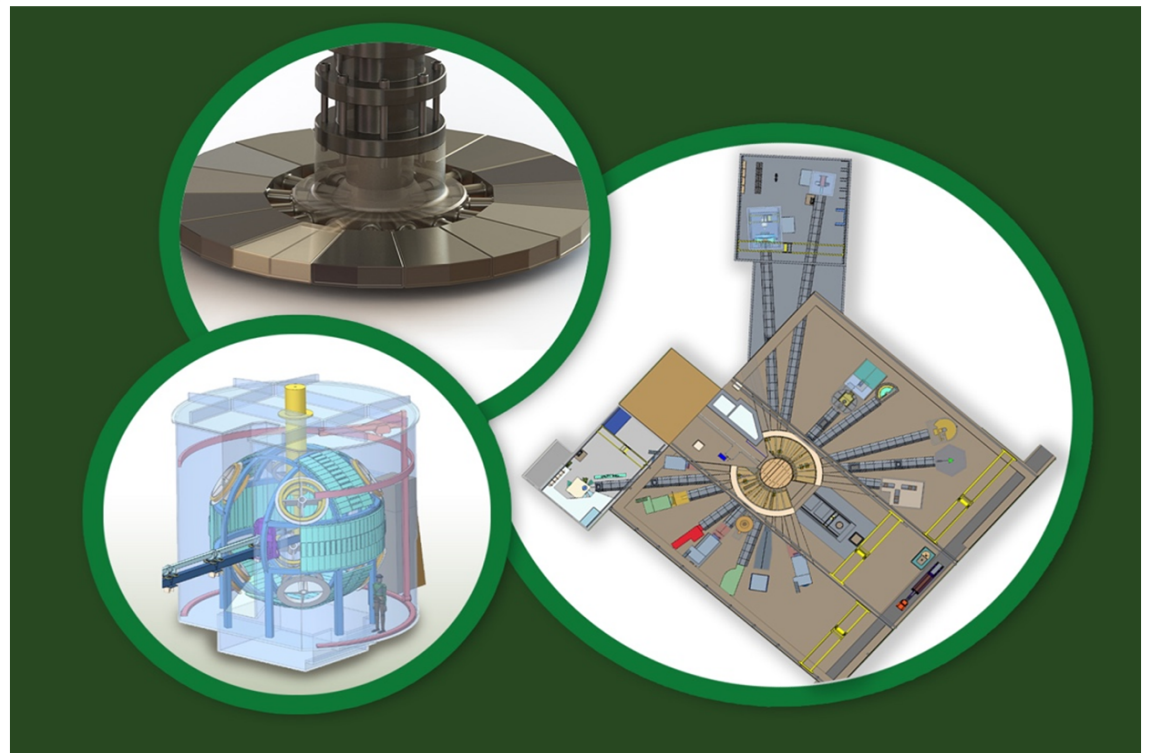


Moderator Optimization for the Second Target Station Final Design



Kristel Ghooos
Lukas Zavorka
Igor Remec

July 2024

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Second Target Station Project

Moderator Optimization for the Second Target Station Final Design

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July 2024

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ABBREVIATIONS

ORNL	Oak Ridge National Laboratory
SNS	Spallation Neutron Source
STS	Second Target Station

EXECUTIVE SUMMARY

This report details the results from the optimization simulations performed for the final design of the Second Target Station (STS). This is a continuation of the analysis performed in 2022 for the preliminary design. To evaluate the impact of the design changes since 2022, the analysis was repeated with updated target and moderator models. Additionally, more degrees of freedom have been considered in the premoderator dimensions which provide a refinement compared to the previous optimization analysis.

We have applied a fully automated optimization workflow in which a detailed unstructured mesh geometry is automatically generated with Attila4MC, starting from a parametrized CREO geometry followed by pre-processing with SpaceClaim. With this geometry, an MCNP run is performed to calculate the brightness metrics, which are subsequently provided to the optimization algorithm in Dakota that provides new parameters and drives the optimization loop until convergence.

The results provide a refinement to and confirmation of the conclusions of 2022. The dimensions of the cylindrical remain unchanged to the 2022 optimized design. For the tube moderator, the premoderator dimensions have been updated. By optimizing the premoderator dimensions as separate parameters on the top, bottom, left and right, a 2% performance increase is achieved.

Parts of this report have been published in [1] and [2].

1 SCOPE

This report details the optimization simulations performed for the selection of the dimensions of the moderators for the final design of the STS. We discuss the results that have lead to the final choice of parameters for the cylindrical and tube moderators.

2 METHODOLOGY AND MODELS

2.1 WORKFLOW

The automated optimization workflow is described in detail in [3, 4]. In summary, six steps need to be performed each iteration:

1. For each new set of input parameters, a CAD model of each of the moderators is generated using a parametrized model in CREO[5].
2. Pre-processing of this model is performed in SpaceClaim to fill the liquid volumes and to help the meshing process[6].
3. An unstructured mesh is generated in Attila4MC for each of the moderators[7].
4. A new input file is written with the meshes embedded in the MCNP geometry. Subsequently, a neutronics calculation is performed using MCNP6.2[8].
5. The brightness metrics are calculated from the MCNP tallies using custom Python tools.
6. Dakota provides a new set of input parameters until the algorithm reaches conversion. In this work, we have used the efficient global and parameter study algorithms[9].

One design iteration needs approximately 5 min for the mesh generation, which is run on a Windows pc, and 1 hr 15 min for the MCNP simulation, which is run on 384 processors on a Linux cluster. The resulting statistical precision on the results is indicated with 95% confidence intervals (CI) in the figures.

2.2 CYLINDRICAL MODERATOR MODEL

Figure 1 provides details about the model of the cylindrical moderator. The cold para-hydrogen moderator is surrounded by a water premoderator and a beryllium reflector. All vessels are made of aluminum. Six geometric parameters can be changed independently within the range indicated between brackets:

- the moderator radius R_m (35 mm - 80 mm),
- the thickness of the premoderator on the side P_s (15 mm - 40 mm),
- the thickness of the premoderator on the bottom P_b (15 mm - 40 mm),
- the thickness of the premoderator on the top P_t (10 mm - 40 mm),
- the radius of the beryllium reflector R_{be} (175 mm - 200 mm),
- the horizontal position of the moderator assembly X_m (-20 mm - 20 mm).

Several geometric dependences are included in the model, such as an adjustment of the thickness of the moderator's vacuum and hydrogen vessels to the size of the vessels. With moderator radius of 50 mm, the

flat and cylindrical wall thicknesses are respectively 5.35 mm and 2.8 mm, while the flat wall thickness of the vacuum vessel and the premoderator vessel are 2.61 mm and 3.38 mm. More details can be found in [4] and [10]. The parameter X_m moves the entire moderator reflector assembly, including the tube moderator, along the incident beam axis with regard to the target.

