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Unperturbed moderator brightness in pulsed neutron sources

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ABSTRACT

The unperturbed neutron brightness of a moderator can be defined from the number of neutrons leaving the surface of a moderator completely surrounded by a reflector. Without openings for beam extraction, it is the maximum brightness that can be theoretically achieved in a moderator. The unperturbed brightness of a cylindrical cold moderator filled with pure para-H_2 was calculated using MCNPX; the moderator dimensions were optimised, for a fixed target and reflector geometry corresponding to the present concept for the ESS spallation source. This quantity does not depend on openings for beam extraction and therefore can be used for a first-round optimisation of a moderator, before effects due to beam openings are considered. We find that such an optimisation yields to a factor of 2 increase with respect to a conventional volume moderator, large enough to accommodate a viewed surface of 12×12 cm^2: the unperturbed neutron brightness is maximum for a disc-shaped moderator of 15 cm diameter, 1.4 cm height.

The reasons for this increase can be related to the properties of the scattering cross-section of para-H_2, to the added reflector around the exit surface in the case of a compact moderator, and to a directionality effect. This large optimisation gain in the unperturbed brightness hints towards similar potentials for the perturbed neutron brightness, in particular in conjunction with advancing the optical quality of neutron delivery from the moderator to the sample, where by Liouville theorem the brightness is conserved over the beam trajectory, except for absorption and similar type losses.

1. Introduction

The European Spallation Source (ESS), which entered in the construction phase in 2013 in Lund, Sweden, aims at starting operations and delivering the first neutrons in 2019 [1]. At 5 MW time average power, and 125 MW peak power, ESS will be the most powerful neutron source in the world for neutron scattering studies of condensed matter. Neutrons will be produced by a 2.5 GeV proton beam impinging on a target made of tungsten. ESS will be the first high-power long pulse source [2], the pulse length of the beam will be of 2.86 ms, with 14 Hz repetition rate.

A key for a highly performing neutron source is the optimisation of the configuration of the target, moderator and reflector assembly [3]. The use of tungsten as spallation material will ensure a high neutron yield per incoming proton; the high density of tungsten favours the production of neutrons in a small volume, increasing the probability that neutrons will eventually be slowed down by the moderators placed next to the target. The presence of a reflector surrounding the moderators is essential to increase the neutron intensity from the moderators. For a long pulse facility such as ESS, the recommended moderator type is a coupled, pure para-H_2 moderator [4], because it delivers the highest brightness per proton. The coupling between moderator and reflector (i.e. the absence of any neutron absorbing material to shape the pulse length) guarantees the highest peak flux from the moderator surface; pulses are shaped in time by choppers placed in the beam lines.

The goal of the neutronic optimisation is to determine the configuration that delivers the largest spectral brightness in the wavelength region of interest. The brightness of a neutron source is the number of neutrons emitted per unit time, per unit solid angle, per unit energy (or wavelength), per unit area of the surface. Unlike the flux, the brightness of a neutron beam does not depend on the distance from the source: it is therefore a quantity that characterises the neutron source and depends on its design. Requirements coming from the beam extraction (such as needed viewed moderator surface, and number of beam ports) influence the design choices. In fact, neutrons are extracted via the beam extraction system, consisting of beam ports with neutron guides starting at about 2 m from the moderator surface. Openings in the reflector allow for viewing the surface of the moderators. The angular coverage of the openings, and their positioning, affect the overall performance of the moderator. Other requirements that have an effect on moderator design come from engineering, such as heat load on the moderator cryogenic parts.

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Ultimately, the overall performance of a neutron source depends on the source brightness, the moderator surface area, and the quality of neutron optics, which is inherently poorer than light optics. In case of perfect optics with unlimited aperture, the best solution would be a source of some reasonable size with maximum brightness, which could be imaged without losses to the sample, eventually magnified or reduced. In this paper we aim at discussing and optimising the brightness of a moderator without considering perturbation by the beam extraction system, and the problem of beam optics.

