SNS 107080100-TD0002-R00

Supplement to

Extended Q-range, High Intensity, High Precision Small Angle Diffractometer

FOR SNS

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Spallation Neutron Source

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A U.S. Department of Energy Multilaboratory Project

SPALLATION NEUTRON SOURCE

Argonne National Laboratory • Brookhaven National Laboratory • Thomas Jefferson National Accelerator Facility • Lawrence Berkeley National Laboratory • Los Alamos National Laboratory • Oak Ridge National Laboratory

SNS

Introduction

The Extended Q-Range Small Angle Scattering Instrument (EQ-SANS) [1] (Fig. 1) on the 60Hz SNS target is designed to have high intensity, high precision, and large Q-coverage. The machine is located on beamline No. 6, facing the downstream, upper, coupled hydrogen moderator. Its total length is variable between 15 and 18m. Since the completion of the conceptual design [1], two likely improvements to the instrument have been studied. The first one is the insertion of a T0-chopper, which is aimed at reducing the background. The second one is the possibility of using the three bandwidth choppers to separate the inelastic contributions from the scattering intensity. Such separation capability is very much desirable for strongly inelastic scattering systems.

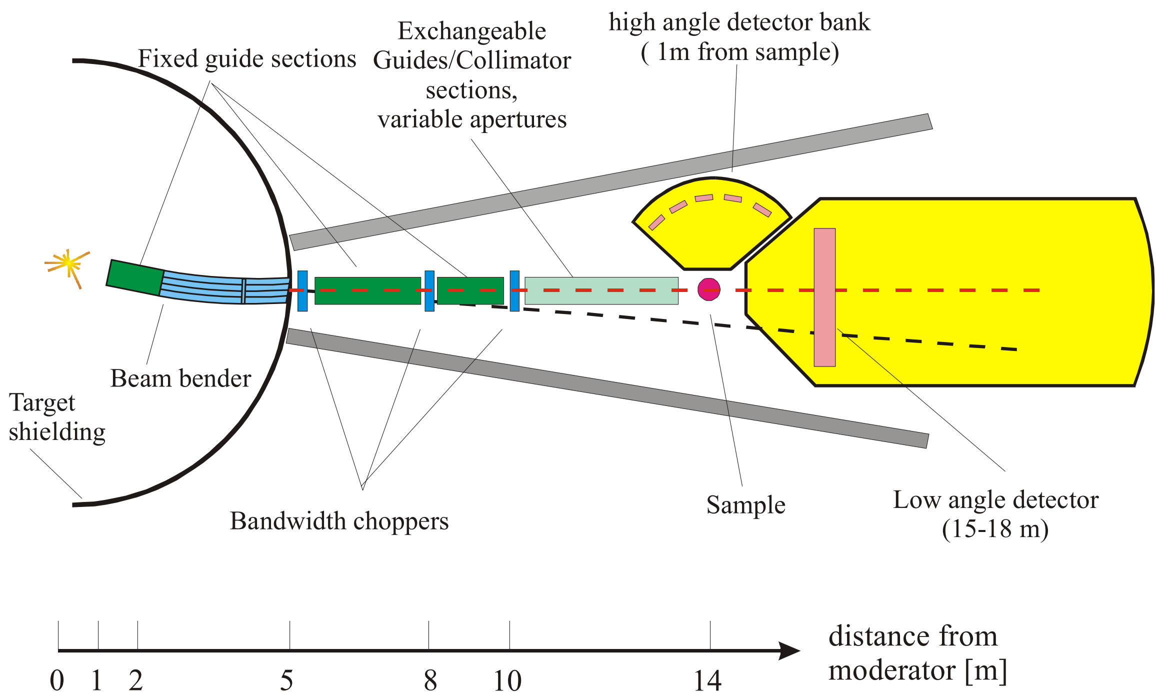

Figure 1. Conceptual sketch of the EQ-SANS adapted from [1].