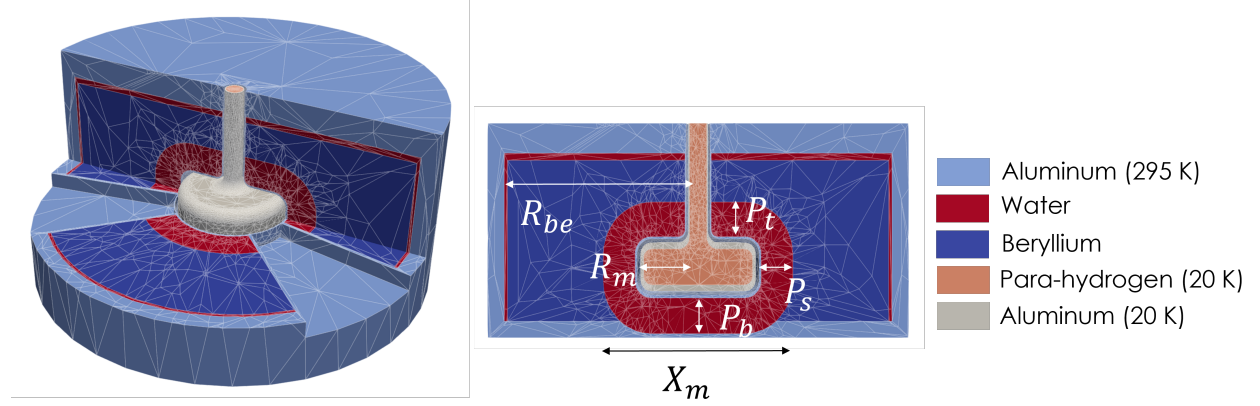


Figure 1. Model of the cylindrical moderator with indication of the parameters and materials.

2.3 TUBE MODERATOR MODEL

Figure 2 provides details about the model of the tube moderator. Three cylinders with cold para-hydrogen are surrounded by a water premoderator inside a beryllium reflector. All vessels are made of aluminum. Six geometric parameters can be changed independently within the range indicated between brackets:

- the tube length L_t (120 mm - 180 mm),
- the thickness of the premoderator on the top P_t (10 mm - 35 mm),
- the thickness of the premoderator on the right side P_r (25 mm - 35 mm),
- the thickness of the premoderator on the bottom P_b (10 mm - 35 mm),
- the thickness of the premoderator on the left side P_l (10 mm - 35 mm),
- the radius of the beryllium reflector R_{be} (175 mm - 200 mm).

The parameter X_m that moves the moderator reflector assembly along the incident beam axis with regard to the target cannot be chosen independently of the value of the cylindrical moderator. In this study, the optimization runs for the tube moderator are calculated with a constant value of X_m . Previous analysis showed that the optimal value is the same as for the cylindrical moderator [11].

2.4 TARGET MODEL AND PROTON BEAM PROFILE

The rotating STS target consists of 20 individual, rotating target blocks. Each block consists of 16-mm thick tungsten plates (58 mm high), separated by thin 0.5-mm tantalum plates, surrounded by a 2-mm thick copper layer and encased in a water-cooled inconel shroud [12]. Figure 3 shows the geometry and meshing of the MCNP model of the target. Also the positioning of the moderators w.r.t. the target is shown. Surrounding the target and moderators is a mixture of steel (95%) and water (5%) modeled in Constructive

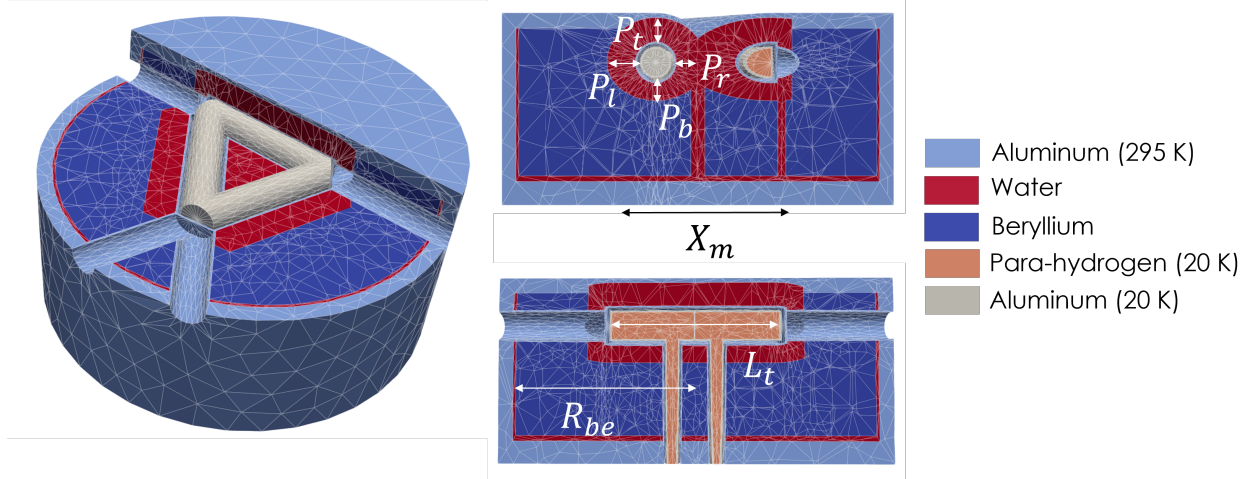


Figure 2. Model of the tube moderator with indication of the parameters and materials.

Solid Geometry (CSG) to represent the cooled shielding that surrounds the target-moderator assembly, see [3] for more details. In order to speed up the MCNP calculations, the simulation considers only three stationary, neighboring target blocks. Previous analyses showed that the contribution to the moderator metrics of the other target blocks further away from the proton beam is negligible. Figure 4 gives an impression of the beam profile on the target face. The beam profile has been accurately modeled with a detailed spatial and directional distribution, based on particle data from accelerator beam profile simulations performed by the STS accelerator system group. This profile has a beam footprint of 60 cm^2 , i.e. 95% of the protons hit the target face within an area of 60 cm^2 .