2. Unperturbed moderators

2.1. Unperturbed moderator brightness

Cold moderators in high-power spallation sources such as SNS [5] and JSNS at J-PARC [6] consist of volumes of liquid H_2 surrounded by reflector material, typically Be. In order to extract the neutrons, openings must be placed in the reflector. The ESS baseline configuration foresees two 60° openings for each moderator, placed approximately face-to-face, so that the moderator surface (of 12×12 cm^2) can be viewed by several neutron extraction beam lines [1]. Because of the reduction of reflector material, the presence of these openings has a strong influence on the performance of the moderator. For comparison, the brightness of a moderator surface of 12×12 cm^2 was calculated in two configurations of the openings: (i) baseline configuration with two 60° openings opposite to each other, capable to deliver neutrons to several beam lines, and (ii) configuration with only one 12×12 cm^2 beam line opening of constant cross-section (0° opening angle). The brightness of (ii) is of 50% higher than (i).

Conventionally, the design process of the target–moderator–reflector configuration takes into account the presence of the openings from the beginning of the optimisation study: the figure of merit used in Monte Carlo calculations for the neutronic performance is the brightness of the moderator surfaces viewed through the openings, calculated with point detector tallies placed at a distance. This kind of optimisation process is certainly effective. However, one could consider as a starting point in the moderator design the ideal case where the moderator is completely surrounded by reflector, without considering the beam openings that decrease its efficiency. Such an *unperturbed* neutron brightness corresponds to the maximum theoretical brightness that can be delivered by the moderator and it is therefore a very interesting quantity to look at: it is a fundamental quantity that does not depend on how the neutrons are extracted, but nevertheless can be expected to be related to the final performance of the neutron source.

Unperturbed neutron fluxes are commonly calculated to estimate the performances of research reactors. In the framework of pulsed spallation sources, unperturbed flux was computed in a few cases in order to compare with the performance of research reactors [7]. In Refs. [7,8] it was pointed out that the ratio between perturbed and unperturbed flux is different in reactors and spallation sources. However, up to now unperturbed moderator brightness has not been used as a parameter in moderator design of pulsed spallation sources.

3. Unperturbed moderator optimisation

We have performed moderator studies by Monte Carlo simulations using the MCNPX 2.7.0 [9] code coupled with ENDF/B-VII data libraries [10]. The nuclear interactions outside the libraries energy range were modelled using the standard Bertini model in MCNPX [11].

We considered a basic model geometry of target–moderator–reflector based on the present ESS concept [1]. The spallation target is a wheel containing pure tungsten in the neutron-producing zone (See Fig. 1). The thickness of tungsten is of 8 cm, the outer diameter is of 2.5 m. The tungsten is enclosed in an iron shroud. The simulated beam footprint is rectangular with dimensions of 16×6 cm^2 and a parabolic shape. The moderators are placed above and below the target. They consist of cylindrical aluminum vessels containing pure para-hydrogen at 20 K. A light water premoderator surrounds each moderator, with the function of partially thermalising the neutrons that will undergo final thermalisation inside the liquid-H_2 of the moderator. The inner reflector is a cylinder of Be of 60 cm diameter and 90 cm height. The outer reflector is a large volume of iron surrounding the inner reflector.

Since the goal of this work is to study the *unperturbed* moderator performance, we had to score neutrons exiting the whole side surface of the moderator. So, we could not make use of conventional scoring by a point detector and benefit from its variance reduction biasing. Instead, we used the surface crossing tally, and scored neutrons exiting the moderator side surface within a narrow cone of 5° angle around the axis, oriented towards the surface normal vector at the point where a particular neutron exited it. The sector angle value was intentionally chosen to be small in order to select neutrons which will potentially arrive to the neutron guide openings (as in a conventional estimation with a point detector) and at the same time large enough to be able to collect enough statistics in reasonable time.