T0 Chopper

On May 23 and 24, 2001, the optics of the SNS reflectometers was reviewed at the Argonne National Laboratory [2]. During the meeting, Ed Blakeman and Charles Slater of ORNL presented shielding and background calculations on the reflectometer. Their results showed that the dose rate at the sample position is about 260 mR/h. The dose rate comes primarily from the secondary fast neutrons scattered downstream off the benders. The EQ-SANS has a very similar neutron optics system to the reflectometers. Similar dose rate can thus be expected on the EQ-SANS. With such dose rate, extra personnel safety precautions have to be put in place. No person can be anywhere near the sample when the scattering experiment is going on. From the neutron experiment point of view, such dose rate will worsen the background significantly, making many experiments on weak scattering systems impossible.

To reduce the dose rate and the background, we looked into the possibility of adding a T0-chopper to the instrument (Fig. 2). The chopper will be located at ~5.5m from the moderator, immediately after the first bandwidth chopper. From Blackman's calculation on the reflectometers, the dose rate at the sample position with a T0-chopper alone is similar to that of with the beam bender alone. It is therefore reasonable to assume that the combination of the beam bender and an additional T0-chopper will drastically reduce the background on the EQ-SANS. Since the geometry of the EQ-SANS is similar but not identical to that of the reflectometers, calculation with the EQ-SANS geometry will be required to obtain a better background estimate. Detailed simulation is also needed to refine the location of the T0-chopper in the future.

In the appendix B of the conceptual design report [1], it was discussed that the T0-chopper will somewhat reduce the beam flux due to the introduced gap. As noted in the report, the simulations were carried out with 1° input beam divergence. The flux reduction by T0-chopper affects primarily the divergent neutrons. Therefore, the flux reduction should have little effect on experiments with long collimation, i.e. experiments with detector positioned at 18m.

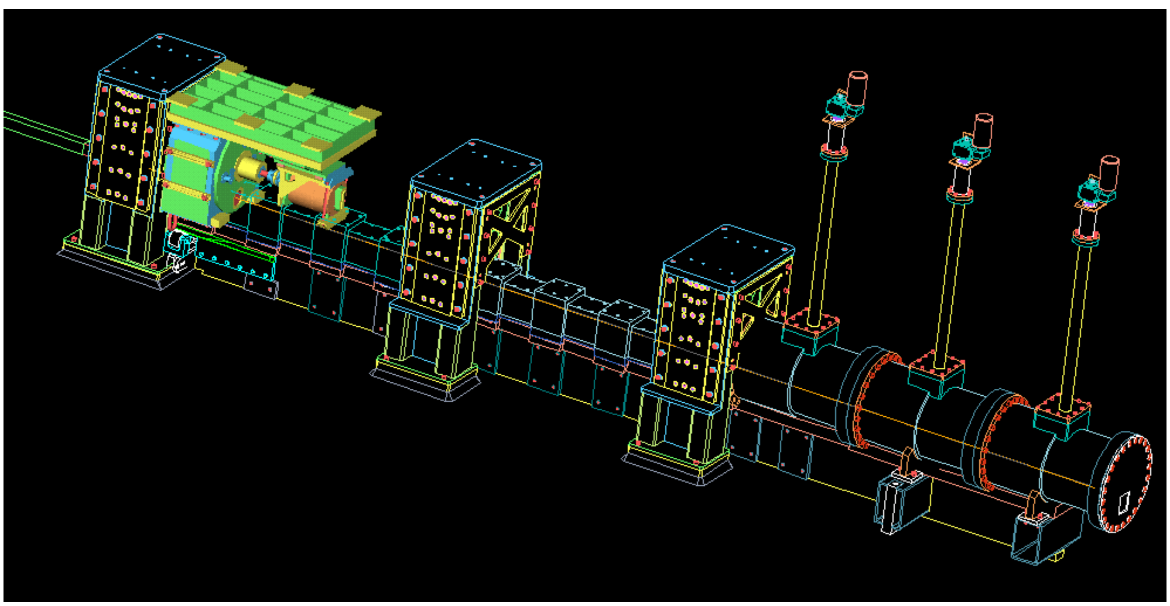

Figure 2. The location of the T0-chopper (shaded). The three bandwidth choppers, neutron guide support, and the three carousels for changing the system collimation are shown. The neutron beam bender is partially shown on the left before the first bandwidth chopper.