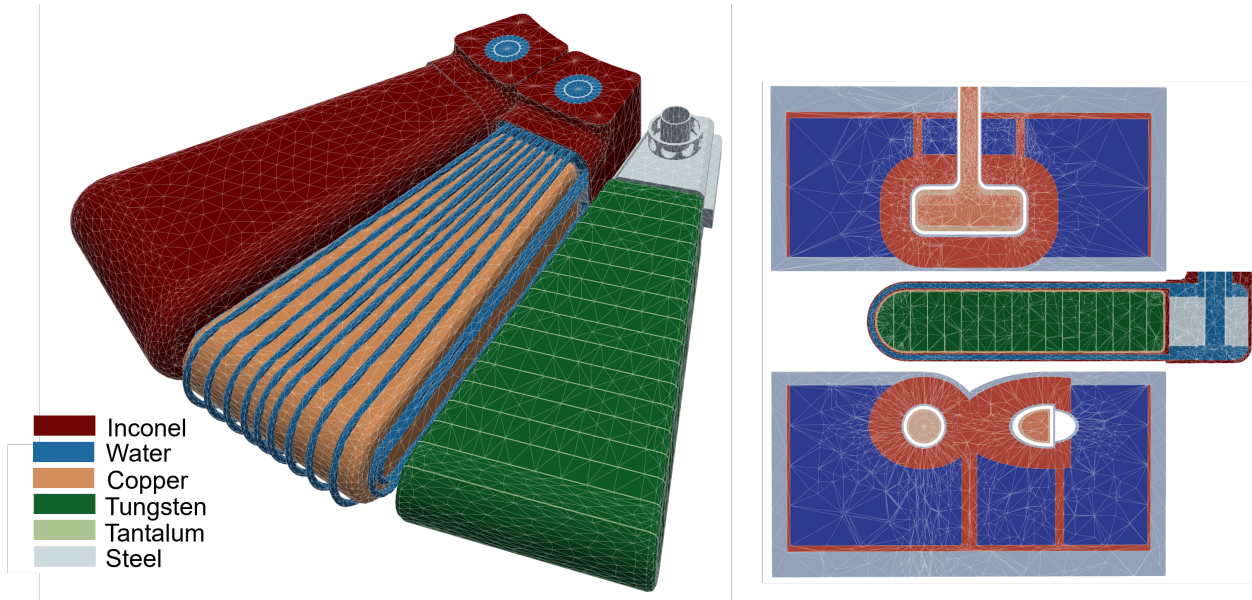


Figure 3. Model of the target with indication of the materials and relative position of the moderators ($X_m = 0 \text{ cm}$).

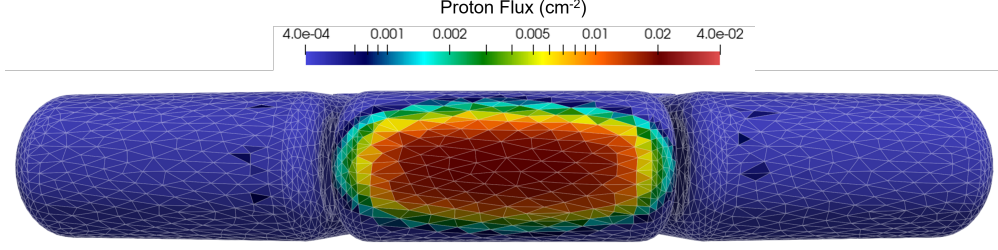


Figure 4. Proton flux on target face.

2.5 BRIGHTNESS METRICS FOR MULTI-OBJECTIVE OPTIMIZATION

The cylindrical moderator provides neutrons to twelve beamlines through four 30 mm by 30 mm openings, while the tube moderator has six circular openings with a 30 mm radius to deliver neutrons to six beamlines. For each moderator, an MCNP point detector tally is placed in one of their beamlines at 10 meters away from the moderator surface. A collimator, simulated using zero importance zones, ensures that only neutrons emitted from the viewed surface of the moderator are tallied. The PEAK brightness metric is defined as the integral of the peak values of the neutron flux up to 10 meV reached in one pulse. The TINT brightness metric is defined as the integral of all neutrons in one pulse for a neutron energy up to 10 meV. A detailed description of the brightness metrics can be found in [13]. A higher PEAK is typically achieved with smaller moderators, while a higher TINT requires a larger moderator. The ideal moderator, however, has both a maximized PEAK and TINT brightness. To consider the trade-off between these two objective, the objective function for the optimization is defined as:

$$\text{Objective} = w_1 \frac{\text{PEAK}}{\text{PEAK}_{\max}} + (1 - w_1) \frac{\text{TINT}}{\text{TINT}_{\max}}, \quad (1)$$

with $\text{PEAK}_{\max}$ and $\text{TINT}_{\max}$ the maximal values that have been obtained for PEAK and TINT respectively. For w_1 , we consider five values: 0, 0.25, 0.5, 0.75, and 1. The resulting five optimal designs are referred to as the Pareto front. When the dimensions are optimized for $w_1 = 0.5$, the optimal combination of both objectives is reached. This is the preferred objective function for the STS moderators based on the feedback from instrument scientists. We refer to this combined metric with $w_1 = 0.5$ as COMB.

3 ANALYSIS AND RESULTS

3.1 CYLINDRICAL MODERATOR

In this section we show the results of the optimization and sensitivity analysis of the cylindrical moderator. Figure 5 shows the relative PEAK and TINT brightness metrics for all samples of the optimization run (black dots), the Pareto front (blue stars), and the configuration that corresponds with the optimal parameters from the 2022 analysis (red star). The parameters associated with the designs on the Pareto front are listed in Table 1 as well as the optimal parameters from the 2022 analysis. A note on the reference values used in the plot is included in appendix D. As expected, the optimal dimensions of the TINT-optimized moderator (with $w_1=0$) are larger than those of the PEAK-optimized design (with $w_1=1$). With a combined objective function ($w_1=0.25$ or 0.5 or 0.75), intermediate dimensions are optimal. The design with $w_1=0.5$ is preferred as the optimal design as both the PEAK and TINT metrics are high ($\geq 95\%$).

of their maximum attainable), while for both PEAK- and the TINT-optimized design, the other metric decreases to $<90\%$ of its maximal attainable value.

Figures 6, 7, and 8 show the results of the parameter study around the optimal designs with $w_1 = 0, 0.5$, and 1 in respectively green, blue and red. In addition to the sensitivity of PEAK and TINT to the parameters in Figures 6 and 7, Figure 8 shows the sensitivity of COMB to the parameters. From Table 1 and the upper right plots in the figures, we clearly see the trade-off that needs to be made between the PEAK and TINT objectives. PEAK is optimized for small moderator radii R_m , while TINT is optimized for larger radii. The COMB metric is highest at intermediate values. The same is visible for the side and bottom premoderator thicknesses P_s and P_b , although less pronounced than with the moderator radius. The metrics have only a very small sensitivity to the top premoderator thickness P_t , the beryllium radius R_{Be} and the position of the moderator X_m . As many of the sensitivities are low, many designs exist that have brightness metrics within 1% of the optimum. This includes the design with the optimal parameters of 2022. We conclude that the model revisions with the new target design do not significantly affect the optimal dimensions of the cylindrical moderator.