The performance of the moderator was estimated as the number of neutrons with $E < 5$ meV integrated over all moderator side surface and time, within 5° sector angle, normalised to the solid angle Ω formed by this cone, and the moderator side

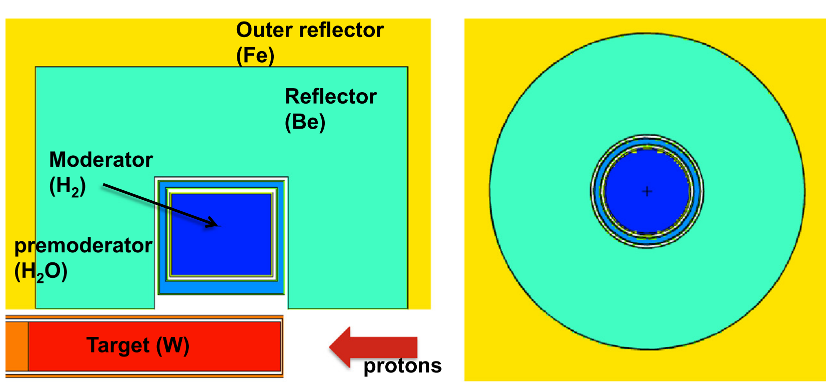

Fig. 1. Side view MCNPX model of the unperturbed moderator (left). Top view of the unperturbed moderator (right).

surface area A:

$$\mathrm{FoM} = \frac{1}{\Omega \cdot A} \int_S dS \int_0^{\infty} dt \int_0^{5^\circ} d\varphi \int_0^{5\ \mathrm{meV}} \Phi(t, \varphi, E)\, dE. \quad (1)$$

This brightness has been used as the figure of merit (FoM) in the current study. The moderator performance study included sensitivity analysis and optimisation. The sensitivity analysis is CPU time expensive, so only two parameters were studied: moderator height and diameter. Optimisation is much faster, so in addition to moderator dimensions, the target offset (offset of the target wheel with respect to the moderator axis along the proton beam direction) was also studied.

Sensitivity analysis. The goal of the sensitivity analysis was to provide information on how the unperturbed moderator brightness changes with moderator size. It was calculated in a grid for different values of moderator dimensions: the moderator height was varied from 1 to 14 cm with 0.5 cm step size, the moderator diameter was varied from 3 to 20 cm with the same step size.

Optimisation. The goal of the optimisation in our study was to fine-tune the optimal value found in the sensitivity analysis on a broader parameter space as described above.

The moderator performance is also affected by its position relative to the target wheel. There are 2 degrees of freedom: vertical and horizontal offsets. The vertical offset (the distance between top of the target and bottom of the premoderator) was fixed at the value of 3.3 cm, because obviously the brightness is expected to be maximum if the moderator is close to the target. The horizontal offset (collinear to the proton beam direction) was optimised, and it turned out that its optimal value (10 cm) is the same for both conventional perturbed and optimised unperturbed configurations.

The thickness of the premoderator was fixed; in particular, the most relevant part of premoderator is the layer between target and moderator, which was fixed at 2 cm. It was previously found in the optimisation studies for ESS that there is saturation of brightness above this thickness [1]. The thickness of the premoderator above and on the sides of the moderator is neutronically less relevant, as it has a negligible effect on the moderator brightness, its main purpose being to facilitate the cooling of the moderator, and it was kept fixed at 1 cm.

The dimensions of optimised moderator (15 cm diameter, 1.4 cm height) were found by fine-tuning the results of sensitivity study by optimisation. We used the optimisation software tool called `Optimiser` [14] with two successively used algorithms: EXKOR (a Bayesian search in one dimension, stepping from one variable to the next) and then MINVAR (a local optimisation routine used to fine-tune the result found by EXKOR) [15,16]. The parameter space used in optimisation includes moderator dimensions and target offset.

3.1. Results

3.1.1. Size effect

Using the geometry of Fig. 1, calculations of figure of merit (1) were performed. A map of FoM values for different moderator heights and diameters was calculated. As shown in Fig. 2, strong variations in brightness are observed. The results peak in a region with diameter in the range 12–20 cm, and height of about 1.5 cm, much smaller than moderators currently used. We find therefore that in the case of a para-H_2 moderator a compact size is capable of delivering a higher brightness, at least for the unperturbed moderator.

