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Solid Mechanics

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Conceptual and Detailed Design of the NMX Beam Geometry Conditioning System

Master's Dissertation by

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Lund, June 2016

Niklas Granlund

ABSTRACT

The European Spallation Source ERIC is a new neutron spallation source being built in Lund, Sweden, with NMX as one of the pioneer instruments. NMX is a Quasi-Laue single crystal neutron diffractometer for the investigation of large biological molecules. Wavelength, size and divergence of the neutron beam reaching the sample have to be controlled to properly match the different experimental needs. The wavelengths are selected using rotating disk choppers. Size and divergence of the neutron beam at the sample position are controlled by the Beam Geometry Conditioning System (BGCS) installed in proximity of the end station.

The purpose of the project is to perform the concept design and development of the Beam Geometry Conditioning System for NMX, to optimize the neutronic performance of the system. The BGCS requires a motorized Pinhole Aperture that is not commercially available. As the Pinhole Aperture is in close proximity to the sample the requirements on the design are rigorous. The footprint of the system and its interaction with neutrons scattered by the sample should be minimized, along with the background noise in terms of beam halo and gamma radiation.

The development of the design has been carried out according to the design process defined by the ESS standard presented in the document *Design Process and Control (ESS-0002411)*. This standard defines the required activities, different roles in the project and who is responsible for each activity. The design process is divided into three main phases, the concept/plan phase, the initial design phase and the detailed design phase. Each phase has to be reviewed and approved before the design may enter the following phase.

The BGCS is broken down into subsystems, individually designed to be assembled to the complete system. The main subsystems are the Collimation System, the Support Tables and the Vacuum System. The focus of the project is the development of the Collimation System, consisting of the Beam Defining Apertures and the Cleanup Apertures. The design has been performed from the basic architecture of the system, the concept design of the BGCS up to the detail design of the Pinhole Aperture.

The main component of this project is the Pinhole Aperture. The design of this system has been evaluated using the concept scoring method, to find the most feasible solution. The result of the concept selection is that the Pinhole Aperture shall consist of a rotating arm that places an absorbing cartridge in line with the neutron beam. The cartridge has a fixed aperture, defining the beam size. To change the aperture size the arm rotates to place the active cartridge in a carousel. The carousel stores cartridges with different aperture sizes, keeping them out of the neutron beam. The desired aperture size is selected by rotating the carousel to place the corresponding cartridge at the arm. The arm grabs the cartridge using magnets and the arm rotates back to place the new cartridge in line with the neutron beam.

There are three main benefits of this system design. The primary benefit is that it is possible to place the aperture close to the sample, which is the most important scientific property as it reduces the beam halo. The second benefit is that specific aperture sizes and shapes may be achieved by manufacturing cartridges matching the needs of the experiment. The last benefit is that the system is easily adjusted for future changes of the requirements. There are many uncertainties regarding which materials to use and the design of adjacent equipment. The system has been validated using Monte Carlo simulations performed with the software McStas.

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1. INTRODUCTION

A brief introduction of the company and the project is presented in this chapter.

1.1 Background

The European Spallation Source ERIC (ESS hereafter) is constructing the new European neutron spallation source in Lund, Sweden. NMX, one of the pioneer instruments, is a Quasi-Laue single crystal neutron diffractometer for the investigation of large biological molecules. To perform the experiment, the instrument will extract neutrons produced by the spallation process in the ESS target. The moderated neutrons are then guided to the instrument end station. At the end station single crystal samples will be studied by exposing them to the neutron beam and collecting the scattered neutrons. The pattern of the scattered neutrons will provide information on the structure of the molecule within the crystal. Wavelength, size and divergence of the neutron beam reaching the sample have to be controlled to properly match the different experimental needs. Wavelengths are selected using rotating disk choppers. The size and divergence of the neutron beam at the sample position are controlled by the Beam Geometry Conditioning System that is installed in proximity of the end station.

1.2 Purpose and Objectives

The purpose of the project is to perform the concept development and design of the Beam Geometry Conditioning System for NMX, to optimize the neutronic performance of the system.

It was foreseen that the concept would require a motorized pinhole collimation system that is not commercially available. As the pinhole collimator is in close proximity to the sample the requirements on precision and stability are high. The absorption process of the undesired neutrons will release gamma radiation. The number of gamma rays reaching the detector system should be minimized, to minimize the background. It is also important to minimize the footprint of the system on the backscattered neutrons. Conceptual and detailed design of the pinhole collimation system was performed to fulfill these requirements.

A concept for the Beam Geometry Conditioning System is to be presented at the end of the project, along with a detail design of the pinhole collimation system including construction drawings. The pinhole collimation system should be ready for prototyping.

1.3 Focus & delimitations

The most challenging task was anticipated to be the design of a pinhole collimation system that can precisely position the neutron absorbers in the proximity of the sample with high precision, stability and minimal footprint. The focus of the project was to perform the conceptual design of the pinhole collimation system in a controlled and documented manner, following to the ESS design process standard.

The thickness and materials of the absorbers used to remove the undesired neutrons are not investigated as these parameters are determined based on detailed simulations performed by the Neutron Optics and Shielding group at the ESS. No forward scattering of the different components of the system is taken into account.

2. NEUTRON SCIENCE

Before the design process commences, it is important to understand the physics underlying the experiments to be performed at NMX, as this is central to the instrument operation. This chapter presents the basic mechanisms behind neutron experiments.

2.1 Neutron

All elements consist of atoms. Atoms, in turn, consist of three subatomic particles, being protons, neutrons and electrons. Neutrons were first discovered in the 1930s (Chadwick 1932). An atom has a nucleus where the protons and the neutrons are located, with electrons surrounding the nuclei in different shell-like layers. The number of protons and electrons of the atom defines the element. The same element may have a different number of neutrons in the nucleus. These different variants of the same element are called isotopes.

Free neutrons interact with matter through the nucleus of the atoms, as the neutron has no electric charge it is not affected by electrical forces caused by the electrons, magnetic moment excluded. Neutrons only interact with the atom through the nuclear forces in the nuclei, which have much shorter range than electrical forces. Thus, neutrons have much higher ability to penetrate matter compared with charged particles (Pynn 1990, 2).

The likelihood that a neutron interacts with a nucleus of an element is connected to a parameter called cross section. Elements with a larger cross section have a higher likelihood to interact with neutrons. There are two different outcomes of the interaction, the neutron will either scatter or be absorbed. When a neutron is absorbed by a nucleus it forms a heavier isotope of the element, in an excited state. The excited isotope is then either stable or not. If the isotope is stable the excess energy is emitted as a photon. If the isotope is unstable it will decay into either the initial isotope by emitting a neutron, or decay into another element and emit alpha and beta particle radiation (Baramsai 2010, 5).

2.2 Scattering

Neutron scattering occurs when a neutron is forced to deviate from a straight trajectory caused by interaction with the nucleus of an atom. The neutron may scatter in any direction. To explain the process, it is easiest to describe the neutron and the nuclei with wave functions, with wavelength, amplitude and phase. Neutron scattering may be either coherent or incoherent. Coherent scattering means that the phase of the neutron is unaffected by the scattering while incoherent scattering changes the phase. The scattering is usually elastic, meaning that the kinetic energy is conserved. Mathematically, it does not matter if the neutron is referred to as a wave or a particle as both models will come to the same conclusions. The wavelength of a neutron is connected to its energy and hence its velocity.

2.3 Diffraction and Interference

When a parallel wave of water hits an obstacle with a slit, the wave will bend and the slit will act as the center of the wave. This phenomenon is called diffraction. If the obstacle has two or more slits, each slit will give rise to a wave. As these waves propagate they will start interacting with each other. The interaction between multiple waves is called interference. At specific location the waves will be in phase and enhance each other by adding up. This is called constructive interference. At other locations the waves will be out of phase and instead cancel each other out, leading to destructive interference. The same effect will be obtained with any kind of waves, such as light. At specific angles the scattered light will be in phase and create constructive interference which will form bright areas, see Figure 1. If a wave of neutrons hit a lattice of atoms the same phenomenon can be observed. The neutrons will scatter off the atoms and, at certain angles, constructive interference will create a pattern like the one in Figure 1. The observed phenomenon is called Bragg diffraction. The connection between the angle, the wavelength and the lattice parameter is described by Bragg's law, see Figure 2.

To achieve this phenomena, the phase of the scattered neutrons must be unaffected by the scattering, *i.e.* coherent scattering. If the scattering is incoherent the phases of the scattered neutrons do not match and the neutrons will not interfere with each other. This means that all incoherent scattering will be noise and not contribute to the interference pattern.

By controlling the wavelength and measuring the angle θ, Bragg's law gives the lattice parameter, also known as the d-spacing. Another important usage of the diffraction is to measure the intensity of the reflections, as this provides information about the distribution of scatterers inside the repeating unit.