EQ-SANS as a multi-chopper machine

Many systems studied by small angle neutron scattering have strong inelastic contributions in the low-Q region. The ability to verify and separate these inelastic contributions is often desired. Even though SNS will have dedicated inelastic scattering instruments capable of measuring the energy transfer spectrum down to relatively low-Q [3], the fact that the EQ-SANS is design to have three bandwidth choppers raises the possibility of operating the EQ-SANS as a multi-chopper machine. The driving force behind such modification is the stated desire to measure and separate the inelastic scattering at low-Q. The constraints are that any modifications on the instrument should not degrade the performance of the machine as a SANS instrument and that the cost for such modification should be minimal.

The three bandwidth choppers are located at 5, 8, and 10m from the moderator, respectively. Two of them can be used for pulse shaping and the third one is used as a frame overlap or pulse selection chopper. In the current discussion, we assume the T1 chopper at 5m and the T3 chopper at 10m (Fig 3) to be the high speed, pulse-shaping ones. Their relative position of 2:1 gives a simple 1:2 ratio between their rotation speeds. If the T3 chopper has a speed of 300 Hz, the T1 either has to rotate at 600 Hz or at 300 Hz but have two openings symmetrically located with respect of the disc center. In practice, due to engineering constraints on the location of the T1 chopper, it may be necessary to use the T2 and T3 choppers for pulse shaping. In this case, one set of possible rotation speeds for T2 and T3 are 300 and 240 Hz, respectively.

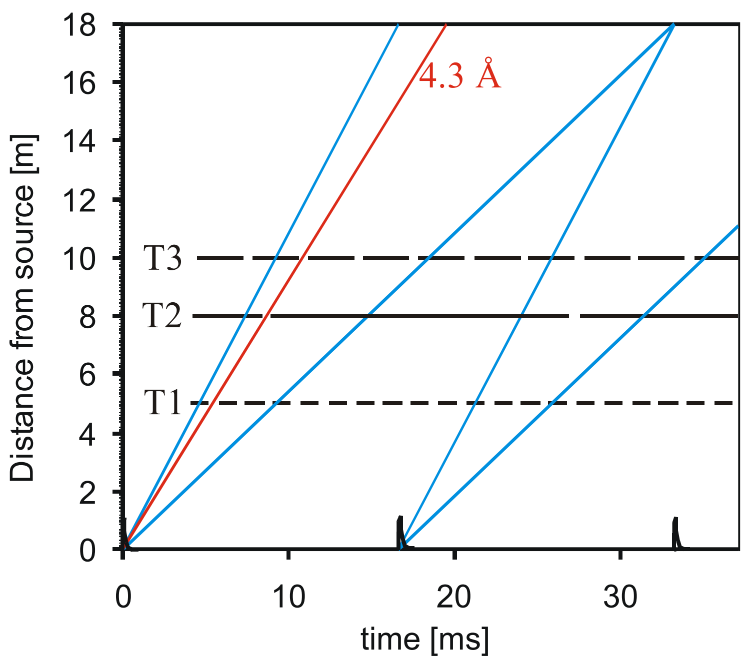

Figure 3. Time diagram of the Extended-Q SANS when operated in chopper mode. The blue lines correspond to the second frame. The red line is the selected neutron pulse. The two high speed choppers T1 and T3 shape the pulse while the 60 Hz T2 acts as a frame overlap chopper. The chopper T1 either rotates twice as fast as T3 or has symmetric, double openings.

Fig 4. shows a simulated neutron pulse in wavelength space measured on the detector at 18m. The chopper setups are as shown in Fig 3. The corresponding incident energy E_i and its FWHM dE_i / E_i are 4.4 meV and ~1.2%, respectively.

When the EQ-SANS is operated in SANS mode, the frame overlap choppers have very wide openings. When the detector is located at 18m, the required opening for T1, T2, and T3 are 100°, 159°, and 198°, respectively. When the detector is at 15m, these openings become 121°, 191°, and 238°. The change in opening angle is achieved by re phasing the two discs of each of the double-disc choppers. Apparently, re phasing the discs will not give us the small openings needed for chopper mode operation. For the T3 chopper, for examples, it is not possible to obtain a 10° opening as assumed in our simulation (Fig 4), since the opening on each of its discs well exceed 185°.

