OPTIMIZATION OF A BI-SPECTRAL BOXED SIDE-BY-SIDE MODERATOR FOR THE TARGET-MODERATOR-REFLECTOR SYSTEM OF THE ESS

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Abstract

Providing bi-spectral neutron beams is one of the main neutronics design criteria for the target-moderator-reflector system (TMR) of the European Spallation Source, to be built in Lund (Sweden). As a first step, the requirements of neutron scattering instruments regarding the neutron spectrum are formulated, a Figure of Merit is defined. In order to maximize the moderator performance to obtain bi-spectral neutron extraction, a parametrized model of the TMR is developed and used within a MCNPX-based optimization framework. This model is then used to study and optimize the moderator performance, especially in the thermal and cold parts of the spectrum. Results obtained with an optimized moderator setup are dicussed and compared with the requirements of the instruments.

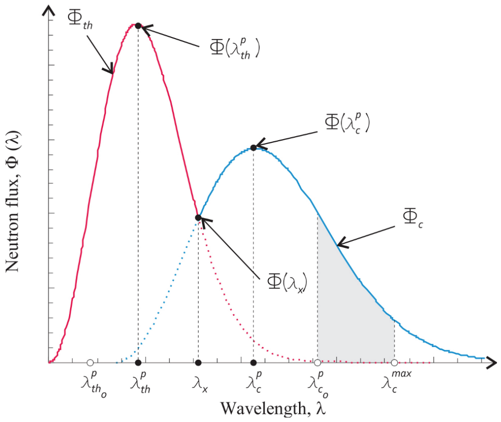

Figure 1: Graphical representation of a bi-spectral neutron spectrum.

INTRODUCTION

At a spallation neutron source [1], significant increase in the performance of the neutron scattering instruments can be achieved if the target-moderator-reflector system (TMR) and the following neutron guides are specifically tailored to the needs of the instruments. In order to define optimal quantities for the Figure of Merit (FoM), a survey has been conducted at Paul Scherrer Institut (PSI) covering the experience of the local instrument scientists which includes also the opinion of the visiting users. Based on this survey we have formulated the optimal neutron spectrum which has two peaks, one in the thermal and one in the cold part (Fig. 1). Furthermore, the maxima should be located between 1.3 and 1.5 Å and at 4.1 Å for the thermal and cold parts, respectively, i.e.

$$1.3\,\text{Å} < \lambda^p_{th_0} < 1.5\,\text{Å},\ \lambda^p_{c_0} = 4.1\,\text{Å} \tag{1}$$

In the best case the relations

$$|\lambda^p_{th} - \lambda^p_{th_0}| \simeq 0,\ |\lambda^p_c - \lambda^p_{c_0}| \simeq 0 \tag{2}$$

should be valid at the same time. It should be mentioned that thermal neutron scattering instruments prefer a maximum at 1.0 Å. On the other hand, the limits given in Eq. 1 are acceptable as long as there is a significant increase in the thermal tail. Additionally, an optimum bi-spectral moderator setup should ensure similar measurement times if either thermal or cold neutrons are used. To be more precise, a maximum factor of 3 between the peak values is acceptable. Thus, the peak values of the neutron flux in the thermal and cold parts of the spectrum have to be maximized.

$$\begin{aligned} \Phi(\lambda^p_{th}) = \text{MAX},\ \Phi(\lambda^p_c) = \text{MAX}, \\ |\Phi(\lambda^p_{th}) - k_1 \times \Phi(\lambda^p_c)| \simeq 0, \end{aligned} \tag{3}$$

where $0.3 < k_1 < 3$.

Besides the above mentioned three criteria, more can be formulated, e.g. maximize the integral neutron flux in specific wavelength bands or position the crossing point between the thermal and cold peaks. The criteria (correct positions of peak fluxes, maximizing peak fluxes, etc.) formulated above have to be properly weighted for an optimal FoM. However, since the instrument parameters planned for the ESS are currently not fixed yet, we took a different approach. Namely, by focusing separately on each criteria we show that the neutron spectrum can be varied in a wide range. As an example, the top moderator of the ESS (Table 1) is chosen for optimization. A parametrized geometrical model of the ESS TMR is built in MCNPX2.7.0 [2] and used within an optimization framework that consists of MCNPX for particle transport simulation, the stand-alone optimizer program that evaluates the FoM value and defines the optimization path in the parameter space, and the automated generator of the input files together with enclosing control scripts [3].