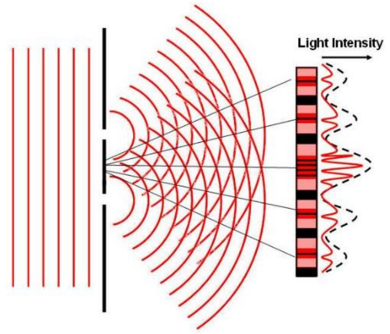

Figure 1 – Illuminating two slits give rise to constructive interference (Cronodon)

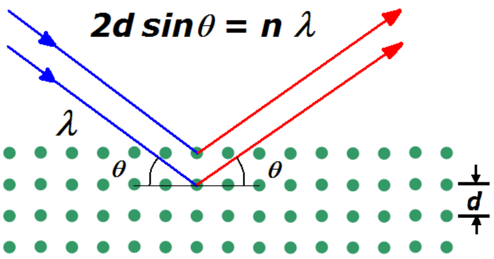

Figure 2 – Bragg diffraction (Wikimedia Commons, 2009)

2.4 Neutrons in experiments

An important parameter when characterizing materials is the distribution of atoms within the structure, as it is connected to the behavior of the material. In order to measure the distribution of atoms, a probe with sufficiently short wavelength is required. It is only possible to measure distances down to the wavelength of the used probe and the wavelength of visible light is approximately a factor thousand larger than atomic spacing. X-rays, on the other hand, are photons with higher energy and thus shorter wavelength than visible light. This makes X-rays a suitable probe for many fields of material studies. However, X-rays interact with materials depending on the amount of electrons surrounding the nucleus of the atom. Materials with higher atomic number have more electrons than materials with lower number and will therefore have higher interaction with X-rays; see Figure 3. This is a good attribute in many experiments, but a limitation in others. There are primarily two cases where this behavior is a limitation. The first case is if the interesting area of the sample is hidden behind a high density material. In this case the high density material will block all the X-rays, obscuring the interesting area. The other case is if the materials in the sample being examined have similar interaction with the X-rays. This will give a homogenous result that is hard to extract any useful information from. A better probe in the described situations are neutrons.

The most significant disparity between neutrons and X-rays is the way they interact with matter. Neutrons, contrary to X-rays, do not interact with atoms based on the amount of electrons surrounding the nucleus, but the structure of the nucleus itself. This allows not only the distinction of different elements, but also different isotopes of the same element. The mass attenuation coefficient for neutrons varies greatly between different elements; see Figure 3. One particularly important property of neutrons is the interaction with hydrogen, as hydrogen has one of the highest mass attenuation coefficients. Here follow two specific examples of experiments demonstrating some of the advantages of using neutrons.

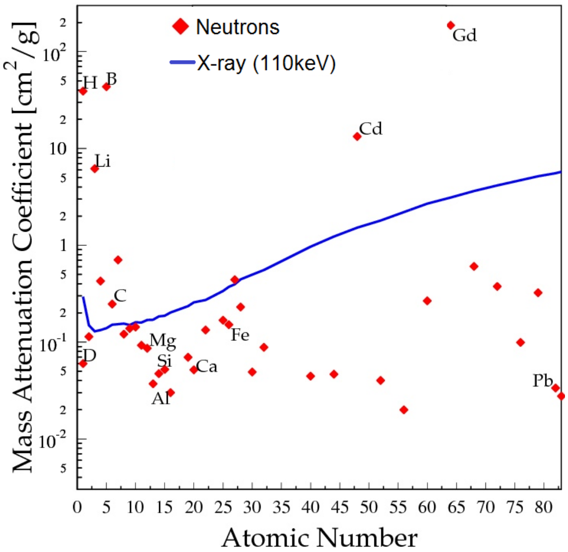

Figure 3 – Mass attenuation coefficient based on atomic number for X-rays and neutrons (McClellan Nuclear Research Center, UC Davis)

The first example experiment has been performed at the National Institute of Standards and Technology (NIST). The experiment aims to make a radiographic image of a flower placed in a lead can. A radiographic image is made by monitoring the amount of the incoming radiation that passes through the studied object and reaches the detector. Making a radiographic image of the can using X-rays will not reveal the flower inside, as the lead absorbs all the X-rays. Performing the same experiment with neutrons instead of X-rays gives a completely different result. Neutrons pass through lead, but the flower contains water and, hence, hydrogen resulting in a higher neutron absorption. The result of is experiment using neutrons is shown in Figure 4.

Figure 4 – Lead can containing a flower used at NIST to make a radiographic image of the flower, result using neutrons shown to the right (National Institute of Standards and Technology)

The second example is of a cartridge for a rifle. In this case, the different probes reveal different information regarding the cartridge. A cartridge can be divided into two main parts, the bullet and the shell. The bullet is made out of lead which is covered with copper. The shell is made out of a tube of brass filled with gunpowder; see Figure 5.

Figure 5 – Arbitrary cartridge showing its inner structure (Wikimedia Commons)

A radiographic image made with X-rays clearly shows the lead bullet and it is possible to see the copper covering the lead. The shell is thicker further back, causing a fading shadow effect in the image. Gunpowder does not interact strongly with the X-rays as it does not contain any high-density elements and is therefore transparent in the image, see Figure 6.

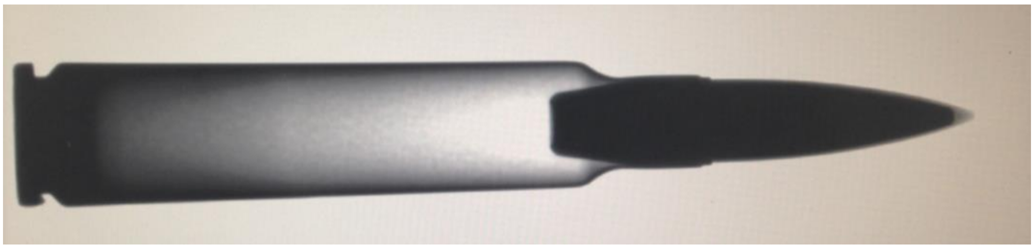

Figure 6 – Radiographic image of a cartridge using X-rays (Vattenhallen Science Centre)

Repeating the experiment with neutrons instead of X-rays reveals the gunpowder, as it contains hydrogen. Approximately 1% of gunpowder is residual water. Cupper also interacts with neutrons, but not to the same extent as hydrogen. The result is that the bullet and the brass shell interact with some neutrons, showing as grey areas. The gunpowder interacts with many neutrons and is therefore black; see Figure 7.

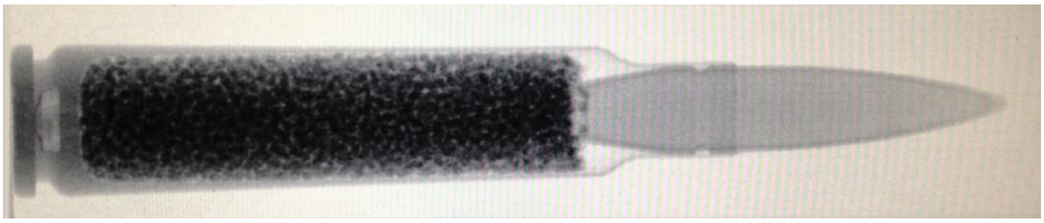

Figure 7 – Radiographic image of a cartridge using neutrons (Vattenhallen Science Centre)

2.5 Macromolecular diffraction

Macromolecular diffraction is a key method in understanding the structure of biological crystals. More than 100 000 protein structures have been determined using X-ray diffraction, providing crucial information regarding an array of biological processes and systems. The usage of neutron diffraction to examine biological molecules has to-date been limited, compared with X-rays. Only 103 protein structures have been determined and registered in the Protein Data Bank using neutron diffraction, to this date (RCSB 2016). It is evident that X-rays and neutrons provide complementary information of the atomic structure, due to their difference interaction with matter. X-rays interact with electrons and thus provide information regarding the electron density of the atoms. Neutrons on the other hand interact with the nuclei of the atoms and therefore provide information regarding the nuclear density (Blakeley 2009). Another key property of neutrons is the ability to locate hydrogen. The location of the hydrogen atoms in the crystal is crucial for the understanding of the structure. A comparison of a protein structure determined using X-rays and neutrons are shown in Figure 8.