To overcome this apparent contradiction between the two operational modes, we design the choppers to have two sets of openings lying on different perimeters (Fig 5). The choppers will be raised or lowered when the machine switches operation modes. For the chopper T2, it can be re phased to have an opening of ~ 22-25°, which should be appropriate enough for its role in pulse selection. Thus, no modification on the T2 chopper is needed.

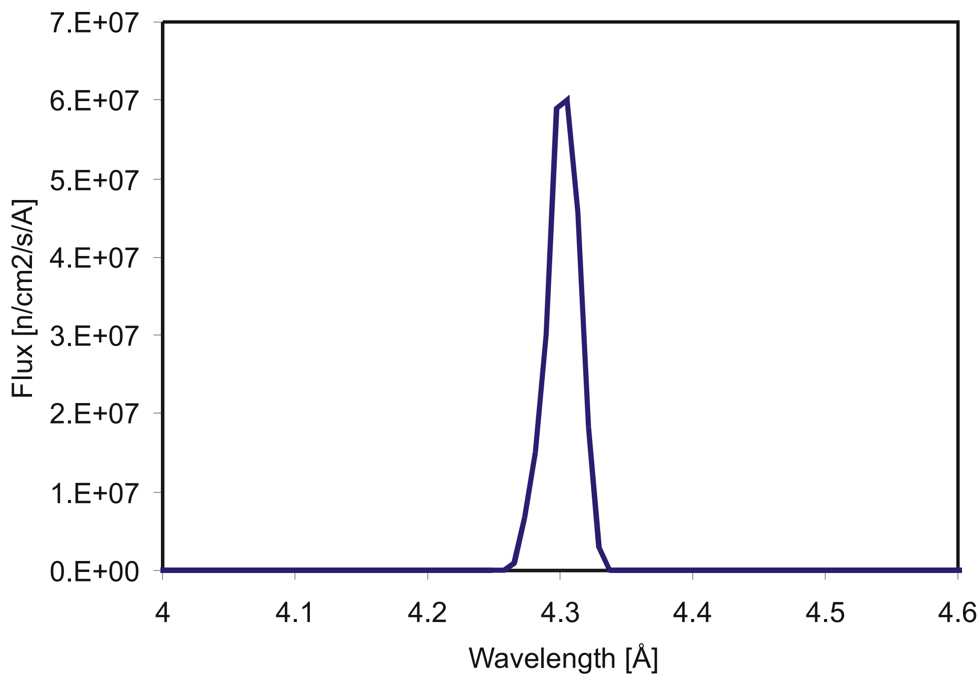

Figure 4. A Monte Carlo simulation of an incident pulse measured on the detector at 18m. The chopper setup is the same as in Fig 2. For all choppers, the distance between the center of the chopper opening and the center of the disc is set to 25 cm. Both the T1 and T3 choppers have 300 Hz counter rotating blades and the openings on the blades are 10°. Chopper T1 have two symmetrical openings while T3 have one. Chopper T2 rotates at 60 Hz and have a wide enough opening to let the pulse at 4.3Å pass through. The neutron pulse corresponds to an energy of E_i ~ 4.4 meV and have a dE_i/E_i (FWHM) of ~ 1.2%.

Therefore, the incurred cost of extending the EQ-SANS to be able to measure inelastic scatterings at very low-Q is the cost of modifying two of the bandwidth choppers. The returned benefit is the flexibility for users to be able to screen out inelastic scatterings without having to conduct experiments on two separate instruments.

