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Simulations of Different Set-ups of D11

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Executive Summary

Monte Carlo simulations have been performed to check ideas for improvements of the collimating guide system of D11. According to the simulations, improved guide characteristics can increase the flux at sample by about 10 to 15 % for short collimation distances. Widening the guide width over the first few meters by 50 % will yield a flux gain of about 40 % for long and intermediate collimation distances, but a loss for short distances. A gain for all collimation distances can be achieved by a reduction of the guide cross section over the last few meters (in addition to the widening). The best performance was found for a quasi-elliptical exit that reduces width and height to 60 % of its nominal size. The effect on divergence of the neutron arriving at the sample was studied.

Introduction

In the framework of the D11 renewal project, simulations have been performed to check ideas to improve the performance of D11. The first idea was to obtain a higher flux at sample by using a collimating guide system of higher quality, i.e. glass of lower waviness and negligible chamfers. The second idea was to widen the guide in order to increase the flux at the sample by reducing the beam divergence.
As a first step, flux measurements of different set-ups (called 'phases') in recent years have been compared to simulations. To avoid difficulties caused by the limited knowledge of the source characteristics, the ratio 'flux at sample with collimating guide system of length L' to 'flux at sample without collimating guide system' was examined (cf. [1]). Then the planned changes were tested by means of simulations. The simulations were performed with the McStas simulation package [2].

Present design of D11

Description of the instrument components in McStas

We have used the characteristic of the vertical cold **source** (VCS) as given in the McStas source component 'source_gen' [3].

Guide characteristics for the 3 phases are given in the tables 1, 2 and 3. In set-up 1, 50 cm guide pieces were used in the simulations as in reality. The other set-ups contain(ed) a mixture of mainly 1 m pieces and some 50 cm pieces. For the sake of simplicity, a constant length of the guide pieces within a section was assumed to simulate these set-ups, the value being as close as possible to 1 m, i.e.

no_of_pieces = ceiling(total_length)
piece_length = total_length / no_of_pieces

Additionally the upper 13 cm of the guide serving the instruments IN6 and D7 are ignored in most of the simulations to achieve better statistics. In one series of simulations, it was checked that this causes no error (cf. Fig. 9). For the aperture in front of the sample, a slit of 13 mm diameter was chosen, which is used in many experiments.

Table 1: Set-up 1 (phase 1)

guide	description	radius [m]	material	gap [m]	length [m]	alu [mm]	w [mm]	h [mm]	R_0	chamfers [mm]	waviness [deg]
0	straight		nickel	2.330	3.580		30	70	0.90	0.1	0.018
1	curved	2700	nickel	0.350	25.500		30	70	0.95	0.1	0.018
2a	straight		nickel	0.000	22.280	16.0	30	70	0.95	0.1	0.018
2b	IN6 -> D7		nickel	0.300	5.400		30	70	0.95	0.1	0.018
2c	D7 -> D11		nickel	0.300	2.335	1.8	30	50	0.95	0.1	0.018
2d	before selector										
2e	after selector										
3	removable		Borkron	0.165	0 - 38	2.0	30	50	0.99	0.2	0.004

Table 2: Set-up 3 (phase 3)

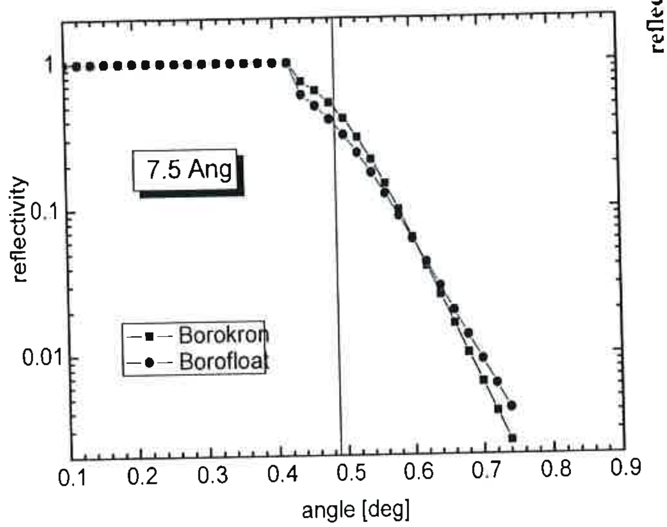
guide	description	radius [m]	material	gap [m]	length [m]	alu [mm]	w [mm]	h [mm]	R_0	chamfers [mm]	waviness [deg]
0	impile		nickel	2.330	3.580	16.0	30	70	0.90	0.1	0.018
1	curved	2700	nickel	0.350	25.500		30	70	0.95	0.1	0.018
2a	straight		nickel	0.000	22.280		30	70	0.95	0.1	0.018
2b	IN6 -> D7		nickel	0.300	5.400		30	70	0.95	0.1	0.018
2c	D7 -> D11		nickel	0.300	1.080	12.8	30	50	0.95	0.1	0.018
2d	before selector		nickel	0.015	0.680						
2e	after selector		nickel	0.030	0.490						
4	removable		Borofloat	0.000	0 - 39	2.0	30	50	0.99	0.8	0.034