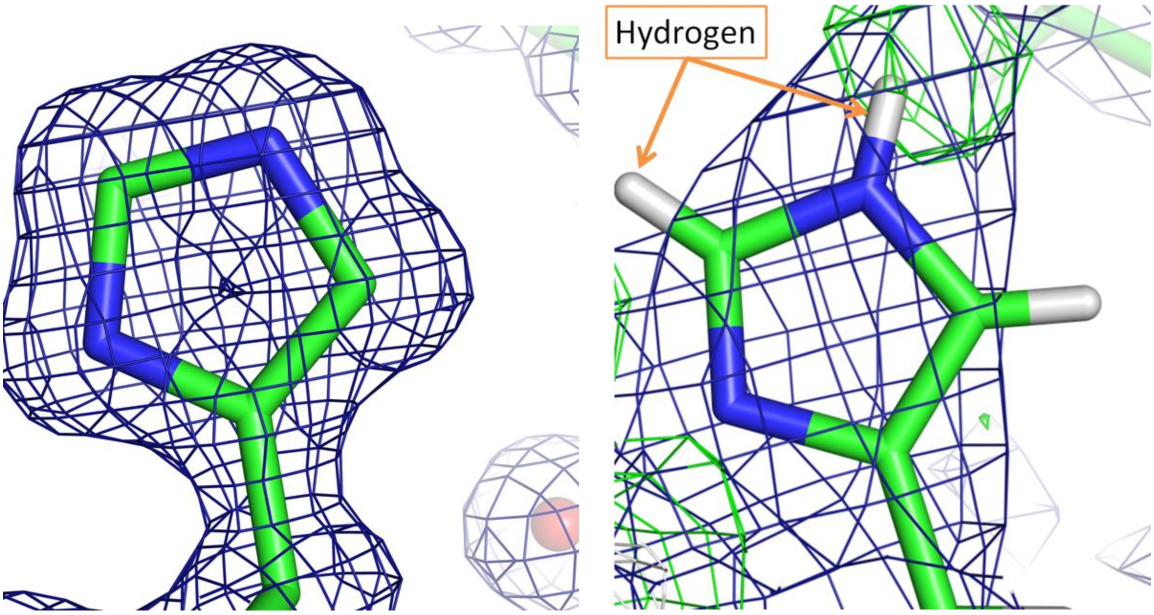

Figure 8 – Protein structure determined using X-rays (left) and using neutrons (right), revealing the location of the hydrogen (E. Oksanen, Vattenhallen Science Centre)

There are two main reasons why neutron diffraction has been used in such limited extent to analyze biological structures, in comparison to X-rays. The first reason is the fact that neutrons were discovered almost 40 years later than X-rays. X-rays were the first probe with sufficient short wavelength to match the spacing between planes in crystals. Hence, X-rays have been the obvious method to analyze crystal structures. This has led to the development of X-ray sources and hence there are more X-ray sources spread around the globe, increasing the availability. The first neutrons were observed in the 1930's, but it was not until the introduction of fission reactors that the flux was high enough to perform the most basic diffraction studies. The first research facility designed specifically to neutron studies was built in the late 60's. However, there have not been any instruments dedicated for neutron macromolecular crystallography until recently. This leads to the second and most important reason, namely that neutron sources have low flux compared with X-ray sources. Flux is basically the intensity of the beam, measured in particles per area and time. Neutron sources have flux in the range of $\sim 10^6$-10^8 neutrons cm^{-2} s^{-1} and X-ray sources in the range of $\sim 10^{10}$-10^{11} photons cm^{-2} s^{-1}. To compensate for the lower flux, neutron beams usually have much larger dimension and wavelength spread. To match the larger dimension of a neutron beam a much larger sample is required compared with X-rays, usually in the range of 1 – 10mm^3 for neutrons compared with 1µm^3 – 0.001mm^3 for X-rays (Blakeley 2009). Preparation of biological crystals is a challenging process that is time consuming, especially with crystals of this size. Growing and preparing the samples are generally the bottlenecks in neutron protein crystallography (Teixeira 2008). To optimize the result of the experiments, it is important to collimate the neutron beam to match the sample size as will be described in the following chapter.

3. THE NMX INSTRUMENT AT ESS

In this chapter ESS and the NMX instrument are presented, describing the Beam Geometry Conditioning System in context of the instrument.

3.1 The European Spallation Source

The European Spallation Source ERIC (ESS) is a new neutron spallation source being built in Lund, Sweden. Spallation is a technique to extract neutrons from a target, instead of using a nuclear reactor. The principle of the spallation, which will be used at ESS, is to accelerate a pulse of protons and to guide them to collide with a target of tungsten. When the protons collide with the tungsten it will release neutrons. The released neutrons will not be immediately suitable for being used by an instrument, as they will have too high energy. They will therefore be decelerated to a more convenient speed by passing through a moderating medium. In the ESS case, this media is water and liquid hydrogen. The moderated neutrons will then be guided to the different instruments. The pulses will be repeated with a frequency of 14Hz, providing ESS with its pulsed beam structure.

ESS is a collaboration between currently 17 European countries. When completed, ESS will be the world's brightest neutron source with up to a hundred times brighter beam than the current leading facilities (European Spallation Source). The first neutrons are expected to be extracted from the ESS target in 2019 and the first user experiments to be performed in 2023. A wide range of instruments will be connected to ESS, applying to many different fields of study. Currently two instruments have entered the detailed engineering design phase, with the NMX Macromolecular Diffractometer as one of these.

3.2 Neutron Macromolecular Crystallography at NMX

NMX will be a Quasi-Laue single crystal neutron diffractometer for the investigation of large biological molecules. To perform an experiment, the instrument will extract moderated neutrons produced by the spallation process in the ESS target and will guide them to the instrument end-station positioned about 150m away from the target station. At the end-station a single crystal sample will be exposed to the neutron beam and diffracted neutrons will be collected by a detector system. The intensities of the diffracted neutrons provide information on the structure of the biomolecule in the crystal.

3.2.1 Quasi-Laue Diffraction and the Time of Flight Principle

All early neutron studies were performed using a neutron beam with a defined wavelength, a monochromatic beam. By removing all neutrons with different wavelengths, the flux reaching the sample was greatly reduced. The reason behind this was the fear that when exposing the sample to different wavelengths, the reflections would be impossible to separate and information lost. It was shown that this is not the case when detectors with sufficiently high resolution were developed (Niimura 1998). In the Laue diffraction method a stationary crystal is exposed to a white beam, *i.e.* a beam with a broad spectrum of wavelengths. By exposing the crystal with all available neutrons, the incident flux is maximized. However, for large unit-cell systems a white beam can cause extensive spatial overlap between Bragg reflections and will also lead to higher background. Quasi-Laue diffraction is an intermediate solution where a restricted spectrum of wavelengths is used to expose the sample. This method gives the best signal-to-noise ratio when investigating large crystals (Blakeley 2009).

The wavelengths of the neutron beam that reaches the sample at NMX will be selected using the time of flight principle and rotating disk choppers. As mention earlier, the wavelength is connected to the energy and thus the velocity of the neutron. The neutrons are selected depending on the time it takes them to travel a certain distance. As the neutrons will be produced in pulses, it will be possible to tune the frequency that a disk with an aperture rotates with to select the neutrons with the correct speed and thus the desired energy. This is the basic principle, but in practice it is more complicated and NMX will use three rotating disks to select the wavelengths.

3.2.2 NMX Samples

Biological crystals are very fragile and are only stable in the mother liquor in which they were grown, or in very similar conditions. To keep the crystals stable during experiment there are three different main methods that can be used. The first method is to place the crystal in a glass or quartz capillary surrounded with two drops of the mother liquor. The crystal is kept in place with the liquor; see Figure 9.

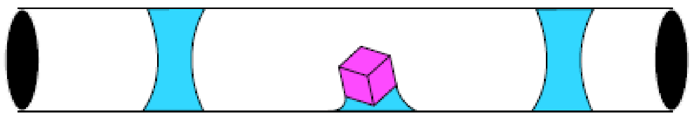

Figure 9 – Illustration of how biological crystal are kept in capillaries (E. Oksanen)

The second method is to place the crystal in a nylon or kapton loop with some mother liquor around it. There are two different variations of this method. Either the loop is kept in a stream of air with the correct vapor pressure or it is flash-cooled to down to 100 K. When the liquor is flash-cooled down to this temperature, it will vitrify without forming ice crystals.

In all these cases, there is mother liquor surrounding the sample. Mother liquor usually contains deuterium, an isotope of hydrogen. Deuterium has a high probability of interacting with neutrons by incoherent scattering. This is the main reason why controlling the neutron beam characteristics is important with biological crystals. The properties of the neutron beam are controlled by the Beam Geometry Conditioning System, installed just upstream of the sample position.

3.3 NMX End Station

The end station at NMX will consist of an assembly of different experimental equipment around the sample position. The main components of the end station will be the goniometer, the detectors, the beam stop and the cryostream.

The goniometer is a robotic arm that positions the sample during the experiments. The goniometer orientates the sample during an experiment to allow the structure of the crystal to be studied in all directions.

There will be three detectors mounted on individual robot arms to be able to place the detectors at different locations depending on the experiment. With this architecture it will be possible to place the detectors above the sample to detect backscattered neutrons. The reason why it is important to be able to collect backscattered neutrons is to be able to measure large d-spacing within the crystals.

During an experiment a large portion of the neutrons will not interact with the sample, instead they will pass through it unaffected. A beam stop will be placed between the sample and the detectors, in line with the neutron beam, to protect the detectors from the neutrons that do not interact with the sample. The beam stop should be as small as possible to not obscure any scattered neutrons, while blocking the full unscattered neutron beam.