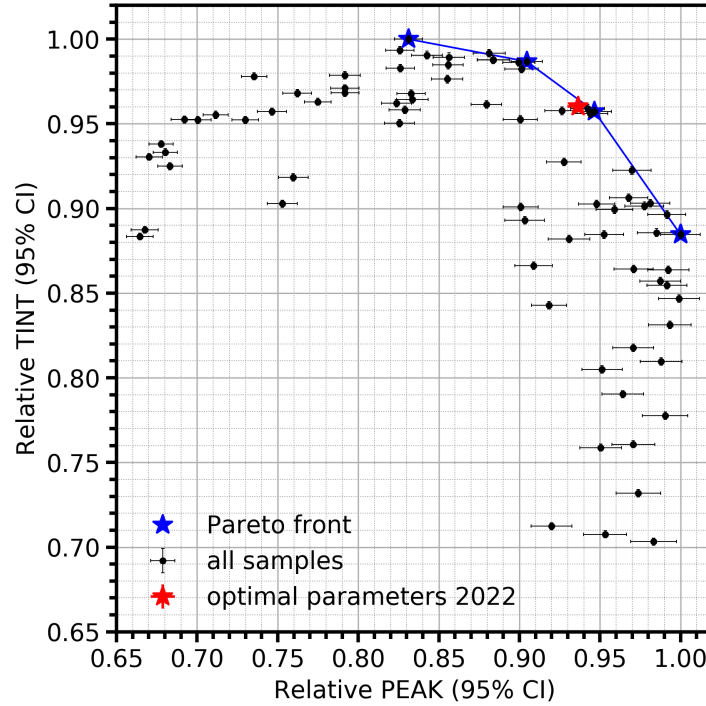


Figure 5. Pareto plot for the optimization of the cylindrical moderator. The black dots, blue stars and red star indicate respectively the results of all samples, the Pareto front, and the design with the optimal parameters of 2022.

w_1	R_m (mm)	P_s (mm)	P_b (mm)	P_t (mm)	R_{Be} (mm)	X_m (mm)	PEAK ($\text{cm}^{-2}\text{s}^{-1}$)	TINT (cm^{-2})
0	61.4	31.7	30.6	23.7	190.4	3.3	7.07E-5	1.67E-08
0.25	55.0	28.9	30.3	22.9	188.1	6.7	7.69E-5	1.65E-08
0.5	50.0	27.9	30.1	22.5	186.1	2.2	8.05E-5	1.60E-08
0.75	43.3	27.1	30.0	21.5	187.4	7.6	8.50E-5	1.48E-08
1	43.3	27.1	30.0	21.5	187.4	7.6	8.50E-5	1.48E-08
Optimal parameters 2022								
0.5	50	29	30	29	175	0	7.96E-13	1.61E-8

Table 1. Optimal parameters and brightness metrics of the designs on the Pareto front for the cylindrical moderator. The optimal parameters of 2022 are listed as well.

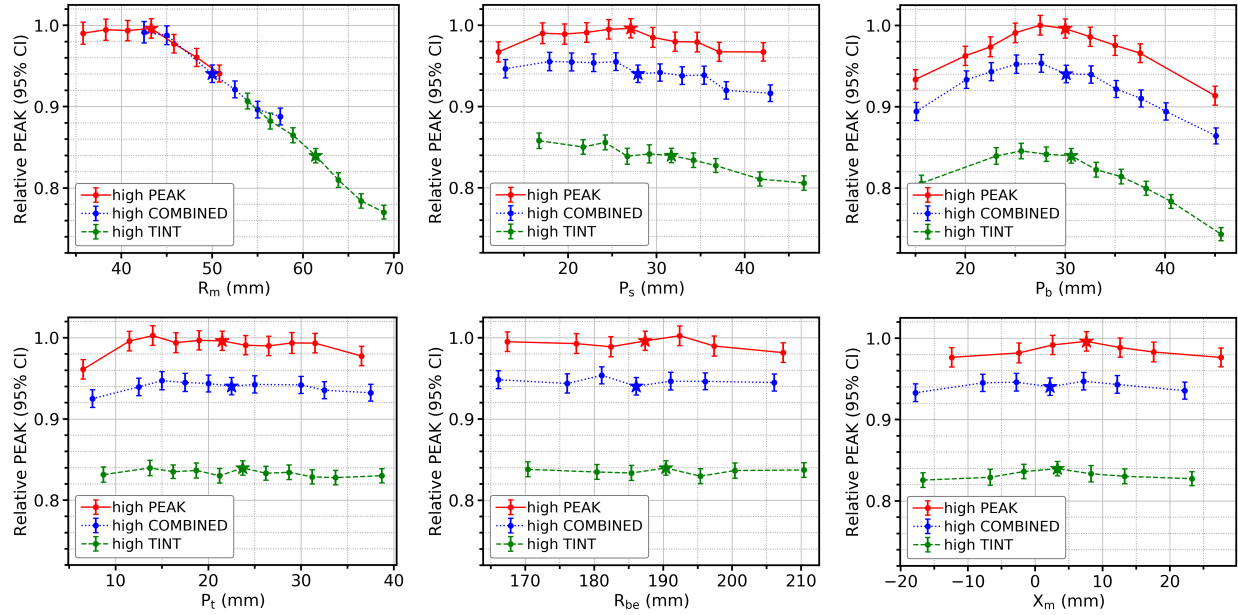


Figure 6. Relative PEAK brightness metric as a function of each of the parameters for the cylindrical moderator for three designs, optimized for respectively PEAK (red line), COMB (blue line), and TINT (green line).

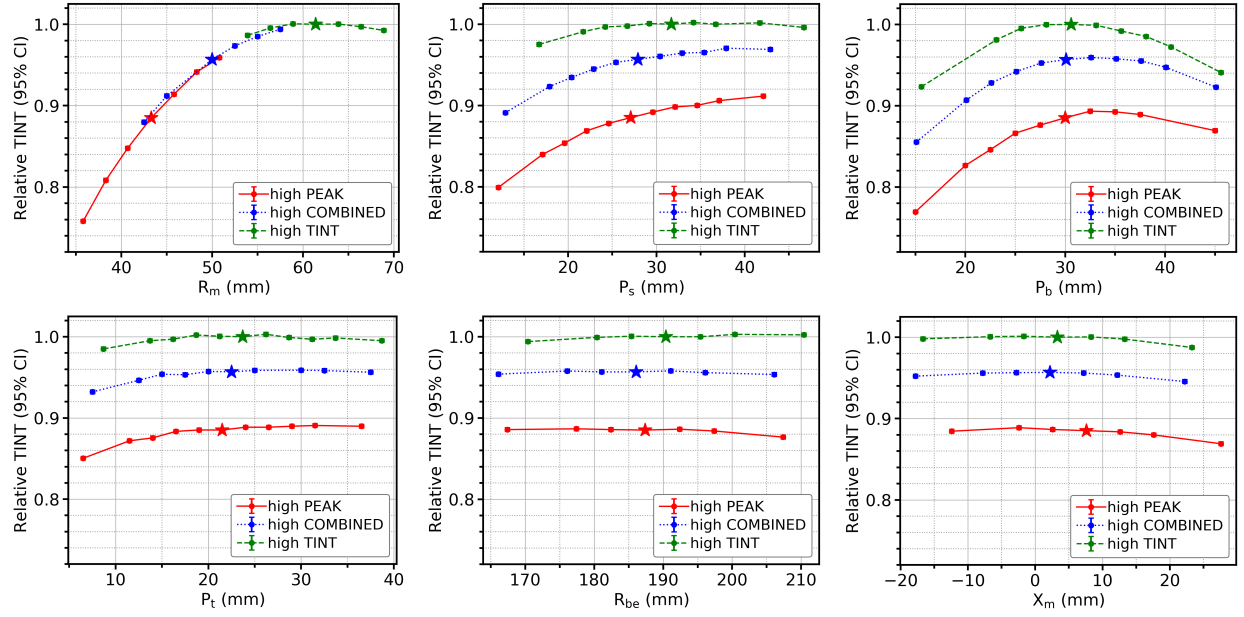


Figure 7. Relative TINT brightness metric as a function of each of the parameters for the cylindrical moderator for three designs, optimized for respectively PEAK (red line), COMB (blue line), and TINT (green line).