The reason for this increase in unperturbed brightness could be a combination of the properties of para-H_2 and of the presence of the reflector. Pure para-H_2 has a scattering cross-section that drops significantly below 50 meV, making the medium almost transparent for cold neutrons. The scattering mean free path of neutrons in para-H_2 in the thermal energy range is comparable to the height of the small, optimised moderator: for a thermal neutron at 25 meV it is of about 2 cm, while for neutrons of 50 meV it is of about 1 cm. A moderator with a disc shape, with the same diameter but a smaller than conventional moderator height, will thus have enough hydrogen to thermalise the neutrons to cold energies. The compact size of this optimised moderator implies more reflector material close to the extraction window. This will favour a directional emission, as discussed below.

The *optimised* and *conventional* moderators, corresponding to the optimised unperturbed moderator giving the highest brightness, and the unperturbed moderator with the present ESS baseline dimensions, respectively, are shown in Fig. 3, and the geometrical parameters are summarised in Table 1.

3.1.2. Directionality

Because of the drop of the para-H_2 scattering cross-section at lower energies, the scattering mean free path of neutrons below 15 meV is more than 10 cm. Therefore, in a pure para-H_2 moderator the whole volume of the moderator is the source of neutrons, as opposed to a ortho-H_2 moderator, in which the neutrons are emitted mostly at the exit surface.

This property may favour directional emission in a disc-shaped moderator. We studied angular emission of cold neutrons from the moderator. In Figs. 4 and 5 the distributions of horizontal and vertical neutron emission angles for two moderator sizes (conventional and optimised, see Table 1) are compared. The vertical angle (Fig. 4) is the angle between the direction of the emitted neutron and the horizontal plane (i.e., the plane perpendicular to the moderator axis). The horizontal angle (Fig. 5) is the angle between the direction of the emitted neutron and the vertical plane normal to the moderator

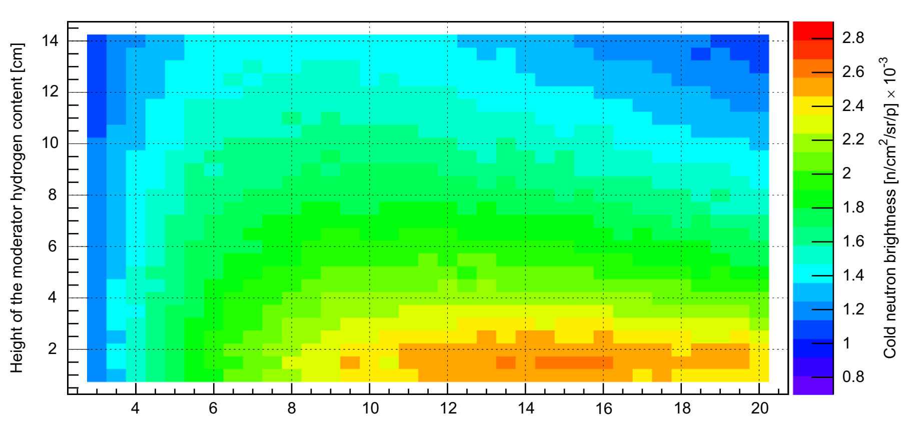

Fig. 2. Map of FoM (1) as a function of moderator dimensions. Relative uncertainty in each bin is less than 1%.

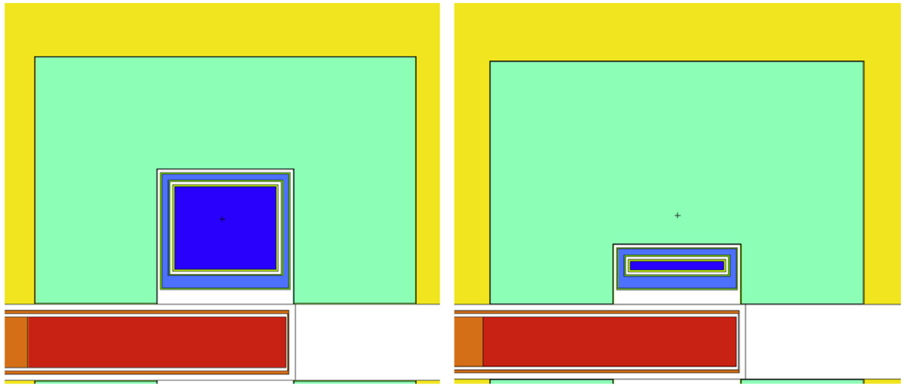

Fig. 3. Left: geometry of the conventional moderator. Right: geometry of moderator optimised for unperturbed brightness.