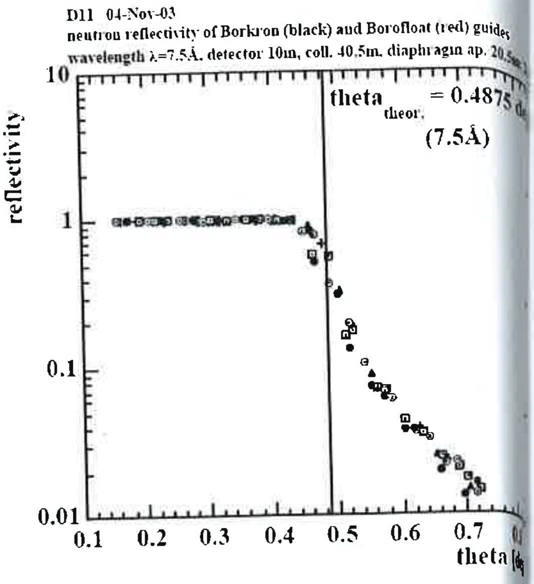
Table 3: Set-up 4 (phase 4)

guide	description	radius [m]	material	gap [m]	length [m]	alu [mm]	w [mm]	h [mm]	R_0	chamfers [mm]	waviness [deg]
0	straight		nickel	2.330	3.580	16.0	30	70	0.90	0.1	0.018
1	curved	2700	nickel	0.350	25.500		30	70	0.95	0.1	0.018
2a	straight		nickel	0.000	22.280		30	70	0.95	0.1	0.018
2b	IN6 -> D7		nickel	0.300	5.400		30	70	0.95	0.1	0.018
2c	D7 -> D11		nickel	0.300	2.335	1.8	30	50	0.95	0.1	0.018
2d	before selector										
2e	after selector										
3	removable p.1		Borkron	0.165	0 - 12.5	2.0	30	50	0.99	0.2	0.004
4	removable p.2		Borofloat	0.000	0 - 26.5		30	50	0.99	0.8	0.034

The parameters determining the **reflectivity curves** were varied to give as good agreement with measurements as possible. According to measurements, a low angle limit of R_0=0.99 was chosen. The resulting curves are shown in Figure 1:

Figure 1: Reflectivity curves of guides in simulations (left) in comparison to measurements by P. Lindner (right)





The **Velocity selector** was simulated as described in component 'V_selector' and the paper "Wavelength calibration and flux measurements with ... DOLORES":

```
num_blades   = 72;
radius       =  0.120 m
sel_length   =  0.250 m
sel_twist    = 48.298 m
thick_bl     =  0. 4   mm
sel_speed    = 60.0*sel_twist/360.0*V2LMBD/lmbd_av/sel_length;
sel_width    =  0.040 m
sel_height   =  0.060 m
```

Flux behind velocity selector

For the instrument in phase 1 (set-up 1), a total intensity of 1.64 E+09 n/s over the whole cross-section was simulated for 6 Å behind the velocity selector. If all neutrons pass through an area of 30 x 50 mm^2, the corresponding flux is 1.09 E+08 n/(cm^2s). In phase 3, this values increases by 15 % to 1.88 E+09 n/s and 1.25 E+08 n/(cm^2s) assuming that the exit window of the velocity selector is large enough to let all neutrons pass, i.e. the exit has at least the size 36.5 x 56.5 mm^2. The measurement result was 1.36 E+08 n/(cm^2s), i.e. the simulation gave a 8 % lower value, which is a good agreement.

88.9 % of these neutrons enter the removable guides, in set-up 1 the fraction is 95.2 %. Thus, there is only a gain in flux of about 7 %.

Flux inside the guide system

Due to the lower m value of glass (m=0.65) compared to the nickel (m=1) coated guide before the selector, the flux inside the guide falls down rapidly on the first meters of the guide. If we assume a sharp cut-off, all neutrons with a higher divergence than the cut-off value of glass (6 Å*0.65*0.1°/Å = 0.39°) should have touched a wall after

$$L = 0.05 \text{ m} / \tan(0.39°) = 7.35 \text{ m}$$

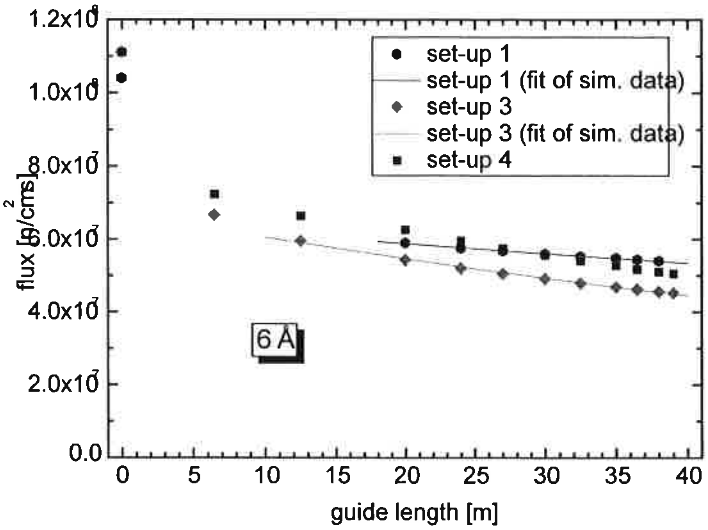


Figure 2: Flux inside guide as a function of guide length

Behind that point the intensity should decrease exponentially

$$I(L) = I(L_0) \exp(-\_(L-L_0)) \quad (1)$$

giving a realistic absorption coefficient _. This fits well the observed decrease in intensity (cf. Figure 2). A slower decrease for the Borkron guides is clearly visible. Fits in a range of 20 – 39 m yield values for _ of 0.0048 m^{-1} for set-up 1 and 0.0096 m^{-1} for 3. Another result is that (for a wavelength of 6 Å) nearly half of the neutrons are lost by the first reflection.