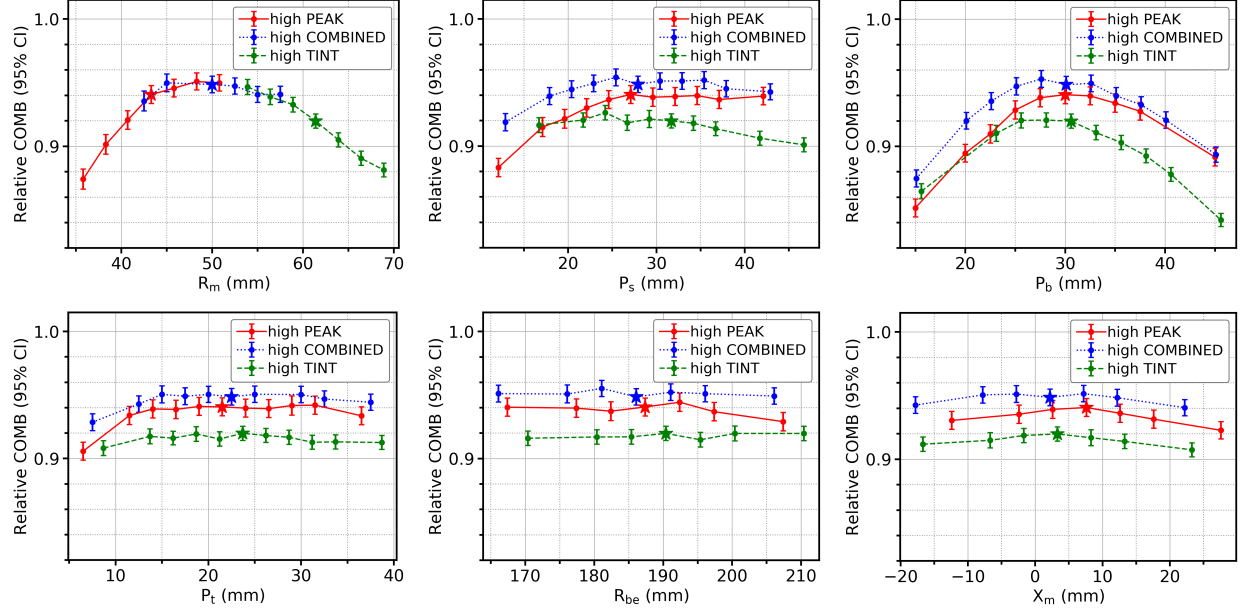


Figure 8. Relative COMB brightness metric as a function of each of the parameters for the cylindrical moderator for three designs, optimized for respectively PEAK (red line), COMB (blue line), and TINT (green line).

3.2 TUBE MODERATOR

In this section we show the results of the optimization and sensitivity analysis of the tube moderator. Figure 9 shows the relative PEAK and TINT brightness metrics for all samples of the optimization run (black dots), the Pareto front (blue stars), and the configuration that corresponds with the optimal parameters from the 2022 analysis (red star). The parameters associated with the designs on the Pareto front are listed in Table 2 as well as the optimal parameters from the 2022 analysis. A note on the reference values used in the plot is included in appendix D. Figures 6, 11, and 12 show the results of the parameter study around the optimal designs with $w_1 = 0.5$ and 1 in respectively blue and red, and around the high TINT design as listed in the last row of Table 2 in green. The high TINT design has a tube length outside of the parameter range of the optimization. The parameter choice is based on the optimized values of the previous analysis [11]. In addition to the sensitivity of PEAK and TINT to the parameters in Figures 10 and 11, Figure 12 shows the sensitivity of COMB to the parameters. Inspection of the list of the parameters of the Pareto front in Table 2 reveals large differences in the choice of the different premoderator thicknesses, which were not considered in the 2022 analysis. Similar to the results of the cylindrical moderator, the trade-off between PEAK and TINT is determined mostly by the choice of the moderator dimension, in this case the tube length T_l . Also the top premoderator thickness P_t , which determines the distance between the target and the moderator, has a large effect on the values of the brightness metrics, followed by the premoderator thickness on the left and the bottom, P_l and P_b . The beryllium radius R_{Be} and the premoderator thickness on the right P_r have a very small effect on the metrics in the considered range.

In Appendix C, an additional optimization study was performed to further investigate the effect of the premoderator thicknesses. This analysis showed similar values for the optimal premoderator thicknesses as well as a performance increase of 2% compared to the design with the optimal thicknesses of the 2022 analysis. Part of this performance increase can, however, be due to the statistical precision.

w_1	T_l (mm)	P_t (mm)	P_r (mm)	P_b (mm)	P_l (mm)	R_{Be} (mm)	X_m (mm)	PEAK ($\text{cm}^{-2}\text{s}^{-1}$)	TINT (cm^{-2})
0	179.7	27.3	29.2	21.1	34.1	199.0	5	7.59E-5	2.13E-08
0.25	179.7	27.3	29.2	21.1	34.1	199.0	5	7.59E-5	2.13E-08
0.5	166.7	26.6	29.1	20.0	33.6	194.4	5	7.82E-5	2.10E-08
0.75	140.0	26.2	35.0	19.1	33.4	184.9	5	8.16E-5	1.99E-08
1	120.0	25.2	31.1	21.6	26.7	191.7	5	8.17E-5	1.82E-08
Optimal parameters 2022									
0.5	170	27.5	27.5	27.5	27.5	175	0	7.58E-5	2.06E-08
High TINT configuration for parameter study									
-	205	27.5	35	14	33	200	5	7.24E-5	2.16E-08

Table 2. Optimal parameters and brightness metrics of the designs on the Pareto front for the tube moderator. The optimal parameters of 2022 and the parameters of the high TINT design for the parameter study are listed as well.