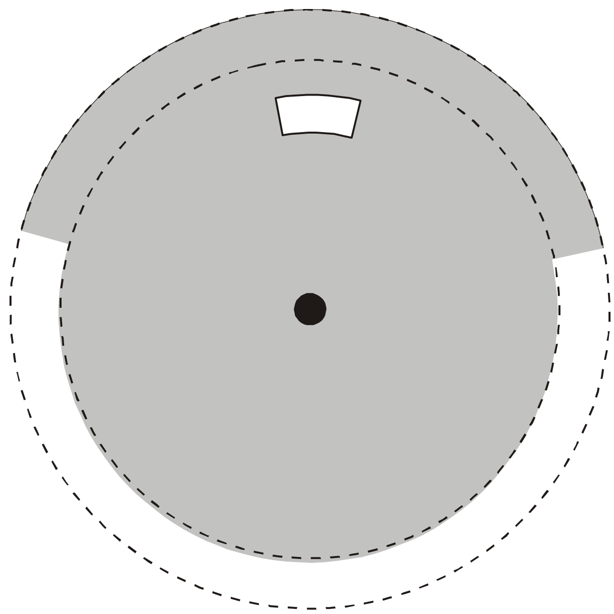

Figure 4. Schematic of a chopper disc for dual mode operation of the EQ-SANS. The large opening on the outer rim is used for SANS operation while the small opening is for chopper operation. By moving the chopper up and down and aligning one of the openings with the neutron beam, different chopper mode can be selected.

References

1. Conceptual Design and Performance Analysis of the Extended Q-range, High Intensity, High Precision Small Angle Diffractometer for SNS, May 2000, Jinkui Zhao, SNS report No. IS-1.1.8.2-6036-RE-A-00
2. A report on SNS Reflectometers Neutron Optics Review, June 2001, compiled by D. Abernathy.
3. SNS Neutron Scattering Instrument Status Report, June 2001, http://www.sns.gov/users/data_sheet_cover_material.pdf

Attachment Reply to suggestions and recommendations from the Scientific Review of the EQ-SANS

(Listed from up- to downstream)

1. The initial 1m of rectangular guide prior to the bender entrance (in core vessel insert) is not necessary and may even be limiting the flux. I suspect that a tapered collimation allowing the bender entrance a full view of the moderator may do better. Figure B4 compares flux at the "end of the bender" with and without this 1m guide, but what was the "collimation" assumed here? (Heenan)

The flux comparison was carried out with ±1° source divergence, which roughly corresponds to 1 m collimation length. Hence, the flux ratio at the end of the benders reflects that of the sample position with 1m collimation.

The main purpose of this 1m rectangular beam geometry in the core vessel insert is to enable the effective blockage of the direct line-of-sight. It is for this reason that a tapered opening allowing the full view of the moderator by the bender is not desired. Inserting a section of straight guide into the beam here should thus increase the flux at the sample position.

Follow ups: full moderator to sample Monte-Carlo simulation was performed for quantitative comparison (Fig 1)