As described earlier, in certain experiments the sample will have to be kept in 100° K. This will be done by the cryostream, which uses a stream of cold nitrogen gas to cool the sample.

The end station will be located inside a shielded room, called the experimental cave. The experimental cave’s main purpose is to prevent neutron and gamma radiation from reaching and harming personnel outside, but also to prevent background radiation from outside of the cave to reach the detectors. Most of the experimental equipment of the end station will be mounted on a large concrete base support. By having all the equipment on the same base, they will move together when exposed to temperature changes or sinking of the support below the cave. The Beam Geometry Conditioning System will also be installed inside the experimental cave. The end station, including an envelope for the Beam Geometry Conditioning System, is shown in Figure 10.

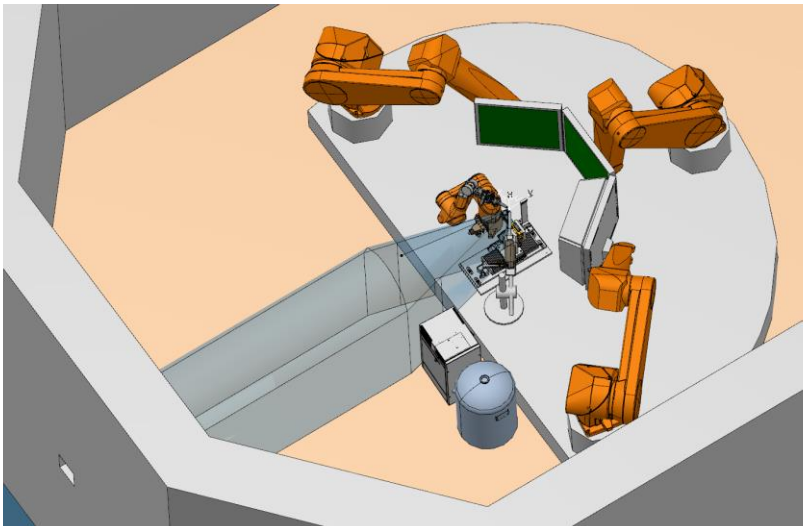

Figure 10 – Illustration of the NMX end station including the envelope model of the Beam Geometry Conditioning System (light blue)

3.4 Beam Geometry Conditioning System

The Beam Geometry Conditioning System is a collimation system that controls the geometry of the neutron beam reaching the sample. The system regulates two characteristics of the beam, being the beam size and the beam divergence.

The beam size is defined by the Full Width Half Maximum (FWHM) of the neutron beam, a definition used in probability theory. The neutrons reaching the sample plane will be distributed across the plane, depending on the distance between the sample plane and the downstream aperture, the size of the aperture and the divergence distribution. The shape of the neutron beam reaching the sample plane will be assumed to be a rectangle. To determine the beam size, the distribution of neutrons reaching the sample plane is integrated on one axis. The beam size is defined as the full width of the projected distribution at half of the maximum value. An illustration of the FWHM is shown in Figure 11. The process of identifying the FWHM will be adjusted to match the actual beam shape. The closer the aperture is to the sample, the sharper will the edges of the distribution be and the projected distribution will resemble a top hat distribution. The edges of the distribution become more diffuse as the aperture moves further away from the sample plane.

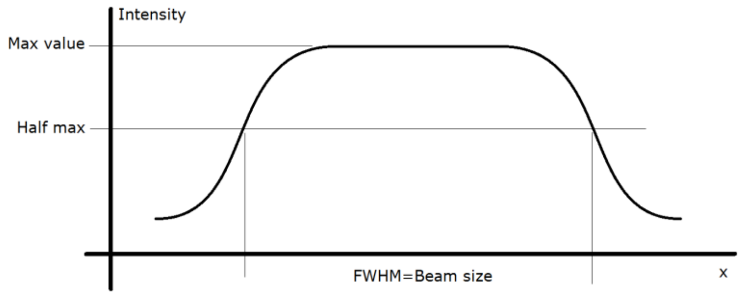

Figure 11 – Illustration of the definition of FWHM

Divergence is the angle between the direction that a neutron is traveling and the axis of the neutron beam. The entire sample should be illuminated with the selected divergence, with minimized contamination of neutrons with higher divergence. The beam divergence is defined according to the illustration shown in Figure 12. To minimize the contamination of large divergence neutrons the distance between the first aperture and the sample should be as large as possible.

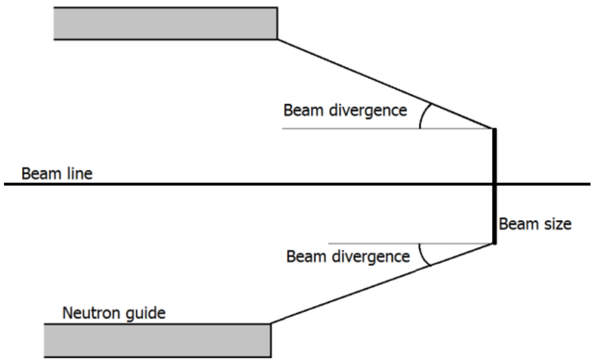

Figure 12 – Illustration of the definition of beam divergence

The reason it is important to control these beam characteristics is to optimize the conditions for the different experiments. The size of the neutron beam should match the sample size, to illuminate the entire sample without having a beam larger than the sample. Over illuminating the sample will allow the neutrons to scatter with the mother liquor surrounding the sample and cause background.

A neutron beam with high divergence will add background due to the different angles at which the neutrons hit the lattice in the crystal, effectively measuring different d-spacing.

Ideally there should be no divergence at all, to obtain the best result. However, crystals are never perfectly ordered. There are defects within crystals where the different crystal planes have a slightly different orientation, called mosaicity. Due to the mosaicity of the crystals some divergence of the neutron beam is acceptable without reducing the quality of the result. By allowing some divergence of the beam, the flux at the sample is increased. Divergence of the same magnitude as the mosaicity may be used. The allowed divergence varies with the crystal being studied and it is therefore important to control.

3.5 Collimation Principle

A collimation system narrows a beam of particles or waves to match the desired characteristics of the beam. This is either achieved by adjusting the direction of the radiation to meet the desired divergence, or by removing the radiation with undesired properties. There is a main kind of collimation system for each method of collimation. Collimation with curved mirrors changes the direction of the radiation and collimation with apertures removes the undesired radiation.

Collimation with curved mirrors is more common when dealing with photons than with neutrons, mainly as neutronic mirrors do not work well with large angles. It is also, generally speaking, a more complex and more expensive solution.

Collimation systems with apertures consist of two aligned apertures, see Figure 13. This is the most common solution used by instruments at neutron facilities. One aperture should be as close to the sample as possible to minimize the halo of the neutron beam and the other aperture should be as far away from the sample as possible to increase the collimation distance. The aperture close to the sample controls the size of the neutron beam. As this aperture is very small it operates as a pinhole and is called the Pinhole Aperture. The aperture far upstream from the sample controls the divergence and is called the Upstream Aperture. The material surrounding the apertures should have a very high neutron cross section to absorb as many neutrons outside of the usable cone as possible. Different kinds of radiation will be emitted depending on the material used by the aperture absorbers. If the radiation emitted is detectable by the detector system, additional shielding is needed to prevent the radiation from reaching the detectors.

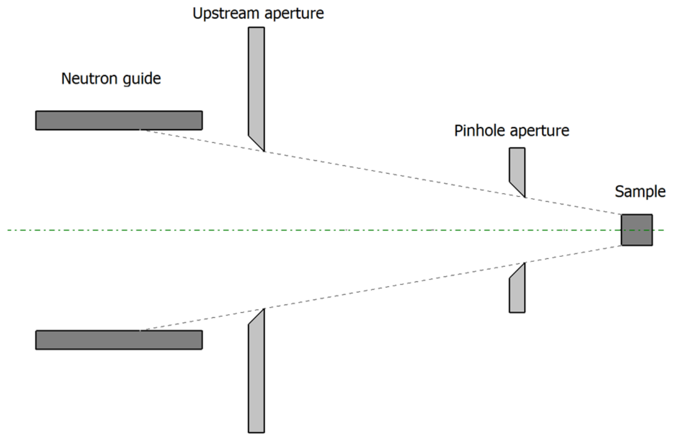

Figure 13 – Illustration of the principle of a collimation system with apertures

As collimation systems with apertures are in general better suited for neutron instruments plus simplicity and cost efficiency are some of the key factors for the design of the system, this is the solution that will be used in the following design of the Beam Geometry Conditioning System.

4. TOOLS AND METHODS

The tools and methods that are used to perform the development of the Beam Geometry Conditioning System are presented in this chapter.