Flux inside the guide system

Peter Lindner has measured the ratio: flux at sample with guide of length L_g to flux at sample without guide for different wavelengths and set-ups. This value shall be called 'relative flux at sample' in the rest of this paper. It will be used to compare simulations and experiments.
Later on, the goal of the simulations with the trumpet will be to find parameters that the 'relative flux at sample' is as high as possible for all wavelengths and collimation lengths.

These curves depend on the performance of the nickel guide in front of the velocity selector, i.e. the primary guide. If its performance is very good, it will transport a high intensity of divergent neutrons to the velocity selector. As a consequence, the gain by the secondary guide, i.e. the relative flux at sample will be high for large guide lengths. Preliminary simulations showed that the relative flux at sample increases stronger in the simulation than in the measurements, if a guide of high quality is assumed. Thus, the reflectivity was decreased until there was agreement between simulation and measurement for one case (6 Å, current set-up (phase 4) and shortest collimation distance). The resulting guide parameters can be found in Tables 1 to 4.

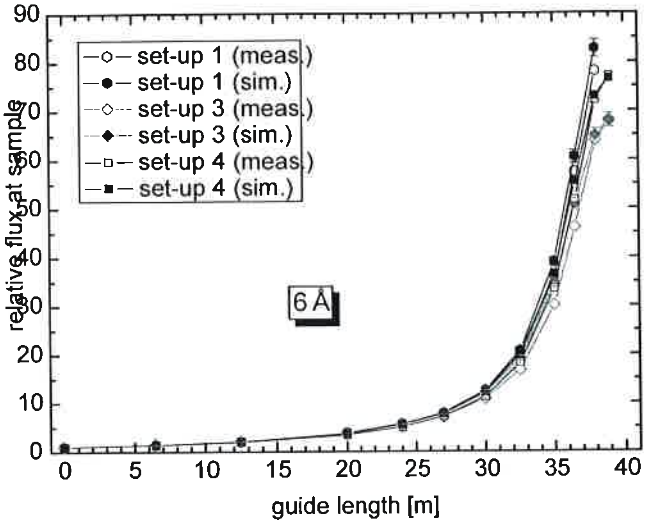


Figure 3: Relative flux at sample in simulations and measurement

If we compare the relative flux at sample now for different set-ups (Figure 3) or different wavelengths (not shown here), we find rather good agreement between simulations and measurements. Remaining discrepancies are probably due to neglecting misalignment and imperfect geometry of the guide pieces in the simulations.

Following the same procedure as done for experimental data, we can determine the guide transmission by calculating the flux per solid angle _ as a function of guide length with _ being the solid angle of the guide exit seen from the sample position:

$$\_ = w \times h / L_1^2 \qquad (2)$$

This can be done up to a guide length of about 34 m. Above this value, the sample is not illuminated any more by the whole guide exit; thus the value of _ used in the calculation is not the 'real' solid angle any more. (For this reason, the fit of the measures values had been restricted to the range below 34 m.)
Figure 4 shows the result in comparison to the transmission calculated from the coefficients obtained from the **experimental** data.

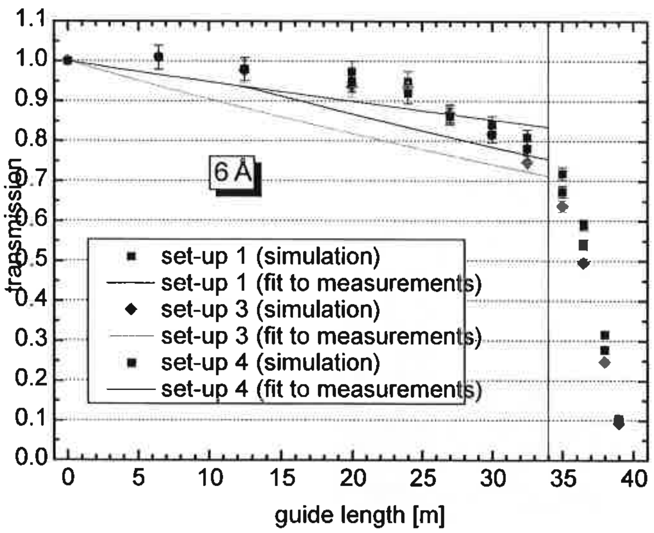


Figure 4: Transmission as a function of guide length obtained from the flux at the sample. Simulation values are compared to fitted curves of measurements

While the resulting transmission for the whole guide length is well described by the experimentally determined transmission coefficients, the function T(L) is different from an exponential decay – even below 34 m guide length. Up to 12.5 m, it is quite close to 1; then it drops down faster and faster. The reasons are the following:

- for 12.5 m guide length or 28 m collimation the neutrons arriving at the sample (of 3 cm diameter) have a maximal divergence of atan(0.0315/28) = 0.064° or a typical divergence of atan(0.010/28) = 0.020°. Those neutrons change their distance to the guide walls by maximally 14.1 mm or typically 4.2 mm while passing through the 12.5 m long guide. That means the majority of the neutrons are not at all reflected in the guide, the others are reflected only once. With an assumed reflectivity of 0.99, the resulting transmission should be above 0.995. (The same holds for the guide length of 6.5 m.)
- The divergence distribution is not at all homogeneous. Divergent neutrons have higher losses caused by a more frequent reflections at the walls or and a higher probability of being absorbed by the chamfers. Additionally the velocity selector favours non-divergent neutrons. The resulting distribution is shown in Figure 5. If the collimation length is decreased, maximal and average divergence of the neutrons arriving at the sample increase. But as their intensity is not as high as that of the non-divergent neutrons, the intensity increases slower – or – if we divide through the solid angle, the flux per solid angle decreases.

Summarising it can be said that this method does not determine the total decrease in flux inside the guide (cf. figures 2 and 4), but that of neutrons of low divergence. Therefore there is good agreement between the values obtained this way from experiments (0.0053 m^{-1} for set-up 1 and 0.010 m^{-1} for set-up 3) and those found in simulations for the flux (0.0048 m^{-1} for set-up 1 and 0.0096 m^{-1} for set-up 3).

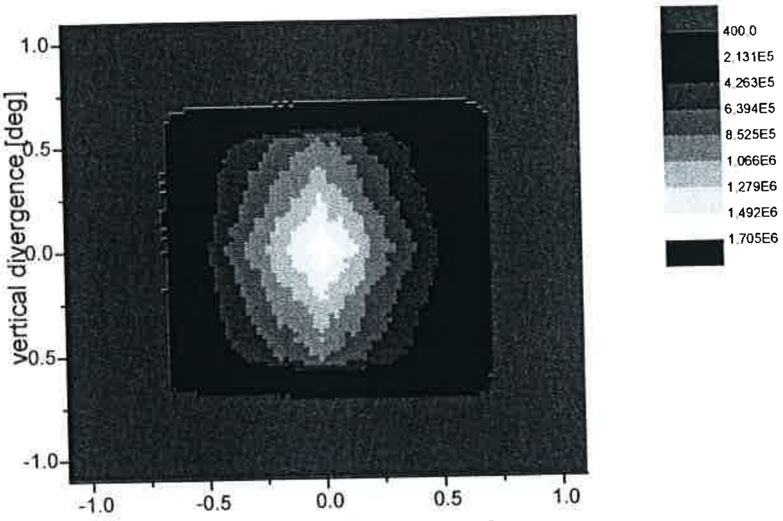


Figure 5: Divergence distribution behind velocity selector (6 Å, set-up 4)

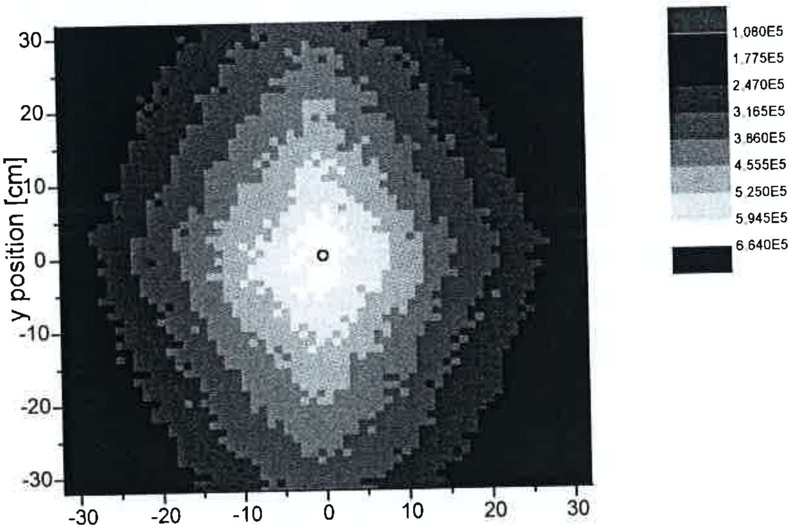


Figure 6: Spatial distribution of flux at sample position (6 Å, set-up 4). The red circle indicates the sample size.

D11 with Trumpet

The guide system is identical to that of phase 3 except that the waviness is supposed to be 0.006 deg and the chamfers 0.01 mm (see Table 4)

Table 4: Parameters of set-up 5 (phase 5)

guide	description	radius [m]	material	gap [m]	length [m]	alu [mm]	w [mm]	h [mm]	R_0	chamfers [mm]	waviness [deg]
0	straight		nickel	2.330	3.580		30	70	0.90	0.1	0.018
1	curved	2700	nickel	0.350	25.500		30	70	0.95	0.1	0.018
2a	straight		nickel	0.000	22.280	16.0	30	70	0.95	0.1	0.018
2b	IN6 -> D7		nickel	0.300	5.400		30	70	0.95	0.1	0.018
2c	D7 -> D11		nickel	0.300	2.335	1.8	30	50	0.95	0.1	0.018
2d	before selector										
2e	after selector										
3	removable		Borofloat	0.165	0 or 6.5	2.0	30->45	50	0.99	0.1	0.006
4	removable		Borofloat	0.165	0 - 32.5		45	50	0.99	0.1	0.006

Different guide options

A straight guide was compared to a guide opening from 30 x 50 mm^2 (w x h) to 45 x 50 mm^2 over the first section or the first two sections, i.e. over 6.5 or 12.5 m. Additionally it was tested whether it is useful to start with a larger width behind the gap. Therefore also trumpets opening from 32 x 50 mm^2 and 36 x 50 mm^2 to 45 x 50 mm^2 over 6.5 m length were checked and even the extreme case of a guide of 45 x 50 mm^2 constant width.