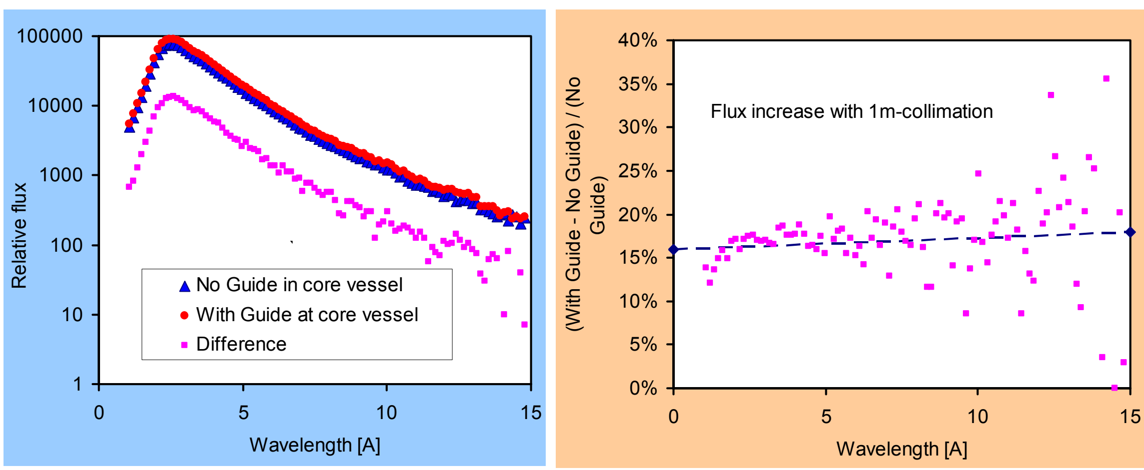

Fig.1 Moderator to sample simulation with and without the core-vessel guides. Left: relative fluxes at the 2cm x 2cm sample with a 1m collimation length (from the end of the guide system to the sample). Right: relative guide gain. The simulation conditions are as the following: (1) The moderator source generate neutrons between 1-15Å with a max divergence of 1°. (2) A slit is located at 1m from the moderator. This is the place where the core-vessel starts. (3a) For simulation with the core-vessel guide: a slit is placed at 1.27m from the moderator and a 1m guide after that. (3b) For simulation without the core-vessel guide: a slit is placed at 2.27m. (4) a curved bender 3.06m long with the radius of curvature of 68m. (5) A straight guide is placed between 5.35 - 13m from the moderator. (6) A 2cmx2cm detector is placed at the sample position of 14m from the moderator. All slits, guides and benders have the same cross-section of 4cmx4cm. The super-mirror coating for the guides and benders is 3.5x*Ni*-Θc, except the convex

on the side of the bender, which is 2x. These geometrical parameters reflect the actual engineering design and differ slightly from those of the conceptual design

2. Has the effect of increasing the guide & bender height to say 5 or 6cm been investigated? This might improve flux at shorter sample-detector distances? (Heenan)

This was briefly considered. A higher beam might increase the total flux. The concern was that with a non-square beam, sample, and beamstop, the quality of the Q-min data will be degraded. Thus the increased flux will mainly benefit shorter sample-detector distances where Q-min is not the primary concern, as was pointed out by the reviewer. However, with the current detector technology, it is more likely than not that the detector at shorter distances will, or close to, be saturated even with the current beam cross-section.

In the following months, we will quantitatively compare the flux of higher beams to the current design. We will also analyze the added cost to the neutron optical system. We will also seek to evaluate the effect of the added background and the radiation dosage at the sample enclosure that might rise from a larger beam.

Follow ups: Flux vs. Guide-height simulation was performed. Under the operation condition for the EQ-SANS, no flux advantage is seen for increased guide height (Fig 2).

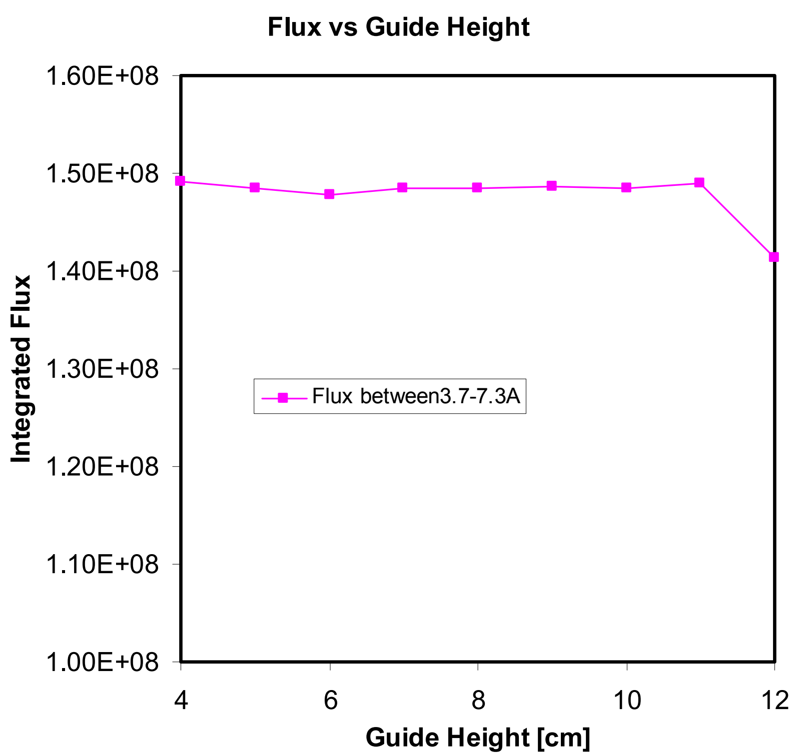

Fig 2. Flux at the sample position vs. Guide-height simulation. The simulation condition is the same as that in the conceptual design document (SNS IS-1.1.8.2-6036-RE-A-00) with 4m collimation. The sample size is kept at 2cmx2cm.

3 Multi-chopper mode operation – Its usefulness, usage, and justification. (Heenan)

The chopper mode operation is not suited for *dedicated inelastic measurements (Heenan)*, rather, it is intended for weak scatters at low-Q such that inelastic contributions to small angle scattering can be separated out.