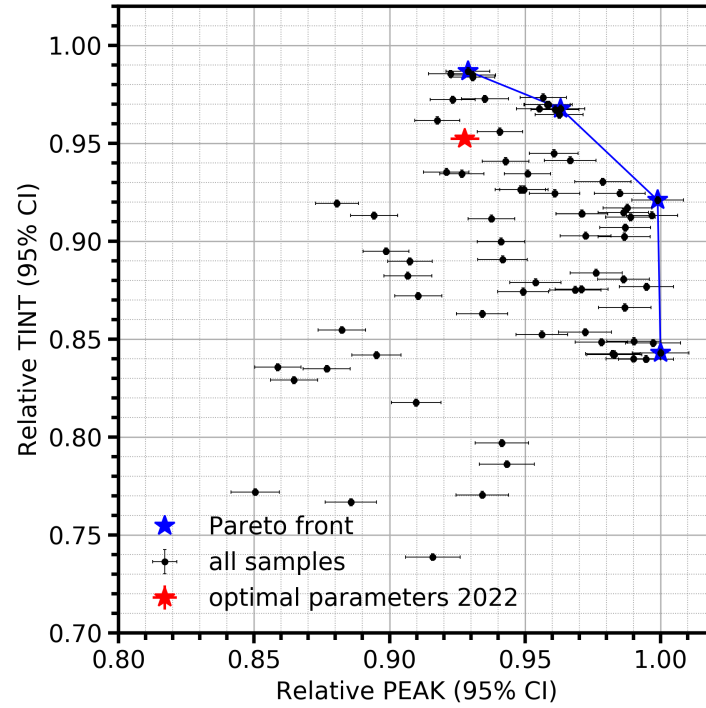


Figure 9. Pareto plot for the optimization of the tube moderator. The black dots, blue stars and red star indicate respectively the results of all samples, the Pareto front, and the design with the optimal parameters of 2022.

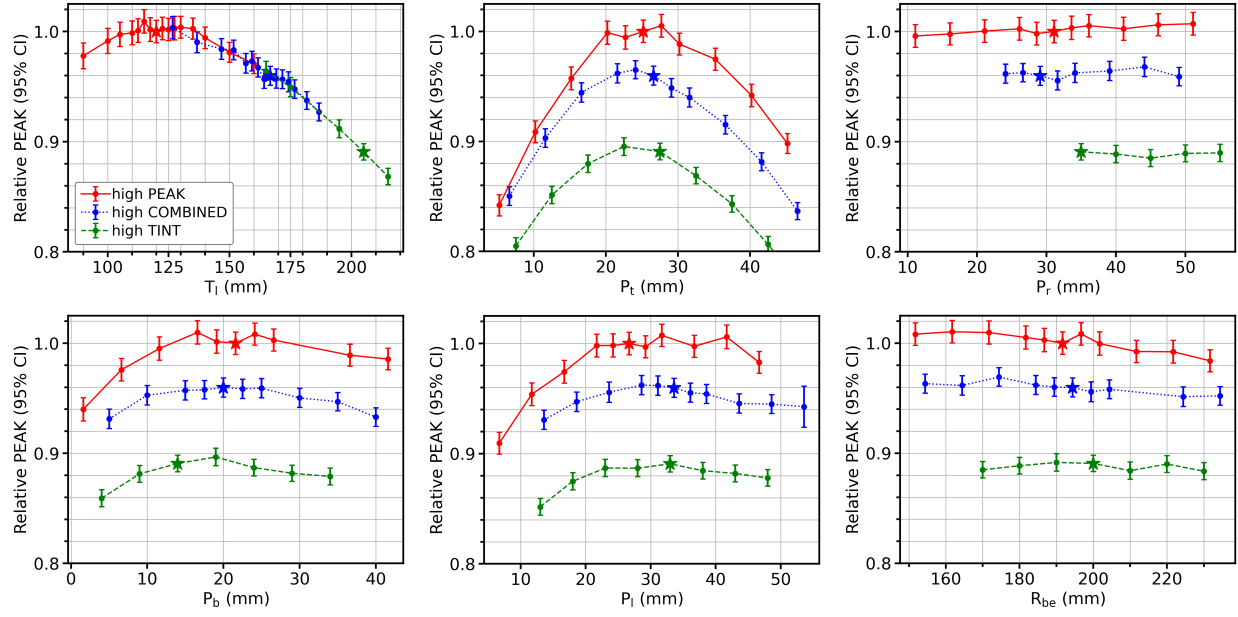


Figure 10. Relative PEAK brightness metric as a function of each of the parameters for the tube moderator for three designs, optimized for respectively PEAK (red line), COMB (blue line), and TINT (green line).

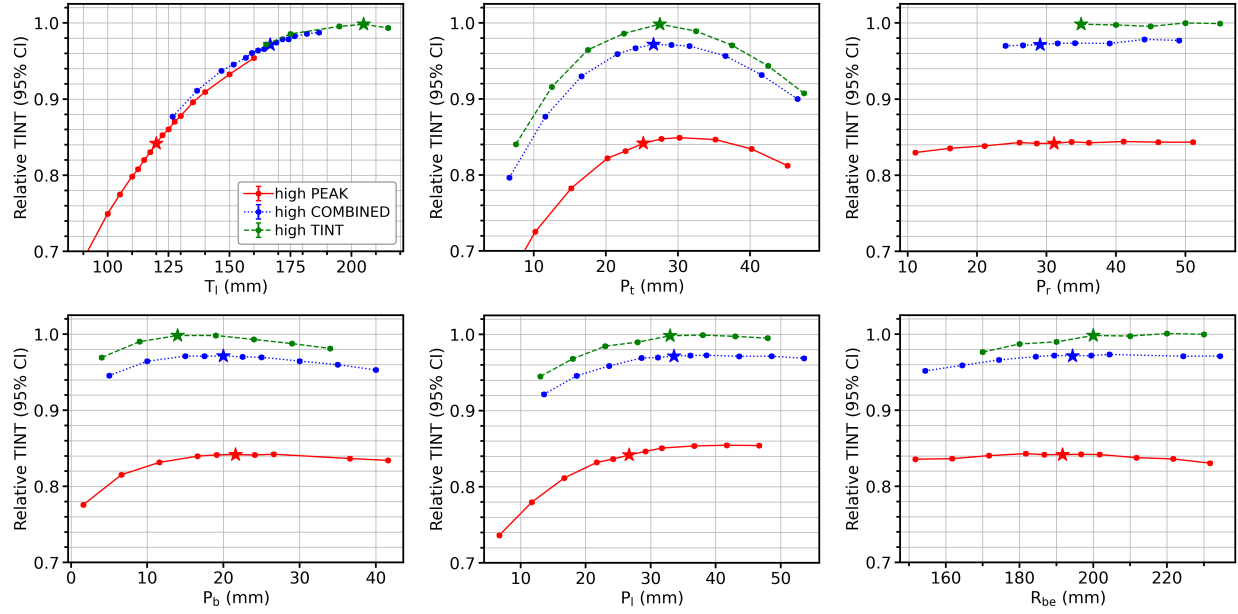


Figure 11. Relative TINT brightness metric as a function of each of the parameters for the tube moderator for three designs, optimized for respectively PEAK (red line), COMB (blue line), and TINT (green line).