Figure 7 shows the gains compared to the straight guide of 30 x 50 mm^2 as a function of guide length. Using an enlarged cross-section at the guide entrance reduces the efficiency of the trumpet. Indeed, the intensity at the entrance is between 3.3 % and 7.5 % higher, but the effect of reducing the divergence is weaker. This seems to be more important than avoiding to lose neutrons at the entrance. The loss for the option of constant width of 45 mm is caused by the fact that those neutrons with a sufficiently low divergence to reach the sample (<0.048° for L_g=34) cannot touch the wall.
The difference between the trumpets of different length is not large. The 12.5 m long trumpet shows a slightly better performance for intermediate collimation lengths - but for the longest collimation (6.5 m guide) the gain in flux is significantly lower. Therefore, the option 30 x 50 to 45 x 50 mm^2 over 6.5 m was chosen.

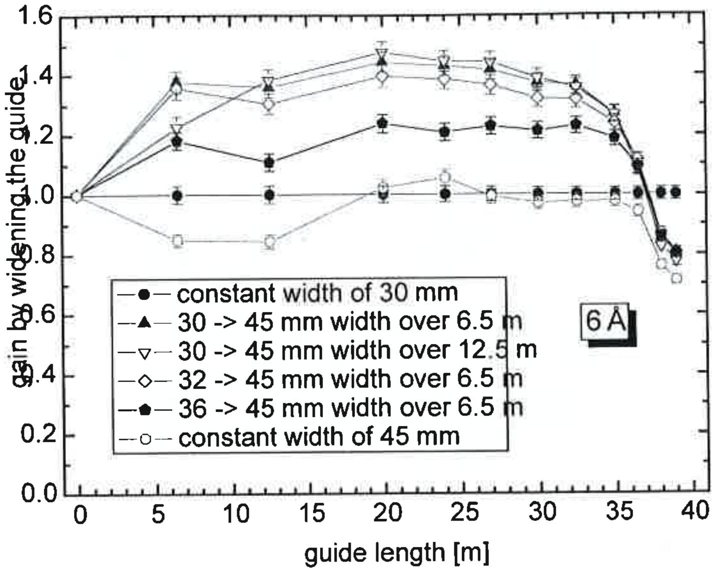


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Figure 7: gain in flux at the sample vs. guide length for different realisations of the diverging trumpet and 6 Å

For intermediate and long collimation lengths, a gain of about 40 % can be reached (see Table 5, Figure 7). This is a really high value, as the enlargement of the cross-section (and thus the maximal value) is only 50 %. For long and short collimation lengths the gain is smaller; for a collimation length less than about 3.5 m the flux at sample is smaller, if a trumpet is used. This is not surprising, because in these cases only the neutrons leaving the guide at its centre contribute to the flux at the sample. Due to the enlarged guide cross section, the flux is lower with the trumpet than it is in the original set-up with the constant cross-section though the intensity is higher. Roughly, the intensity increases by 25 %, while the flux decreases by 20 %.
In addition to these solutions it was tested, whether the guide in front of the velocity selector could be used as trumpet. It turned out that it is too short to decrease the divergence effectively, especially for 4.5 Å. It has a length of 2.33 m and opens with an angle of 0.183°. Therefore neutrons of 0.366° divergence are reflected to be non-divergent, while the 6.5 m long trumpet used in the collimation system converts neutrons of 0.132° divergence to non-divergent neutrons. The intensity of these more divergent neutrons is significantly less because of the existing gaps in the beam-line and the limited reflectivity of the guide. As a consequence, the gain for the short trumpet is only about half of that of the longer trumpet. For 4.5 Å it is even less, because it is already close to the cut-off angle for Ni (0.45°).

To avoid the losses for short collimation lengths caused by the diverging trumpet, a converging trumpet at the end of the guide system was introduced. The last 3 guide sections were chosen for this focussing exit, i.e. it extends from 5.5 to 1.5 m from the sample position (cf. Figure 11). The idea was to reduce the cross section both in horizontal and in vertical direction. First simulations with an exit of 30 x. 30 mm^2 showed a significant gain for short wavelength (4.51 and 6 Å) and even improved performance for the longest wavelength examined (18 Å).