Currently, there is a LDRD project at ORNL to study the effect as well as the separation of inelastic contributions to small angle neutron scattering using multiple bandwidth choppers. We will closely interact with the ORNL team on this subject. One area of attention is the resolution and energy transfer range that are required for such undertaking.

The chopper mode operation is included in the baseline funding. Our design purpose is to preserve further upgradeability with no SANS-performance and minimal cost impact.

4. Pulse rejection to 30Hz. (Heenan)

Pulse rejection has been considered though it is not written in any of these reviewed documents. If every other pulse is rejected (30Hz) and assuming detector is at 18m, One could for example choose to use 1-8.3Å or 3.66-10.99Å neutrons. There will be a leakage between 14.25~15Å for the former and 16.85~17.65Å for the latter cases, respectively. These leakages can be eliminated by adjusting the chopper openings and phases, with the penalty of reducing the total useable bandwidth slightly (by <1Å in both cases).

Operating with longer wavelength, e.g. 7.33-14.65Å, will be more difficult. In addition to the leakage at the longer wavelength of 20.65~21.35Å, there will be a leakage at 0.85~1.65Å.

5. Fourth Frame Operation (Glinka)

Higher Frame Operation was not discussed in the documents. In principle, the instrument should be able to operate in higher frames just like in the lower ones. In the fourth frame and with the detector at 18m, the neutron band will be at 10.99-14.65Å, giving a Q-min of ~ $0.003Å^{-1}$.

6. Need Interchangeable beam aperture at 10m and before sample. (Heenan)

Before the sample, we intend to use manually exchangeable apertures, possibly mounted directly on the sample holder. At 10m, an aperture wheel has been considered, though not designed. Many of these engineering design works will be performed in FY 02.

7. Displace Carousels to improve shielding. (Heenan)

In the current engineering design, these carousels are collinear. This may indeed weaken the shielding effect of the carousels. We will look into the engineering model for offsetting one of the carousels. This will be conducted in FY02.

8. Soller Collimators – design, usefulness etc. (Thiyagarajan/Glinka/Heenan)

The usage of cross Soller collimators in the design has raised many concerns. Besides manufacturing difficulties of the two 1m long collimators with sub millimeter channel widths, reflection and parasitic scattering from the collimator appear to pose a huge technical challenge. Thus the benefit of cross Sollers may not warrant the investment.

The usefulness of the Soller collimators appears now in doubt. We will look into other ways of accessing lower Q-min, such as *longer detector to sample distance (Heenan*) and using *fourth frame (Glinka)*. In particular, we will look into the cost increase of extending the scattering tank.

9. Sample Area Access. (Thiyagarajan/Glinka/Heenan)

The current design of the sample area has not been fully reflected in the design criteria document (DCD). The current layout calls for horizontal personnel access to the sample area. Heavy equipments are lowered down from the top platform, presumably on the level as the mezzanine.

Viewing the sample at any time during an experiment (Thiyagarajan) is possible but may be limited by the personnel protection requirements. We will look into using video equipments to monitor the sample.

Large sample area (0.75-1m) with adjustable sample table (Thiyagarajan) is in fact the current design. The low angle detector tank is designed to be retractable to accommodate large equipments.

We will work closely with the SNS sample environment group to ensure the smooth operation of the large equipments on the Extend-Q SANS.

We are building a mock up stand for the whole sample detector tank and sample area at ANL such that we can have a real feeling about how much space there will be for use access. Issues such as *Floor level (Thiyagarajan*) will also be looked into in the mock up.

10. High angle detector bank – costs, configuration, normalization (Chen/ Thiyagarajan/Glinka/Heenan)

The current design of the high angle detector is not fully reflected in the DCD. Together with the SNS detector group, we have been looking into using position sensitive ^{3}He-tubes for the high angle detector bank (*also suggested by Glinka*). This should address the price tag issue while provide good performance. *Detector coverage beyond 40°* (*Thiyagarajan*) should not increase the instrument cost significantly with the tubes and such coverage does seem to be useful for studying such systems as *the perturbation of the solute to the structure of the solvent and the phenomenon of hydrophobic hydration (Chen)*.

