gallmeier, HFIR Cold Source Upgrade Options, ORNL/TM-2018/820 SNS-106100200-TR0235-R00



Experiment: Motoki Ooi et al. brightness change relative to 35 % para-H

Motoki Ooi et al., Experimental studies of the effect of the ortho/para ratio on the neutronic performance of a liquid hydrogen moderator for a pulsed neutron source, Nucl. Inst. Meth. A, 659, pp. 61-68 (2011).