4.1 Design Process

The development of the design is performed according to the design process defined by the ESS standard presented in the document *Design Process and Control (ESS-0002411)*. The standard defines the required activities, different roles in the project and who is responsible for each activity. The different roles are the project engineer, the designer, the lead engineer and the instrument lead engineer. In this project the project engineer and the designer are the same person, as are the lead engineer and the instrument lead engineer. Henceforth there are only two roles in the project, the designer and the lead engineer. The designer is responsible for the delivery of the project, the mechanical and engineering design and the detailed drawings. The lead engineer is the owner of the project and responsible for the reviews and approval of the design. A third person who will be supporting the project is the instrument scientific project leader, mainly supporting by reviewing the different steps of the design process to ensure that the system meets the scientific requirements.

The design process is divided into three main stages. The first stage is the concept/planning phase. This is the start-up of the project. The lead engineer presents the initial design specification to the designer. Based on these specifications, the designer defines the Engineering Design Specification (EDS). The EDS contains the system requirements, the envelope boundaries and the different interfaces. The EDS is reviewed by the lead engineer and the designer. As the EDS is approved the design process enters the second stage, the initial design phase.

As the name indicates, the initial design of the project is performed at this stage. The concept development is performed by the designer according to the EDS. 30-50% of the design should be completed at this stage. Different concepts are evaluated and the best design should be selected for further development. The concept selection is done by the designer in accordance with the lead engineer, based on how well the concepts satisfy the requirements. The initial design should be reviewed and approved by the lead engineer along with the designer before the development enters the third stage, the detailed design.

At the detail design stage the design should be 100% completed. All calculations and analysis should be completed. The final design should be reviewed and approved by the lead engineer before the designer creates the detailed drawings. Finally the detailed drawings should be reviewed and approved and the design process complete.

The Beam Geometry Conditioning System is a large system that will be divided into subsystems. Each subsystem will mainly be developed individually and then assembled into the full system.

4.2 Computer-Aided Design

The main tool for the development of the system is the CAD software CATIA® v6, a three-dimensional modelling system used at ESS. CATIA® is initially used to identify the design space of the system, by creating an envelope model that should contain the completed design. All parts and assemblies should then be modelled to fit within the envelope using CATIA®. The construction drawings will also be created using CATIA®.

4.3 Monte Carlo Simulations Using McStas

The Monte Carlo method is a numerical analysis technique to solve a range of mathematical and physical problems, based on probability theory. The procedure is to sample a large series of random numbers from a specified distribution, usually in the range of zero to one. Depending on the probability of an event to occur, a limit is set to divide the random numbers in whether the event occurred or not. By counting the times that the events occur according to the random number, and in what order, it is possible to draw conclusions regarding the scenario. The accuracy of the calculation increases with a large amount of sets of random numbers. The key to a successful Monte Carlo calculation is to have the correct probability that the event will occur in reality and the method of sampling random numbers.

One of the most used applications of the Monte Carlo method is transportation of subatomic particles. The mathematical model of the interaction between these and a nucleus is complex and in many cases it is impossible to obtain a solution without Monte Carlo calculations. A neutron traveling in a material may either scatter or be absorbed by the nuclei of the material. In between these interactions the neutron will travel in a straight line. The probable length a neutron travels in between two interactions is related to the neutronic cross section of the material. It is possible to predict the probable travel path a neutron will take through a material with Monte Carlo simulations. Repeating the simulation for many neutrons provides information of the average behavior of a neutron beam. This method is fundamental to many different areas in neutron facilities, from the neutron guide system to absorbers and shielding (Dupree, Fraley 2002).

McStas is an open source software, based on Monte Carlo calculations, for neutron scattering experiments. The Monte Carlo method is used in McStas to predict the neutron interactions and ray tracing is used to create images of the beam. Ray tracing is a method for creating images following the path from an imaginary camera to an imaginary pixelated screen, calculating what the camera will see in each pixel of the screen. This is used to simulate different kinds of detectors, such as intensity detectors and divergence detectors. The result of the detectors can be presented on a linear or logarithmic scale. The two options provide different information. A linear scale shows the peak in intensity of the beam more clearly than with a logarithmic scale. The logarithmic scale on the other hand provides information regarding the true size of the beam, as areas with lower intensity are shown more clearly.

In this project McStas is used at two different phases of the design process, for setting up the basic architecture of the system and for validating the functionality of the completed collimation system. McStas has two uses when setting up the basic architecture, to understand the properties of the neutron beam leaving the neutron guide in terms of divergence and to find the optimal position for the Pinhole Aperture.

To get as accurate results as possible, the entire NMX instrument is simulated in McStas, from the ESS neutron source up to the sample, including the neutron guides and choppers. An existing model of the NMX instrument up to the end of the neutron guide will be used. The Beam Geometry Conditioning System will be modelled throughout the design process, as the system is developed.

4.4 MATLAB

The result from the McStas simulations will be imported to MATLAB® to be evaluated. MATLAB® is a software and programming language for numerical computation, matrix manipulation and plotting functions. The main purpose of using MATLAB® is to calculate the beam size in terms of FWHM and to calculate the beam halo.

5. ENGINEERING DESIGN SPECIFICATION

This chapter contains the specification according to which the design of the Beam Geometry Conditioning System should be done, the Engineering Design Specification (EDS). The EDS has been defined by the designer according to the initial design specifications presented by the instrument lead engineer. The EDS has been reviewed and approved by the instrument lead engineer and the instrument scientific project leader and is published as a separate document in the ESS document managing system, CHESS. The specifications presented in this chapter are extracted from the EDS document.

5.1 Concept of Operation

The Beam Geometry Conditioning System should collimate the neutron beam from the neutron guide window up to the sample, to match the needs of each experiment. The system controls the beam size and the beam divergence. This is achieved by removing the unwanted neutrons using absorbing slits. The collimation system has two main slits, one far away from the sample to control the beam divergence and one close to the sample to control the beam size. The beam size and the beam divergence should be adjustable to match the different experimental needs.

5.1.1 Installation

The installation of the system will be divided into two steps. The first step is to install the support structure for the collimation system in the experimental cave. The second step is to install the collimation system. Slits and vacuum tubes should be aligned with the theoretical neutron beam axis using laser tracker. The alignment will be performed by the ESS Survey and Alignment Group.

5.1.2 Commissioning

The commissioning and verification of the system will be performed in two steps, a cold and a hot commissioning. The cold commissioning of the system is done by verifying that the movement of the slit blades matches the predicted, by movement of the motors.

The hot commissioning is done by exposing the system to a neutron beam with a detector at the sample position. Each axis should be adjusted separately and compared with the result of the detectors, to ensure that the functionality of the system satisfies the requirement. At this stage the neutron beam is diagnosed and the system is aligned with the effective, actual neutron beam axis.

5.1.3 Operation

If needed, diagnostic procedures can be performed on the system to verify the functionality, *e.g.* homing the positions of the axis.

If needed, diagnostic procedures can be performed on the neutron beam to characterize it. This may be done by scanning the beam to find the center of the intensity.

To perform an experiment the user inputs the desired beam characteristics into the experimental control software. The needed parameters are sample size, beam divergence and center of sample position. The control system converts the inputs into position and size of the slits.

5.1.4 Decommissioning

For any materials that are activated, the ESS procedure for active materials will be followed during decommissioning.

5.2 System Requirements

5.2.1 Functional Requirements

Table 1 – Functional requirements extracted from *System_Requirements_BTS_13.6.4.1*

Requirement	Rationale	Verification
Beam maximum size The BGCS shall define at the sample a beam of neutrons with a maximum size (full width half maximum) of 5 x 5 ± 0.1 mm.	This is the largest envisaged sample size (see 13.6.4.1 (2))	Measurement of the beam intensity profile at sample
Beam minimum size The BGCS shall define at the sample a beam of neutrons with a minimum size (full width half maximum) of 0.2 x 0.2 ± 0.02 mm.	This is the smallest envisaged sample size (see 13.6.4.1 (2))	Measurement of the beam intensity profile at sample
Beam maximum divergence The BGCS should define at the sample a beam of neutrons with a maximum divergence of ±0.2°.	This is the largest envisaged sample mosaicity (see 13.6.4.1 (3))	Measurement of the beam divergence at sample
Beam minimum divergence The BGCS shall define at the sample a beam of neutrons with a minimum divergence of ±0.02°.	This is the smallest envisaged sample mosaicity (see 13.6.4.1 (3))	Measurement of the beam divergence at sample
Beam size selection The BGCS should allow the beam size to be selected in 0.05 ± 0.02 mm steps in both height and width independently.	This is a small fraction of the expected beam size (see 13.6.4.1 (4))	Measurement of the beam intensity profile at sample
Beam divergence selection The BGCS shall allow the beam divergence to be selected in 0.02° steps.	This is a small fraction of the expected beam divergence (see 13.6.4.1 (5))	Measurement of the beam divergence at sample
Neutron background The BGCS should absorb 99.9% of the thermal and cold neutrons outside the selected beam size and divergence	The collimating elements need to absorb the neutrons that are not used in the experiment (see 13.6.4.1 (7,11))	Measurement of the beam intensity profile at sample
Gamma ray background The BGCS should not expose the detector system to radiation that detector system cannot distinguish from thermal neutrons.	Any neutrons absorbed in the collimating elements produce secondary particles, which add to background if they reach the detectors (see 13.6.4.1 (12))	Analysis & simulation
Accessible solid angle The BGCS should not obscure neutrons scattered by the sample within an angular range of ±165° from the neutron beam axis in the top hemisphere.	To make use of the longer wavelength neutrons that are scattered to higher angles at a given d it has to be possible to detect these neutrons (see 13.6.4 (2) and ConOps)	Test
Beam halo The BGCS should define at the sample a beam of neutrons with a distribution such that more than 90% of the neutrons are within the beam size area.	Reduce the background noise by reducing the over illumination of the sample	Measurement of the beam intensity profile at sample

Accessible solid angle definition

When the neutron beam hits the sample some neutrons will interact with the sample and be scattered. The neutrons can be scattered in any direction. One way to describe the direction of the scattered neutrons is to measure the angle to the neutron beam, with 0° in the beam direction. Neutrons can be scattered up to 180°. It should be possible to detect neutrons that are backscattered up to 165° in the top hemisphere, creating a 15° cone that should contain all equipment. There should be no equipment outside of the cone, as it would obscure the backscattered neutrons to the detectors. The cone is centered on the axis of the neutron beam and focused on the sample plane. The cone is illustrated in Figure 14.