Even though the sample area is designed for large equipment access (~ 1m radius), we will incorporate the suggestion of *having the high-angle detector be removable (Glinka)* such that future experiments are not limited by space.

The high angle detectors are not in the current project baseline, though we are confident that with the SNS project progresses, we will be able to free enough money to install the high angle detectors. In the same time, we are also looking into alternative detector technologies such as cross fiber scintillators (Li-Gd-B). The gamma ray discrimination technology on the Li-Gd-B system appears to be able to reduce the detector background to the same level of a ^{3}He detector. It may take a long time for such technologies to result into useable products. Once the technology matures, however, it will allow us to equip both the high and low angles with high counting rate, low background, and low cost detectors.

Normalizing between the high and low angle detectors (Chen/Heenan) may indeed present some challenge. We will work closely with the SNS data acquisition group on the normalization issue. We will also try to learn from experiences on SAND at IPNS.

11. Low angle detector and detector tank

The absolute Lateral positioning accuracy is irrelevant (Heenan) for determining the beam center. However, since the detector will most likely be moving back and forth during an experiment, or at least between experiments, we believe lateral positioning reproducibility is important. Otherwise the detector beam stop will have to be constantly realigned. We will look into relaxing the accuracy requirement and the cost saving it may result.

The scattering tank travel (Heenan) has been reduced to ~ 1.5m to save cost and space. Though we will look into extending it again for accessing lower Q-min (refer to 8), or to have a longer tank.

We will incorporate the recommendation of *using fused silica or c-axis cut sapphire as the low angle scattering tank window (Heenan)* in our design.

Moving the low angle detector or tank sideways (*Heenan*) appear to be difficult from the engineering point of view. We have considered moving the tank briefly in the very beginning of the conceptual design phase, but since have abandoned the idea. Moving the detector within the tank is difficult with the current tank diameter. But it would be relatively easy to achieve when a larger tank is used. We will investigate these options.

The tapered cone on the detector tank (Heenan) should be adequate for 1m sample to detector distance. However, we will work closely with the SNS sample environment group to ensure that the cone will work with large sample equipments that may be used on this instrument.

13. Sample geometry, sample exchanger. (Glinka/Heenan)

The conceptual design specifies that the *Maximum sample size (Heenan)* should be ~ 2cm. Larger samples should be possible, though may no longer be optimal for pinhole setups, since the neutron guides and benders are designed to have the crosssection of 4x4 cm^2.

Sample geometry is indeed a difficult issue since the *low and high angle detectors work best with either flat or cylindrical samples respectively* (*Glinka/Heenan*). As it appears that there is no easy solution for deciding the sample geometry, decision has to be made on a case-by-case base.

We have not finished the detailed engineering design of the sample exchanger. It will have to be *vertical moving (Heenan)* as suggested.

12. Beam monitor, transmission monitor, beam stops (Heenan)

Beam and transmission monitors are being considered, though not yet incorporated in the engineering design. The main reason for this is that we have not determined what kind of beam monitor will work best to cover the wide energy range required on this instrument. We are working closely with the SNS detector group to resolve this issue. The location of the beam monitor is considered at 10m.

For the transmission monitor, we have considered two possible techniques. One is to use an attenuated pinhole in the detector beamstop as has been used elsewhere. The other one is to put a small scintillation detector on the detector beamstop or to put scintillating materials on the beamstop and readout the light from a camera fixed on the scattering tank.

We will work with the detector manufacture on the *beam stop positioning device (Heenan)*. The mechanism used by the ORNL 5m SAXS machine appears to be adequate. It uses thin wires to hold the beam stop. The wires can move up and down, or left and right.

14. Shielding (Heenan)

We are planning to conduct Monte-Carlo simulations on the shielding, similar to what have been done on other instruments. These simulations should help us determine the best shielding configuration. In doing so, we will take all the recommendations into account. Depending on the funding situation, these simulations may be performed in FY02.

15. Shutter (Heenan)

We plan to get at least one carousel back into the baseline and use it at the secondary shutter. We will use the shielding calculation (ref. 14) to verify whether it will be sufficient to block the beam.

16. Software (Heenan)

Data collection and moving motors around (Heenan) are being designed and worked on by the SNS data acquisition group, as well as the detector and sample environment groups.