CALCULATIONAL MODEL

The top moderator of the ESS TMR is modelled as a box-shaped (12×24×12 cm^3 for thickness, width and height) double-walled AlMg3 can (0.3 cm wall thickness)

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Table 1: Baseline Parameters of the ESS Pulse [4]

Parameter	Unit	Value
Proton kinetic energy, E	GeV	2.5
Average beam power, P	MW	5
Pulse repetition frequency, f	Hz	14
Macro-pulse length, τ	ms	2.857

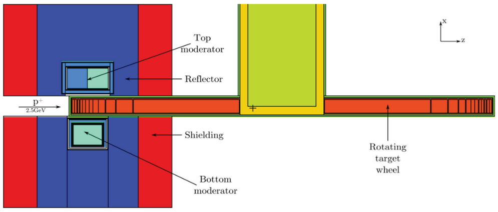

Figure 2: MCNPX model of the ESS TMR.

containing liquid para-hydrogen (20 K) and ambient temperature light water in side-by-side arrangement. The void gap between the moderator and the pre-moderator is 0.5 cm. The pre-moderator encloses the moderator on 4 sides leaving the beam ports open. The void gap between the lower pre-moderator and the target is 1.1 cm. The cylindrical reflector is made of Beryllium surrounded by Iron (Fig. 2). The MCNPX model is parameterized and contains 31 parameters in total which enable the variation of dimensions and materials within the optimization procedure. For the optimization presented in this paper only 3 parameters are used, namely the moderator offset in y and z and the water-to-hydrogen ratio.

$$\Phi_\Omega(\lambda) = \frac{\Phi(\lambda)}{\Omega \cdot \Delta\lambda} \; [\text{n/cm}^2\text{/p/sr/Å}] \tag{4}$$

The optimized quantity is the neutron flux (see Eq. 4) at a point detector (F5 tally) which views the surface (12x24 cm^2) of the moderator with a solid viewing angle of 1.422×10^{-3} sr (Fig. 3).

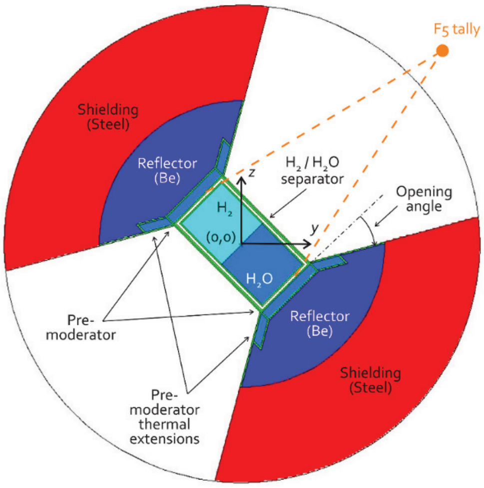

Figure 3: Top view of the side-by-side moderator.

Table 2: Parameter Values after Optimization with Different FoMs

Parameter	FoM$_1$	FoM$_2$	FoM$_3$
Moderator offset in y [cm]	-3.00	-0.97	-0.05
Moderator offset in z [cm]	-5.00	2.03	0.00
H_2/H_2O ratio	0/100	100/0	68/32

Table 3: Results Using Different FoMs

Quantity	FoM$_1$	FoM$_2$	FoM$_3$
λ^p_{th} [Å]	1.03	1.03	1.02
$\Phi_\Omega(\lambda^p_{th})$ [10^{-3} n/cm^2/p/sr/Å]	1.45	0.21	0.37
λ^p_c [Å]	2.46	2.46	2.49
$\Phi_\Omega(\lambda^p_c)$ [10^{-3} n/cm^2/p/sr/Å]	0.21	0.60	0.37

RESULTS

FoMs

First, FoMs for maximizing the thermal and cold peak neutron fluxes are used:

$$\text{FoM}_1 = \Phi(\lambda^p_{th}) \text{ and } \text{FoM}_2 = \Phi(\lambda^p_c) \tag{5}$$

These are obtained if the moderator box is completely filled with either water or liquid para-hydrogen, respectively. These are the limiting cases, i.e. provide the highest possible thermal (red curve in Fig. 4) or cold (blue curve in Fig. 4) neutron flux. However, they do not provide a bi-spectral neutron spectrum. This can be obtained with FoM$_3$

$$\text{FoM}_3 = \min(\Phi(\lambda^p_{th}), \Phi(\lambda^p_c)) \tag{6}$$

aimed at balancing and maximizing the thermal and cold peak neutron fluxes at the same time (green curve in Fig. 4).

Neutron Flux

The optimized parameter values are given in Table 2. The positions and magnitudes of the peak neutron fluxes are summarized in Table 3. The neutron flux using FoM$_1$ is 0.21×10^{-3} n/cm^2/p/sr/Å at 2.46 Å, where the cold peak is found using FoM$_2$. The neutron flux for FoM$_2$ is 0.21×10^{-3} n/cm^2/p/sr at 1.03 Å, where the thermal peak is found using FoM$_1$ lies. Thus, the range of k_1 (see Eq. (3)) is obtained: [0.34 ... 7.07].