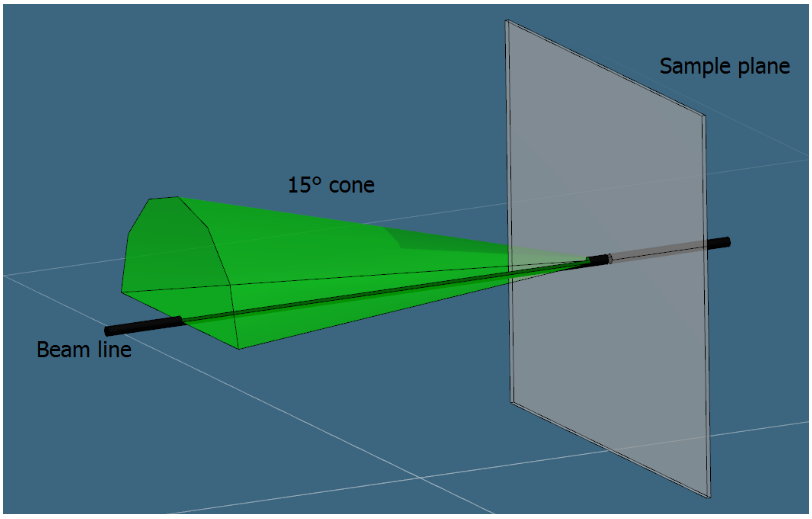

Figure 14 – Illustration of the definition of the accessible angle

5.2.2 Constraint Requirements

Table 2 – Constraint requirements

Requirement	Rationale	Verification
Design space The system shall be contained within the envelope model ESS-0052092	Ensure that the system do not interfere with other components, such as the goniometer	Check drawings
Support areas The system shall be supported on the areas identified in the envelope model ESS-0052092	Match support interface between the system and the experimental cave	Check drawings
Stability The centroid of the collimated beam shall remain within 10% of the beam size from the effective sample position (as identified by the goniometer)	Ensure that the beam is illuminating the sample at all time	Calculating temperature expansion
Structural materials Structural materials shall be agreed with NOSG	Avoid using materials with unwanted neutron interaction properties	Check with NOSG
Centring cameras The BGCS should provide support for the sample centring cameras	Reduce the amount of standalone supports	Check drawings
Cryostream The BGCS should provide support to the cryostream and other possible equipment to install at the side	Reduce the amount of standalone supports	Check drawings
Air travel The neutrons should not travel more than 1000 mm in air from the neutron guide window up to the sample.	Reduce the amount of air scattering, contributing to background	Check drawings
Axis All axis should be motorized, encoded and manually operable via knob on the motor	Controlled motion of the axis	Check drawings
Maintenance It should be possible to maintain the system (including installation) using the experimental cave overhead crane	No need for external lifting systems required	
Upgrades The system should allow upgrades by installation of future components	New demands on the system might arise	Flexible supports
Shielding accessibility The system should avoid unauthorized personnel to access the shielding components of the BGCS	Reduce the risk that shielding is removed	Locks
Secondary shutter The BGCS should leave 500mm of free space after the guide window	Allowing installation of a secondary shutter or diagnostic equipment	Check drawings
Beam diagnostic The pinhole should be adjustable ±15mm in y and z (x is along the beam) and should allow to diagnose the beam profile	To center the peak in intensity of the neutron beam on the sample	Check drawings
Repairs The BGCS should be accessible for repairs while the *proton beam is on target,* from within the experimental cave.	The instrument will be more fault tolerant hence increasing throughput of experiments (see ConOps)	Check drawings

5.3 Design Envelope

The system shall be contained within an envelope model. The design envelope shall contain information regarding the accessible design space, the location of the concrete base for the experimental equipment, the floor height of the experimental cave and where the system may be supported. As the design of the components surrounding Beam Geometry Conditioning System is ongoing and not fixed, the design envelope may be updated throughout the design process of the Beam Geometry Conditioning System. The initial design envelope is presented in Figure 15.

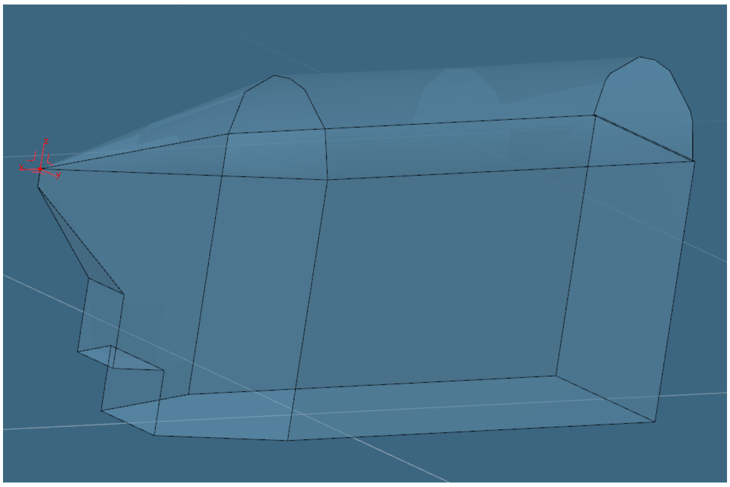

Figure 15 – Initial design envelope

5.4 Validation plan

The design of the system shall be validated according to the following steps.

Beam size

McStas simulations will be performed by the designer, according to previous McStas description. A 200 x 200 pixels neutron detector will be placed at the sample position to count the neutrons reaching the plane. The detector provides a matrix with the number of neutron hits in each pixel the YZ-plane. The result from the detector will be integrated onto one axis, giving a 1 x 200 vector. The full width half maximum of this reading will be calculated, defining the beam size. To validate the results of the McStas simulation, NOSG, the neutron optics and shielding group at ESS, will run additional simulations.

Beam halo

The halo is calculated from the same McStas simulation as the beam size. By counting the neutrons that hit the sample and the total numbers of neutrons reaching the sample plane it is possible to calculate the percentage of the neutrons hitting the sample.

Beam divergence

The beam divergence reaching the sample plane is calculated by hand-calculations, based on geometry and line of sight. The calculations are validated using McStas.

Assembly size

The design of the system will be visually evaluated using the envelope model ESS-0052092 throughout the project. The boundaries of the beam size are the limiting cases and therefore the main focus.

Shielding and absorbers

Absorbers and shielding shall be designed based on recommendations of NOSG, regarding material, thickness and position for the shielding and material and thickness for the absorbers. The design shall be validated by simulations performed by NOSG.

Stability

The final design should be analyzed using ANSYS® Workbench. A thermal expansion simulation containing the BGCS, the goniometer and the concrete base support will be performed for a temperature change of ±2°C. The difference in position between the goniometer and the beam line should not exceed 10% of the sample size.

Maintenance

To ensure that the system is maintainable using the experimental cave overhead crane should no part of the assembly weigh more than 500kg. Every component heavier than 25kg should be designed to be lifted by the overhead crane. This will be validated by applying correct materials to the CAD models and calculate the weight using CATIA®.

Final design

The final design should be evaluated for each requirement to ensure that they are all fulfilled. The fulfillment of the requirements will be graded according to *fully fulfilled*, *partly fulfilled* and *not fulfilled*. Requirements graded as *partly fulfilled* shall have a specification on the conditions needed to fulfill the requirement and an explanation regarding the reason it was not fully fulfilled. If a requirement cannot be fulfilled, the designer should communicate this to the instrument lead engineer as soon as possible.

6. BEAM GEOMETRY CONDITIONING SYSTEM

The Beam Geometry Conditioning System can be divided into smaller subsystems. These subsystems are mainly developed individually and then assembled into the full system. The identified subsystems are presented in Figure 16 and a schematic assembly of the system is shown in Figure 17. In this chapter the different main subsystems are briefly introduced.