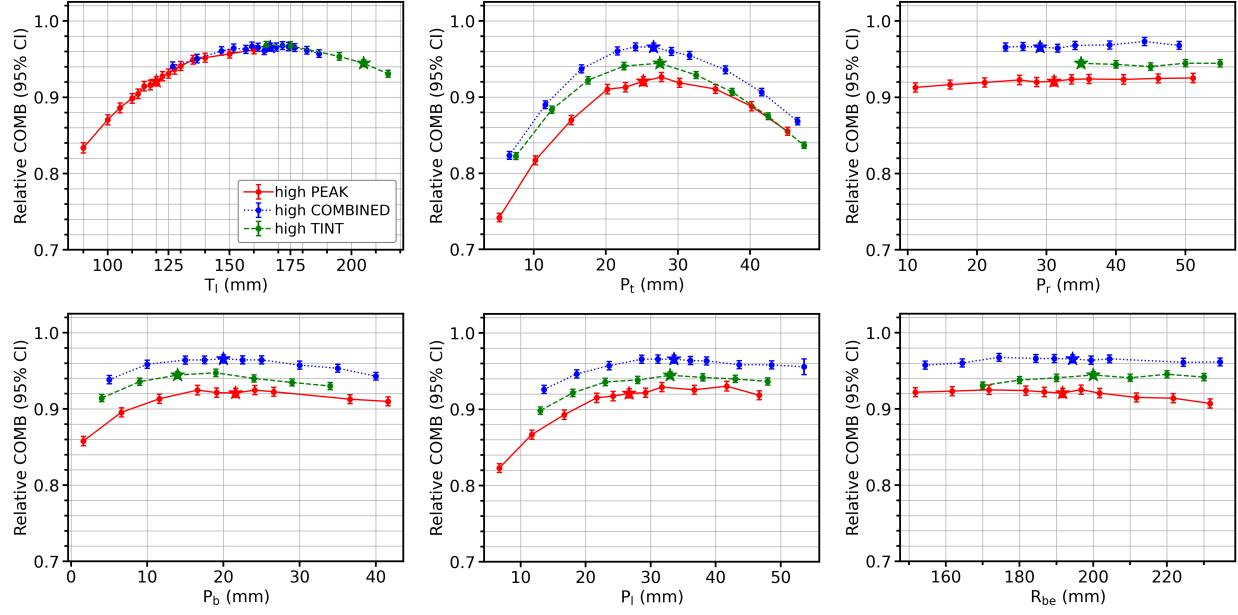


Figure 12. Relative COMB brightness metric as a function of each of the parameters for the tube moderator for three designs, optimized for respectively PEAK (red line), COMB (blue line), and TINT (green line).

4 CONCLUSIONS

We performed an optimization analysis with updated target and moderator models for the final design of the STS moderators. The dimensions of the cylindrical remain unchanged to the 2022 optimized design and are based on the optimal combined metric COMB. For the tube moderator, the premoderator dimensions have been updated which leads to a small performance increase ($\leq 2\%$) compared to a uniform premoderator dimension. The final selection of the parameters is listed in Table 3.

Table 3. Final parameter selection for the cylindrical and tube moderator.

	R_m (mm)	P_s (mm)	P_b (mm)	P_t (mm)		R_{Be} (mm)	X_m (mm)	PEAK ($\text{cm}^{-2}\text{s}^{-1}$)	TINT (cm^{-2})
Cylindrical moderator	50	29	30	29		175	0	8.04E-5	1.61E-8
	T_l (mm)	P_t (mm)	P_r (mm)	P_b (mm)	P_l (mm)	R_{Be} (mm)	X_m (mm)	PEAK ($\text{cm}^{-2}\text{s}^{-1}$)	TINT (cm^{-2})
Tube moderator	170	26.5	30	20	32	175	0	7.66E-5	2.07E-8

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APPENDIX A. COMPUTER HARDWARE AND SOFTWARE

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The mcnp module loaded on Saturn is

mcnp/mcnp6.2mod_20231115

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APPENDIX B. LOCATION OF COMPUTATIONAL INPUT AND OUTPUT FILES

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The main input and output files are archived in

sts_archive/S.03.04_Mod/Optimization_2024_FinalDesign/

on Saturn.

**APPENDIX C. ADDITIONAL OPTIMIZATION TO INVESTIGATE
OPTIMAL PREMODERATOR THICKNESSES FOR TUBE
MODERATOR**

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An additional optimization is performed to further investigate the optimal premoderator thicknesses. The tube length, beryllium radius, and moderator shift are kept constant at 170 mm, 175 mm, and 0 mm, respectively. A pareto set optimization with several values of w_1 was performed. However, the resulting designs do not show a consistent trend in parameters, but just one optimal configuration, which is given in Table 4. This often occurs when the sensitivity of the maximum to the parameters is low. Figure 13 shows the relative PEAK and TINT brightness metrics for all samples of the optimization run (black dots), the optimal configuration (blue star), and the configuration that corresponds with the optimal parameters from the 2022 analysis (red star). Figures 14 and 15 show the relative PEAK and TINT brightness metrics for all samples of the optimization run. This gives an impression of the sensitivity of the brightness metrics to each of the parameters. This is, however, not a parameter study as all premoderator thicknesses are chosen differently in each of the samples instead of changing one parameter while keeping the others constant. These results confirm that a better choice of premoderator thicknesses increases the moderator performance metrics by approximately 2%. Some of this increase, however, may be due to statistical uncertainty.

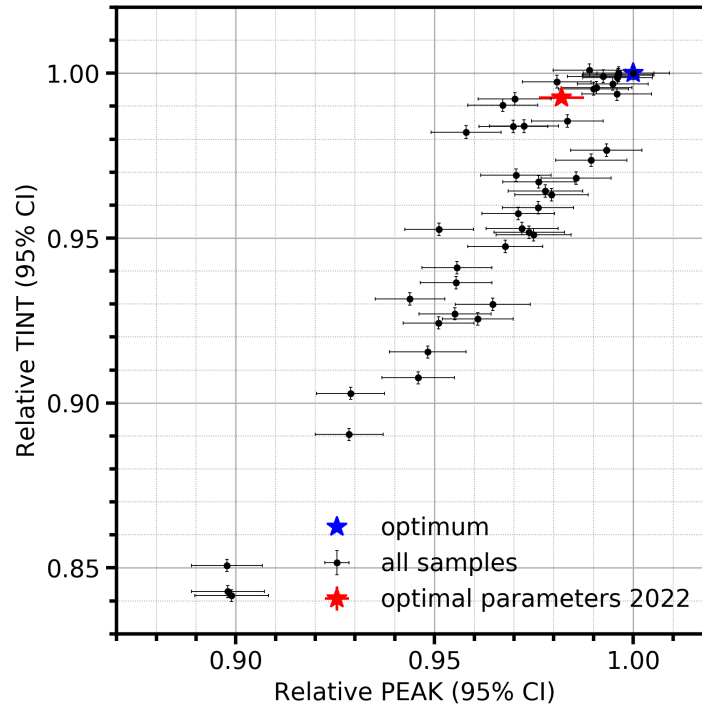


Figure 13. Plot of all runs of additional tube moderator optimization study of the premoderator thicknesses. The black dots, blue star and red star indicate respectively the results of all samples, the optimum, and the design with the optimal parameters of 2022.