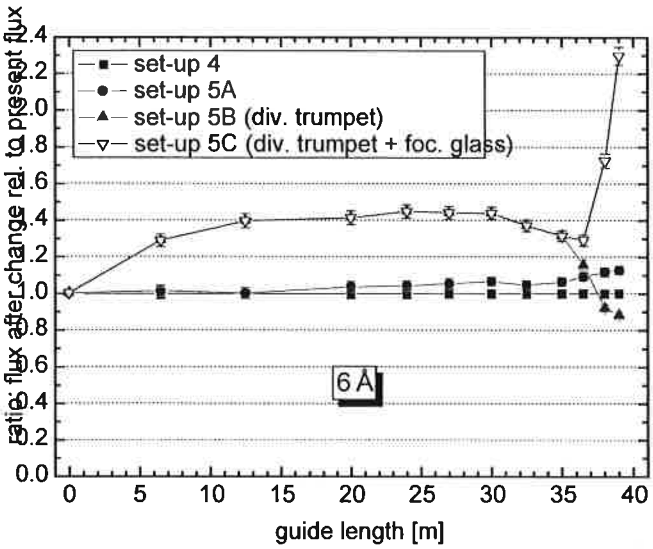


Figure 8: change in relative flux at sample compared to the present situation as a function of guide length for different guide designs, an exit size of 30 x 30 mm^2 and a wavelength of 6 Å.

At this point is was checked if the approach to ignore the upper part of the guide was justified. The same simulation was performed for set-up B and C and some of the collimation lengths. The main features are the same for both series of simulations. The gains are higher for the 20 cm guide, but the difference is within statistical error (see Fig. 9). The difference is probably due to an underestimation of the reference flux (no guide) for the 20 cm simulation. The statistics are poor in spite of the by a factor of 2 higher number of events used for the 20 cm series (and accordingly long simulation times.)

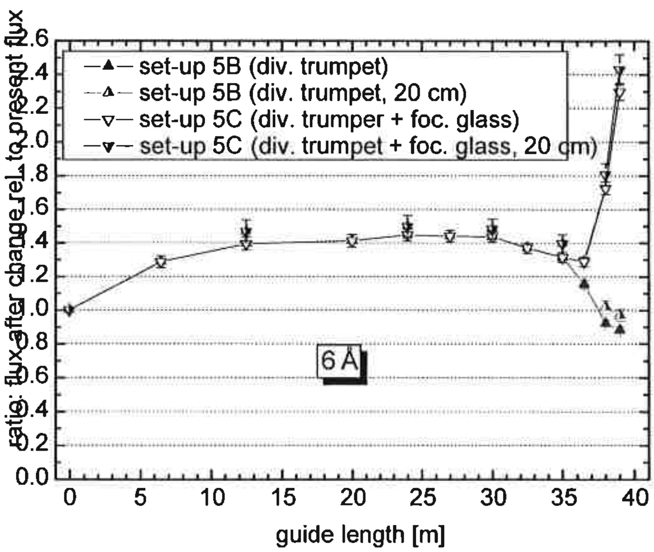


Figure 9: comparison of simulation with real height of primary guide (20 cm) and approximation to use only the lower 7 cm of the guide. Simulation parameters as in Fig. 8.

To find the optimal solution, the exit size was varied systematically. The ratio of width to height was kept constant, while its size was varied from 100 % of the guide width and height to about 40 % in steps of 10 %. Figure 10 shows the result for two wavelengths. The optimal size depends on the wavelength, for 4.5 Å it is about 60 %, for 18Å about 85 %. A trumpet with variable exit size could be adapted to the wavelength. Ideas for that exist, but were not yet realised.

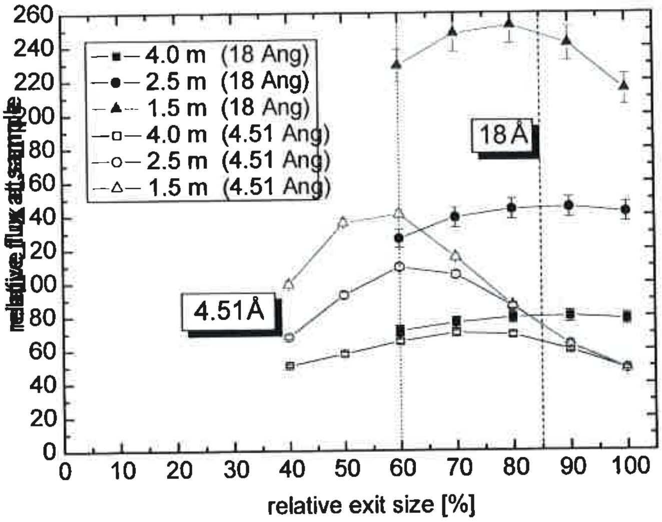
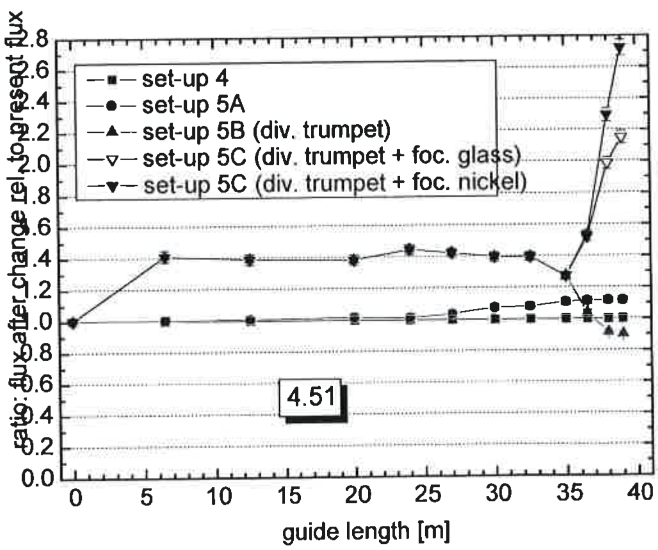


Figure 10: relative flux at the sample for different exit sizes of a linear trumpet and wavelength of 4.51 and 18 Å.