Table 1
Geometrical parameters of optimised and conventional moderators.

Moderator	Diameter (cm)	Height (cm)	Opening (°)
Optimised unperturbed	15	1.4	None
Conventional unperturbed	16	13	None
Conventional perturbed	16	13	$2\times60^{\circ}$ viewing a 12×12 cm^2 surface

surface, at the point where the neutron is crossing the surface. The optimised moderator shows a strong effect at small vertical emission angles, while the effect on the horizontal angle is less pronounced.

Directional emission in moderators has been achieved so far by using grooved moderators or reentrant holes [3,12,13], for thermal or cold neutrons. The principle behind these moderators is that by cutting grooves inside the moderator it is possible for the instruments to view the cold, more intense flux inside the moderator [12]. The emission is anisotropic, giving a preferential direction. In the case of cold neutrons, the moderating medium is either liquid H_2 with a mixture of ortho/para concentration, or other media such as methane. It is very interesting to observe such a strong directionality effect for a small disc-shaped moderator. In this case, the directionality is not a property of the moderating medium (which is transparent to cold neutrons), but a property of the geometrical configuration of the moderator. The directionality is a direct consequence of the compact geometry of the optimised moderator, combined with the long mean free path of cold neutrons in pure para-H_2 and the large surface of reflector around. Long wavelength neutrons are emitted from the whole volume of the moderator and have only one direction to escape the moderator.

3.1.3. Perturbation effect

For a perturbed moderator neutrons are extracted through openings in the reflector. We consider as an example the typical case of openings of 60°, intended like at ESS to serve several instruments. The viewed surface of the moderator is of 12×12 cm^2. In Fig. 6 the FoM as a function of the angle of emission in the surface of the cylindrical moderator is shown. For the perturbed cases, there are two openings, shown by rectangles. The surface brightness is lower in these openings. The maximum perturbation effect is a factor of 1.8–1.9 (ratio between black and red curves), giving a maximum theoretically achievable unperturbed moderator brightness of a factor of 3.7 higher than the viewed perturbed brightness of the conventional moderator (ratio between the blue and the dip of the red curves).

The brightness of the perturbed moderator is in excellent agreement with a conventional point detector calculation, calculated at 5 m distance from the moderator surface and looking at the 12×12 cm^2 surface: a point detector tally gave an integrated brightness between 0 and 5 meV of 0.73×10^{-3} n/cm^2/sr/proton, corresponding to the dip of the red curve in Fig. 6.

For reference, we added the results for a Cd decoupled moderator, in optimised configuration, which gives a brightness about 10 times lower than for the coupled moderator.

Fig. 7 gives the dependence on the position along the height of the moderator for the same four cases. The brightness distribution for a conventional moderator decreases with increasing distance from the target, with a minimum at about 20 cm from the center of the target. It has already been observed [4] that for a conventional moderator the brightness distribution on the moderator emission surface has a minimum at the center of the surface, which is somehow confirmed for the unperturbed case. Our results for the smaller moderator show that the unperturbed brightness distribution is maximum at the center of the side surface, in agreement with the directional emission shown in Fig. 4: it is indeed an optimised moderator for cold neutron emission from the side surface.

4. Discussion

Our study of the unperturbed cold moderator brightness lead to the surprising result that it can achieve as much as nearly 4 times the perturbed moderator brightness in the common moderator – beam extraction configurations. Since the perturbation of removing reflector for allowing neutrons to be extracted inevitably reduces the moderator brightness, the unperturbed brightness can be considered as an upper limit for the perturbed one that can theoretically be made available for beam lines. The unperturbed brightness can be considered as a fundamental source parameter, as it is at reactors sources.