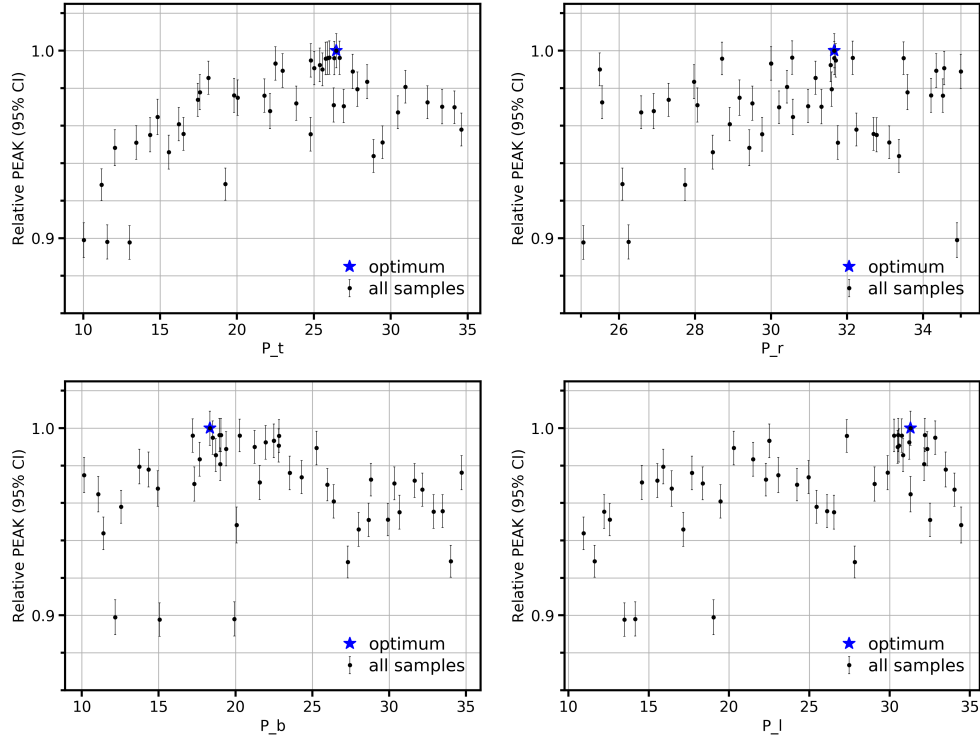


Figure 14. Relative PEAK brightness metric as a function of each of the parameters for the tube moderator for all samples in the optimization run. The black dots and blue star indicate respectively the results of all samples and the optimum.

Table 4. Optimum and reference parameters of 2022 for additional analysis of the tube moderator.

	T_l (mm)	P_t (mm)	P_r (mm)	P_b (mm)	P_l (mm)	R_{Be} (mm)	X_m (mm)	PEAK ($\text{cm}^{-2}\text{s}^{-1}$)	TINT (cm^{-2})
Optimum	170	26.5	31.7	18.3	31.3	175	0	7.72E-5	2.07E-8
Parameters 2022	170	27.5	27.5	27.5	27.5	175	0	7.58E-5	2.06E-8

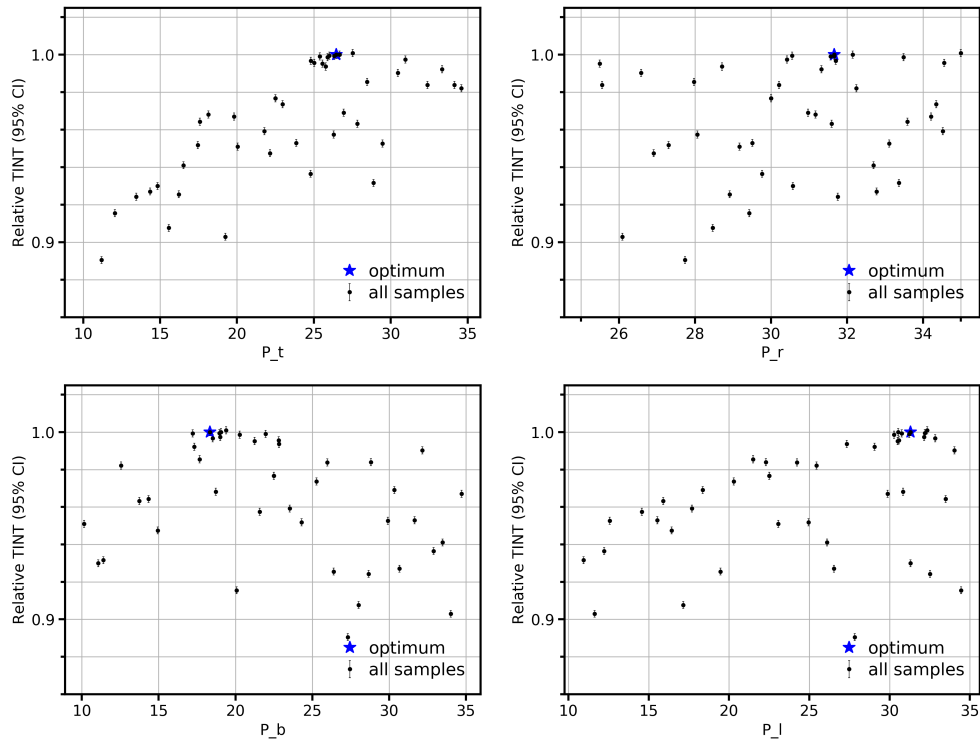


Figure 15. Relative TINT brightness metric as a function of each of the parameters for the tube moderator for all samples in the optimization run. The black dots and blue star indicate respectively the results of all samples and the optimum.

**APPENDIX D. NOTE ON THE REFERENCE VALUES USED IN THE
FIGURES**

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Cylindrical moderator Both the reference for PEAK and TINT are taken a posteriori from the results of the Pareto set run (see Table 1). This is evident from Figure 5, in which the Pareto front $w_1 = 0$ and $w_1 = 1$ numbers are exactly 1 on TINT and PEAK respectively.

For the parameter study, the baseline design (around which the parameter study is performed) is evaluated again in MCNP, however, with values for the parameters that are rounded compared to the output of the Pareto set run. The resulting PEAK and TINT are statistically equivalent, but since the relative error for PEAK is about 0.7%, this results in a visible difference on the plot (Figures 6, 7, and 8).

For COMB, equation 1 is used with $w_1=0.5$. Therefore, the optimal middle configuration has the following value for the COMB metric:

$$\text{COMB} = 0.5 \frac{8.05\text{E-}5}{8.50\text{E-}5} + 0.5 \frac{1.6\text{E-}8}{1.67\text{E-}8} = 0.9526. \quad (2)$$

For COMB to be 1 (as defined here), the design would have to achieve both the maximal PEAK value and the maximum TINT value, which is of course not possible. The plot does not have COMB exactly at 0.9526 because of the statistical precision.

Tube moderator The reference for PEAK is taken a posteriori from the results of the Pareto set run (see Table 2). This is evident from Figure 9, in which the optimal design with $w_1 = 1$ is exactly 1 for PEAK. For the reference for TINT, the result from the Pareto set run (for the design with a tube length of approximately 180 mm) was extrapolated based on previous analysis to the best-guess value at a tube length of 205 mm, where the TINT optimum is expected. For the parameter study in Figures 10, 11, and 12 again slight statistical variations are expected.