An exit of 70 % of width and height of the guide, i.e. 31.5 x. 35 mm^2, which is the optimum for 10 Å (not shown here), seems to be a good compromise for the whole wavelength range used. Simulations of different wavelength (4.5, 6, 10, 12 and 18 Å) were performed with that size. The simulations show gains compared to a straight guide for all wavelengths and all collimation lengths (see Figure 11). A nickel coating of this focussing exit yields higher gains for short wavelengths, but not for long wavelengths.



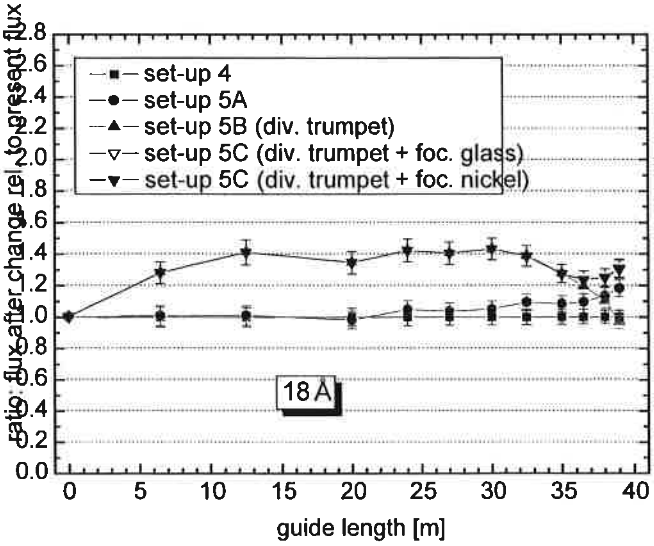


Figure 11: change in relative flux at sample compared to the present situation as a function of guide length for different guide designs and wavelengths and an exit size of 31.5 x 35 mm^2.

Finally, a quasi-elliptical shape was simulated for the exit. It consists of straight parts within each section; but the size is decreased more distinctly towards the sample (see Figure 12).

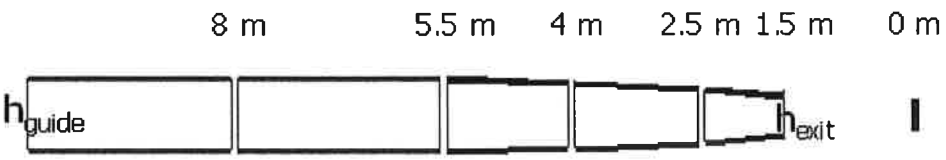


Figure 12: design of a focussing trumpet with quasi-elliptical shape

The result was that the performance can be improved compared to a linear guide, especially for short wavelengths and the shortest collimation (see Figure 13).

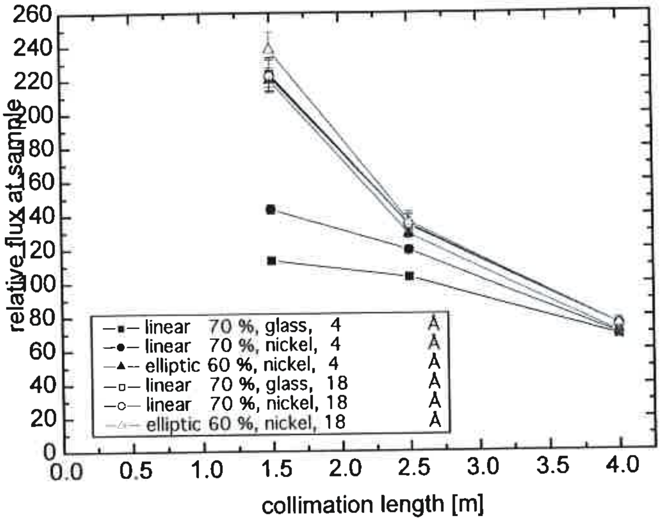


Figure 13: relative flux at sample for different options of the focussing exit

Resolution

The increase in flux at sample causes a higher divergence of the neutrons reaching the sample. The horizontal divergence is shown in Figure 14 for different set-ups. This reduces the resolution in Q of the measurement. The determination of the resolution by Mildner and Carpenter [4] takes the whole trajectories from source (= guide exit in this case) to detector into account. This does not allow separating the incoming divergence from the outgoing divergence. Therefore the approach of independent errors by incoming and outgoing divergence [5] was used. This approach underestimates the error a bit (cf. last 2 columns in Table 5). But it allows taking the properties of the neutron beam into account. From the Bragg condition and its SANS approximation

$$Q = 4\pi / \_ \sin(\_/2) \approx 2\pi \_ / \_ \qquad (3)$$

it follows that

$$\__Q^2/Q^2 = \_\_^2/\_^2 + \_\_^2/\_^2 \qquad (4)$$

The approach is now:

$$\__Q^2/Q^2 = \_\_{_{,in}}^2/\_^2 + \_\_{_{,out}}^2/\_^2 + \_\_^2/\_^2 \qquad (5)$$