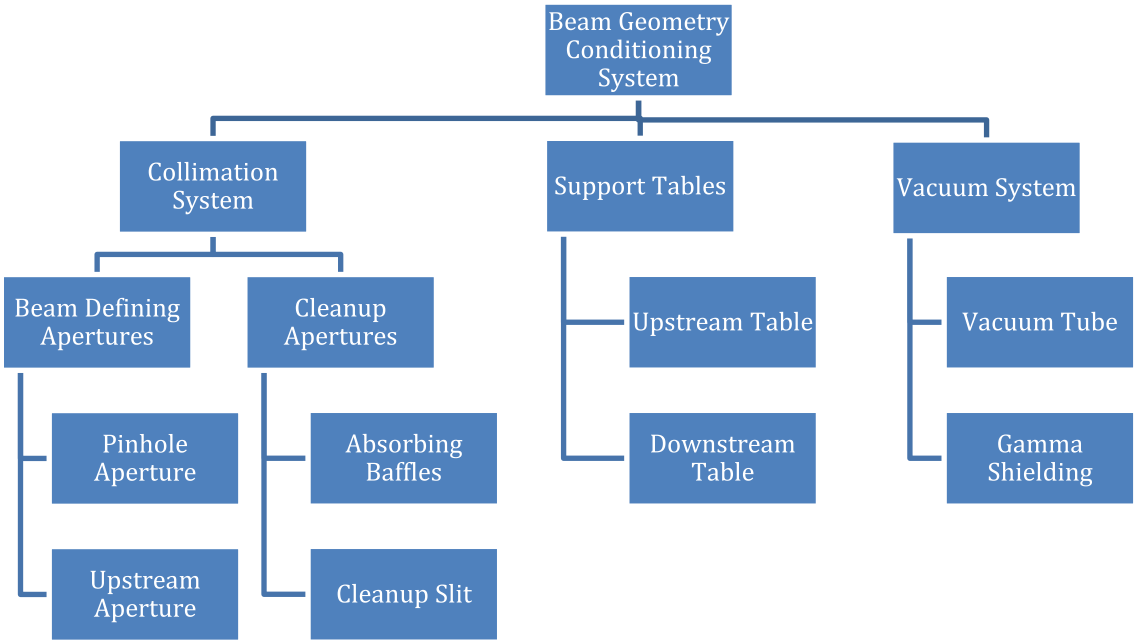

Figure 16 – Beam Geometry Conditioning System divided into subsystems

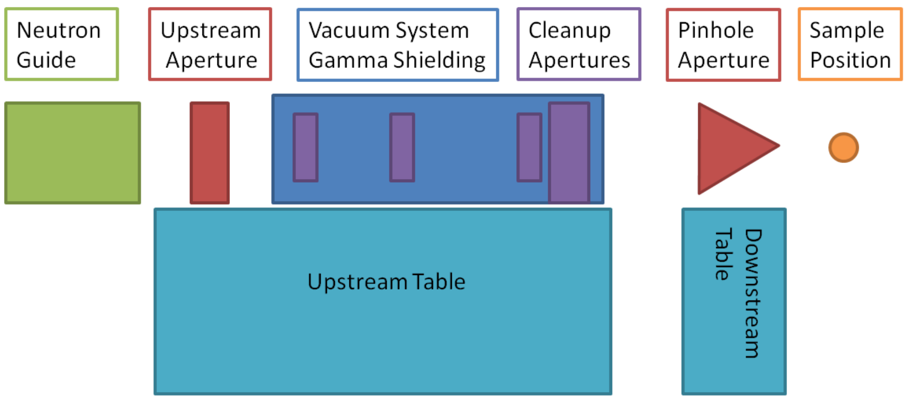

Figure 17 – Schematic assembly of the Beam Geometry System

6.1 Collimation System

The Collimation System is the core of the Beam Geometry Conditioning System. The Collimation System is divided into two different subsystems, the Beam Defining Apertures and the Cleanup Apertures. The Beam Defining Apertures consist of the two adjustable apertures that define the geometrical properties of the neutron beam. The aperture close to the sample controls the size of the neutron beam that reaches the sample. As this aperture is very small it is called the Pinhole Aperture. The Pinhole Aperture is a key component to the system, as its design sets the boundaries for the angle in which backscattered neutrons can be detected as well as the distance between the sample and the aperture.

To minimize the background noise from the absorption of the unusable neutrons the absorption should occur as far upstream as possible. This is achieved by cleaning up the beam before it reaches the Pinhole Aperture. It is foreseen that the cleanup of the beam will be done in two steps, using Absorbing Baffles and adjustable slits. The cleanup of the beam is done within the Gamma Shielding.

6.2 Support Tables

The Beam Geometry Conditioning System and, more specifically, the Collimation System has to be placed in line with the neutron beam. This is achieved by mounting the system on two support tables. The reason for having two separate tables is to increase the flexibility of the system. The table that is close to the sample is the Downstream Table and is mounted on the concrete support base of the experimental equipment. The table furthest away from the sample is the Upstream Table. The Upstream Table should have a flexible interface for mounting different kinds of experimental equipment.

6.3 Vacuum System

Neutrons traveling in open air may interact with the different elements in the air and scatter, causing background noise. To reduce the air scattering the neutron beam should travel as much as possible in vacuum. The system requirements state that the neutron beam should have a maximum travel of 1000mm in air from the neutron guide window to the sample. The Vacuum System is closely connected with the Absorbing Baffles, as the Vacuum System supports the baffles.

7. BASIC ARCHITECTURE

The first step in designing the Beam Geometry Conditioning System is to investigate how the basic architecture should be set up. In this chapter the placement of the different apertures is considered, to understand the outline of the design.

7.1 Two Sample Positions

NMX has two sample positions. The main sample position is used for investigating biological molecules and the secondary sample position for material science. The main objective of the Beam Geometry Conditioning System is to collimate the neutron beam to match the sample at the main sample position. It should however also be a part of the collimation system for the secondary sample position. This is achieved by having the option to adjust the apertures to match the secondary sample position or, if required, removing the Pinhole Aperture from the neutron beam, while being able to remount it in a repeatable fashion. The secondary sample position will have to have a separate aperture in close proximity to it to complete the collimation system. The distance between the two sample positions is 650mm.

As the Beam Geometry Conditioning System should be a component in the collimation system for the secondary sample position, it is required to design the system with this in mind. The placement of the sample positions relative to the neutron guide window and the design of the Upstream Aperture along with the Cleanup Apertures should be done according to the secondary sample position. The Pinhole Aperture should not take the secondary sample position in account and only be designed to match the main sample position.

7.2 Neutron Guide Window

The main parts of the Beam Geometry Conditioning System are the Beam Defining Apertures. However, it is not only the placement of the Upstream Aperture that controls the divergence of the beam. The distance between the sample and the neutron guide window sets the boundary of the maximum divergence of the neutrons that are able to reach the sample. The optimal distance between the secondary sample position and the neutron guide window is calculated according to Figure 18. The maximum amount of neutrons will reach the sample at this distance, with a specific maximum divergence.

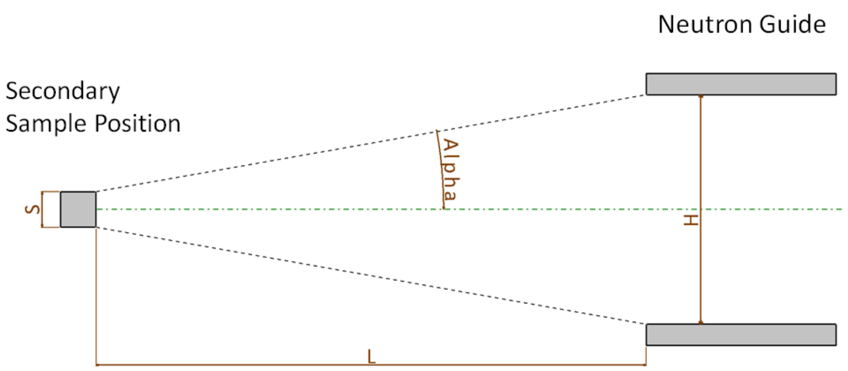

Figure 18 – Optimal distance between the secondary sample position and the neutron guide window

The size of the neutron guide window is fixed at 30 x 30mm. The sample size varies from 0.2mm up to 5mm and the divergence from 0.02° up to 0.2°. Large samples and high divergence require shorter distance, thus the largest sample size and the highest divergence are the limiting parameters. To be able to illuminate the entire sample with the required divergence the distance from the neutron guide to the secondary sample position (L in Figure 18) may not exceed 3581mm. The distance should not be significantly smaller than this either, as it would limit the collimation distance and decrease the distance between the sample and the absorption of the unusable neutrons. It is important to remove the unusable neutrons as far upstream from the sample as possible, to reduce the background from the absorption. By reducing the collimation distance, the contamination of high divergence neutrons at the sample increases. However, the calculated distance requires the sample to be mounted in the perfect position, with very little margin for errors. Reducing the distance gives a leeway when placing the sample and still having the possibility to achieve the correct divergence.