It is of significance that the optimum moderator size for maximising unperturbed brightness has a very low height, so the total number of neutrons leaving its vertical cylinder surface envisaged for beam extraction is about 4.5 times less than that for the conventional size, 13 cm height unperturbed moderator. Actually, the total number of neutrons emitted increases monotonously with the moderator height. These observations about the brightness of unperturbed moderators provide some new insight for the understanding of the complexities of neutron moderation, and are the primary conclusions of the present study. It has to be emphasised that the moderator brightness is by far not the only parameter that determines the useful neutron flux on the samples in the instruments. The number of neutrons emitted over the total

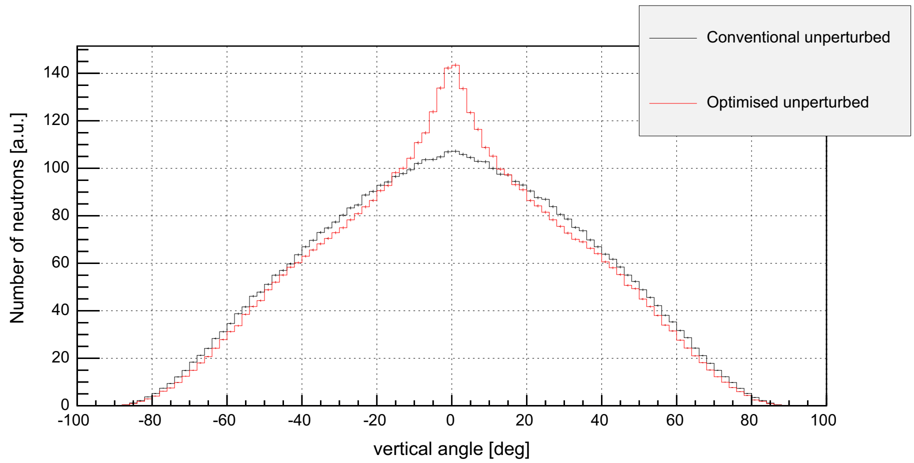

Fig. 4. Distribution of vertical emission angles of cold neutrons ($E<5$ meV) exiting the side moderator surface for conventional unperturbed moderator ($H=13$ cm, $D=16$ cm) and optimised unperturbed configuration ($H=1.4$ cm, $D=15$ cm). The histograms are normalised so that their integrals are equal.

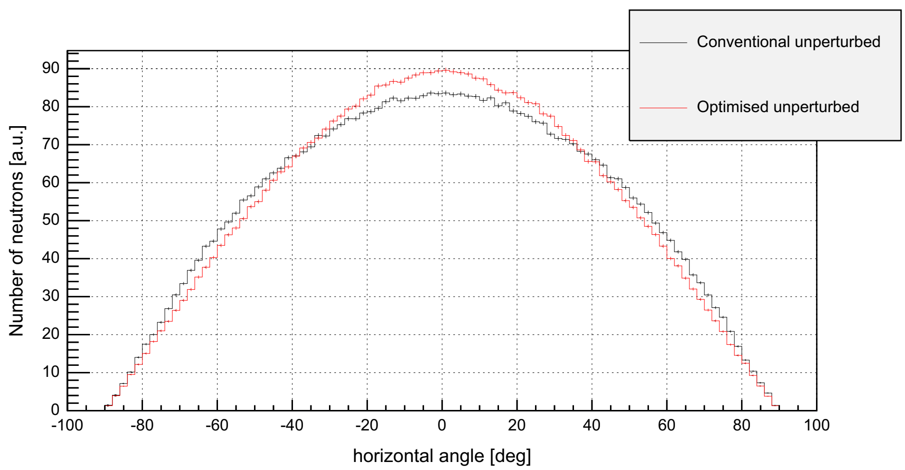

Fig. 5. Distribution of horizontal emission angles of cold neutrons ($E<5$ meV) exiting the side moderator surface for conventional unperturbed moderator ($H=13$ cm, $D=16$ cm) and optimised unperturbed configuration ($H=1.4$ cm, $D=15$ cm). The histograms are normalised so that their integrals are equal.