The deviation $\_\_{_{,in}}$ of the incoming beam has been determined by calculating the second moment of the divergence distribution (of the neutrons reaching the sample) given by the simulations. The deviation $\_\_{_{,out}}$ of outgoing beam has been calculated analytically by integrating over the sample area and a detector element giving

$$\_\_{_{,out}}^2/\_^2 = (x_2^2 + y_2^2 + \_R_x^2 + \_R_y^2) / (12 R^2) \qquad (6)$$

(R is the distance from the centre of the detector to the point of detection. _R_x and _R_y are the detector element sizes in horizontal and vertical direction and x_2 and y_2 are width and height of the sample.)
A sample size of 11.5 x 11.5 mm^2, a sample - detector distance of 1.5 m, a detector resolution of 10 x 10 mm^2 and 9 % FWHM wavelength spread were assumed. Resolutions were calculated for a position of detection (0.25 m, 0.25 m) from the centre.

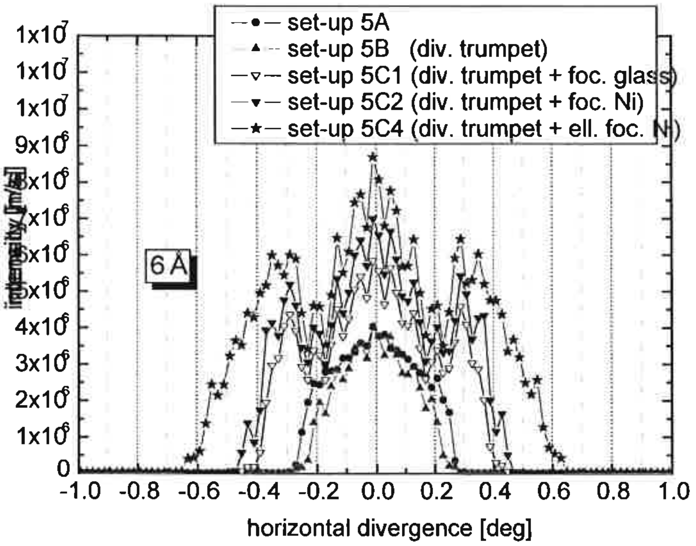


Figure 14: divergence distribution for different options of the focussing exit

Table 5 summarises the FWHM values of _Q/Q for the shortest collimation length of 1.5 m, two wavelengths (4.51 and 18 Å) and different set-ups. For 4.5 Å an increase of _Q/Q by11% is found for the linear trumpet and by 21% for the quasi-elliptic trumpet. For 18 Å, _Q/Q decreases by 4% and 5% resp.
For longer collimation lengths, the incoming divergence is determined by geometrical conditions. As long as this is the case the resolution is independent of the collimation [5]. The value _Q/Q for this case is 15.9 % for the straight and 17.2% for the widened guide and the parameters given above (cf. Table 5).
When the divergence transported by the guide is lower than the geometrically possible divergence between guide exit and sample – which is the case for short collimation lengths and especially for short wavelengths – the value of _Q/Q drops, i.e. the resolution improves. Only this drop is reduced by the focussing exit. The resulting values of _Q/Q are still below the long collimation limit (of 17.2% or 15.9 %), because the reduced exit size decreases the geometrically possible maximal divergence.
For the quasi-elliptical shape, this limit is reached and delivers practically identical values for short and long wavelengths of _Q/Q ≈ 12.8% (or corrected about 13.5%). With the linear trumpet and the larger exit, the divergence of the 4.5 Å neutrons is in between the limits given by the geometrical condition and the reflectivity curve of the guide; thus we find also an intermediate value of _Q/Q of 11.5% (corr. 12.2%). Without a trumpet it is about 10.5 % (11.2 %).
On the other hand, the divergence and thus _Q/Q increases for the 18 Å neutrons to _Q/Q =13% (13.7%) with the linear trumpet and to _Q/Q = 13.5 % (14.2%) without a trumpet due to the increased exit size and the geometrically possible higher divergence.

Table 5: FWHM values of divergence at sample position (as found in the simulations) and resulting resolution in comparison to the theoretical resolution determined from geometrical considerations (L_1=L_2=1.5 m; sample 11.5 x 11.5 mm^2; detection at (0.25, 0.25) m; detector resolution 10 mm; wavelength resolution 9 % FWHM)

	exit			**4.51 Ang**			**18 Ang**				**geom.**	**limits**	
option	width [mm]	height [mm]	hor. div. [deg]	vert. div. [deg]	appr. resol.	hor. div. [deg]	vert. div. [deg]	appr. resol.	hor. div. [deg]	vert. div. [deg]	appr. resol.	exa reso
A	30.0	50.0	0.319	0.335	10.5%	0.621	1.040	13.5%	0.834	1.332	15.3%	15.9
B	45.0	50.0	0.273	0.336	10.4%	0.621	1.050	13.5%	1.206	1.332	16.6%	17.2
C1	31.5	35.0	0.487	0.529	11.3%	0.685	0.869	13.0%	0.871	0.957	13.8%	14.5
C2	31.5	35.0	0.529	0.627	11.7%	0.686	0.870	13.0%	0.871	0.957	13.8%	14.5
C4	27.0	30.0	0.697	0.786	12.7%	0.723	0.815	12.9%	0.762	0.834	13.0%	13.7

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