The following conclusions can be drawn when comparing the results to the user desired optimal spectrum:

- The position of the thermal peak is slightly shifted to smaller wavelengths.
- The position of the cold peak is clearly at smaller wavelengths.
- The obtained variation of k_1 indicates that there exists an intermediate position of the moderator separator where the thermal and cold peaks are equal. This is achieved when using FoM$_3$ (see green curve in Fig. 4).

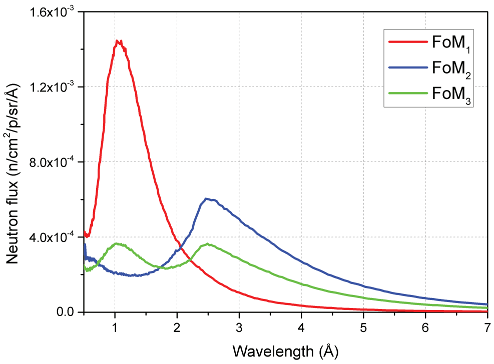

Figure 4: Neutron flux, optimized using different FoMs.

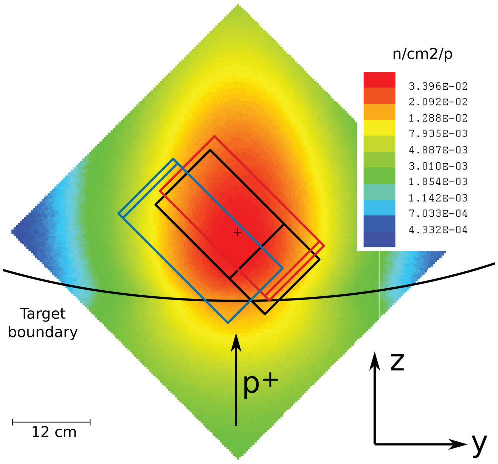

Figure 5: Neutron flux distribution between the target and the top moderator for neutron energies above 1 MeV. The optimized positions of the moderator box above the target are indicated for FoM_1 (blue), FoM_2 (red) and FoM_3 (black). The volume filled with H_2 is the moderator compartment to the left/top.

The fast neutrons produced during spallation are moderated in the water and the liquid hydrogen. Thus, the higher the fast neutron flux coming from the target to the moderator, the higher the cold and thermal flux will be. The fast ($E > 1$ MeV) neutron flux distribution is calculated in the void gap between the target and the moderator (Fig. 5). Since the maximum achievable cold peak neutron flux (0.60×10^{-3} n/cm^2/p/sr/Å) is lower than the maximum achievable thermal peak neutron flux (1.45×10^{-3} n/cm^2/p/sr/Å), when using FoM_3 the separator wall of the moderator box is shifted to increase the volume of the H_2 moderator.

Absolute Peak Brightness

The absolute peak brightness can be calculated by taking into account the proton beam parameters:

$$B(\lambda) = \Phi_\Omega(\lambda) \cdot I_p \ [\text{n/cm}^2\text{/s/sr/Å}] \tag{7}$$

Table 4: Cold and Thermal Absolute Peak Brightness

FoM	λ^p_{th} **[Å]**	**Thermal peak [n/cm²/s/sr/Å]**	λ^p_c **[Å]**	**Cold peak [n/cm²/s/sr/Å]**
FoM_1	1.03	4.52×10^{14}	2.46	0.64×10^{14}
FoM_2	1.03	0.65×10^{14}	2.46	1.89×10^{14}
FoM_3	1.02	1.14×10^{14}	2.49	1.14×10^{14}

where I_p is the peak current:

$$I_p = \frac{P \cdot 6.24 \cdot 10^{18}}{E \cdot f \cdot \tau} = 3.125 \times 10^{17} \text{ protons/s} \tag{8}$$

The peak values for the different FoMs are given in Table 4. Compared to the similar TMR of the LPTS of the ESS 2003 Project [5], and taking into account the differences in the pulse repetition frequency and macro-pulse length, the values are similar. On the other hand, bi-spectrality has its price, namely a lower cold neutron flux compared to pure H_2 moderators, e.g. [6] reports 2.35×10^{14} n/cm^2/s/sr/Å at 2 Å.

SUMMARY

The developed MCNPX-based optimization framework has been successfully applied to the TMR of the ESS, which included a box-shaped side-by-side moderator. Several FoM options have been presented showing the potential of the developed method. Further investigations with improved FoMs are planned taking into account the different criteria of the bi-spectral spectrum with proper weighting factors according to the instrument needs.

ACKNOWLEDGMENT

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