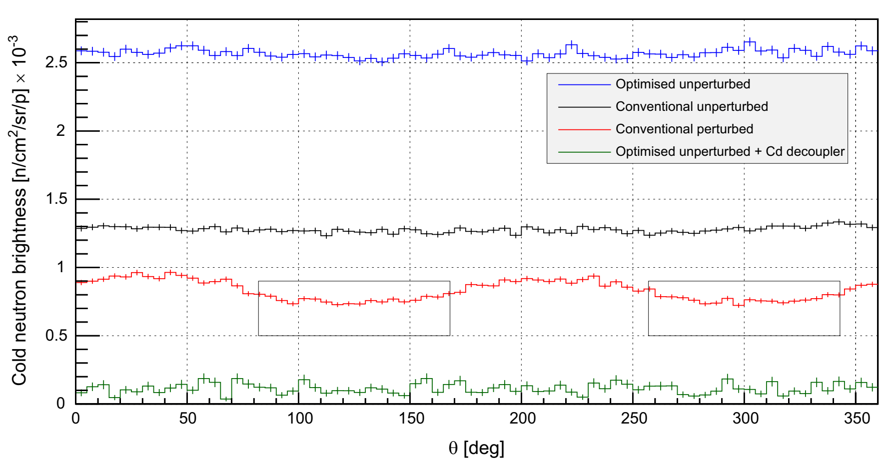

Fig. 6. FoM as a function of the horizontal coordinate of the emission point from the moderator side surface. The brightness is lower in correspondence to the openings. The rectangles indicate the reflector openings on the moderator surface for two 60° beam extraction sectors, corresponding to the initial ESS baseline. All curves have been calculated by the surface crossing estimator method explained about in Section 3. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

viewed moderator surface and in particular the neutron optical beam delivery system between moderator and sample also play fundamental roles. The determination of the optimal combined configuration will be a much more complex and time consuming effort, and it will crucially depend on the evolution of neutron optical concepts and capabilities. Thus the conventional large moderator geometry used as comparison in the present study is certainly very close to the optimal for the currently common neutron guides and beam cross-sections to be delivered to the neutron scattering instruments. Nevertheless, our results on the

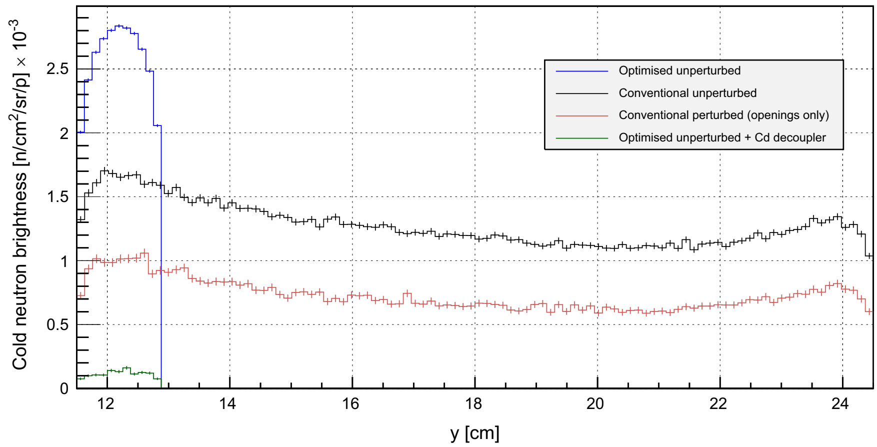

Fig. 7. FoM as a function of the vertical coordinate of the emission point from the moderator side surface. For the perturbed moderator, the distribution is calculated as the average over the openings (marked by rectangles in Fig. 6).

unperturbed moderator can be considered as an important hint for optimising the moderator – beam extraction lay-out for maximum number of neutrons within a desired beam divergence (generally in the range of 1–2°) over the area of the sample, what finally really matters. It is hard to predict the final optimised lay-out and geometry at this stage, but our results suggest that it can be in the direction of smaller moderator heights.

The great difference between moderator height and diameter for the optimum unperturbed brightness may look surprising. The diameter might be related to the sizable volume of proton energy deposition and fast neutron creation in the target, determined by the beam foot print and the proton penetration depth. There is, however, little technical room to change these parameters substantially, while there is quite some freedom to vary the size and shape of the moderators.

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