Due to the arguments above, the distance between the secondary sample position and neutron guide window is chosen to be 3500mm. This will leave ±0.3mm leeway for the placement of the sample, which is larger than the resolution of the goniometer. As the distance between the two samples positions are 650mm, the distance between the main sample position and the neutron guide window is 2850mm, providing a ±5mm leeway.

7.3 Beam Defining Apertures

With a fixed distance between the neutron guide window and the sample positions it is possible to start investigating the placement of the Beam Defining Apertures.

7.3.1 Upstream Aperture

The Upstream Aperture should be as close to the neutron guide window as possible. There is a requirement to leave 500mm of free gap between these two components, for a secondary shutter and other future diagnostic equipment. Due to this requirement, the Upstream Aperture is restricted to be placed 2350mm from the main sample position. At this distance there are no limits on the size of the aperture, meaning it can be constructed as a slit with four absorbing blades moving perpendicular to the beamline.

7.3.2 Pinhole Aperture

The Pinhole Aperture is only a part of the collimation system for the main sample position and not for the secondary. The Pinhole Aperture will be positioned to clear the neutron beam or be entirely removed from the neutron beam area when the secondary sample position is used. Hence, the following description refers to the main sample position only.

The size and placement of the Pinhole Aperture affects many parameters. The size of the aperture depends on the sample size and the distance to the sample. The aperture should allow the entire sample to be illuminated with a neutron beam with 0.2° beam divergence. To fulfill this, the size of the aperture should increase depending on the distance, according to Figure 19. However, a larger aperture size allows more neutrons to reach the sample plane, increasing the beam size. The beam size is calculated according to the Full Width Half Maximum of the neutron distribution at the sample plane, see Figure 20. The distribution will be more spread out with larger distance, increasing the halo. To fulfill the requirements regarding beam size, beam halo and beam divergence at the same time, the distance between the sample and the aperture needs to be very small, especially for small sample sizes. It is likely that it is not mechanically possible to place the Pinhole Aperture this close to the sample. In this case the aperture size should be reduced, which limits the beam divergence reaching the sample, effectively reducing the neutron flux. This action will allow the distance to be increased while maintaining the beam size and beam halo.

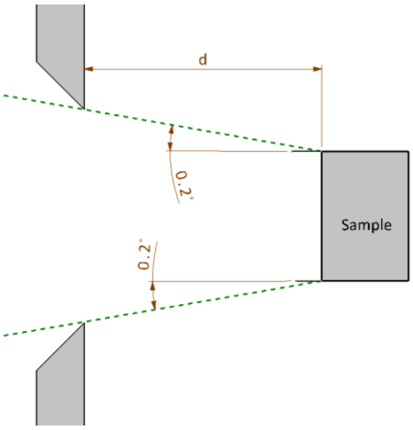

Figure 19 – Aperture size depends on the distance to the sample

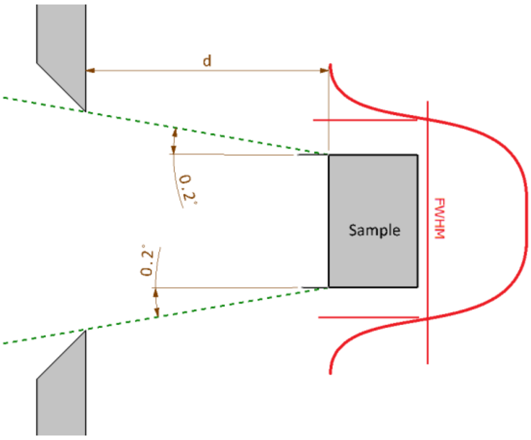

Figure 20 – Illustration of the FWHM

The halo is defined as the neutrons that reach the sample plane outside of the desired beam size. It is the neutrons outside of the FWHM of the distribution in Figure 20. These neutrons will not interact with the sample but instead interact with the surrounding matter, the mother liquor in the case of biological crystals. To minimize the halo the aperture should be as close to the sample as possible. However, this limits the available design space in the top hemisphere, see Figure 21. The requirements state that 90% of the neutrons reaching the sample plane should hit within the beam size. The optimal distance cannot easily be calculated analytically and will be determined numerically using McStas simulations.

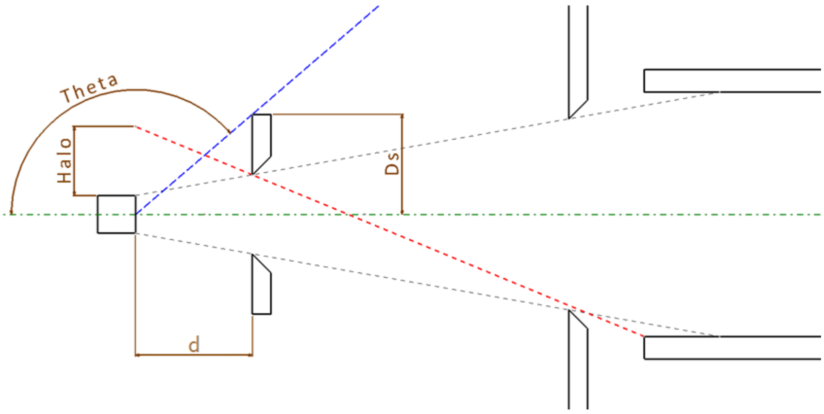

Figure 21 – Illustration of the design space (Ds) and the halo

It is evident that the design challenges are connected with small sample sizes, as the sample to aperture distance is most restricted in these cases. An early prediction is that the smallest sample size requires the distance to be in the 5mm range. The available design space in this case is 1.3mm. There is no obvious solution to this problem that can be concluded at this stage of the design phase, it has to be further investigated. What is clear at this stage is that it will not be possible to adjust the size of the aperture in a purely perpendicular motion to the beam axis. The aperture will have to change its position along the beam axis, depending on the sample size.

7.4 McStas simulations

As described earlier, McStas is used to simulate the neutronic behavior of the design. The neutronic model of the entire NMX instrument, from the ESS neutron source up to the end of the neutron guide, is used to perform the simulations. This is integrated with the neutronic model of the Beam Geometry Conditioning System developed throughout the project. At this stage of the design phase McStas is used to investigate two different subjects: to understand the characteristics of the neutron beam leaving the neutron guide window and to find the optimal position of the Pinhole Aperture.

The following simulations are performed with a sufficient large number of neutrons to get satisfying results. As the simulations are not connected to a specific operation and the numbers of neutrons might differ between different simulations, there will be no scale or absolute values on the intensity in the figures created by the detectors.

7.4.1 Neutron Guide Window Divergence

To understand the prerequisites for the design it is important to know the characteristics of the neutron beam leaving the neutron guide window. The size of the beam is equal to the size of the window, which is 30 x 30mm. The divergence is not as evident. To investigate the divergence of the neutron beam leaving the neutron guide window a divergence monitor is created at the window. The result from the detector is shown in Figure 22.

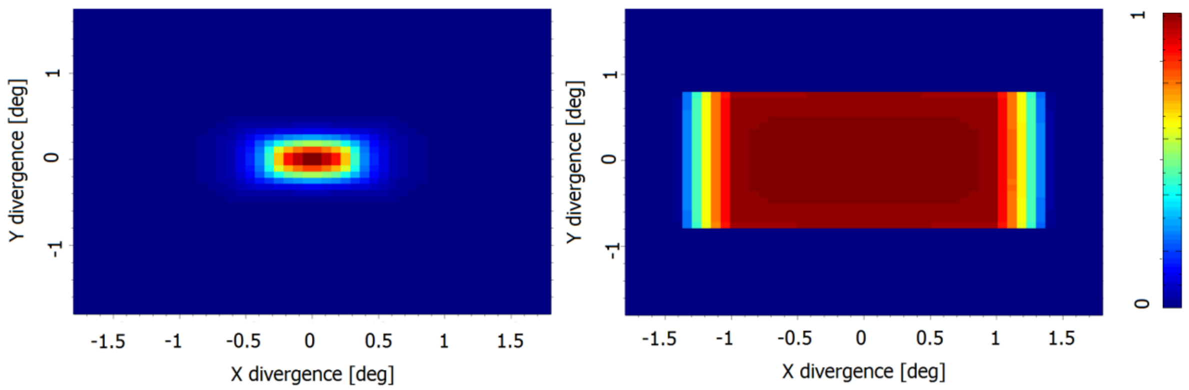

Figure 22 – Beam divergence of the neutron beam leaving the neutron guide window (Left: linear scale, Right: logarithmic scale)

Most of the neutrons have a divergence lower than 0.5°, as seen in Figure 22 (left). However, the figure with logarithmic scale, Figure 22 (right), reveals that a few neutrons have a divergence up to 1.4°. Also, the divergence is higher in the horizontal plane than in the vertical. The reason behind this is the shape of the neutron source. It is expected that this issue will be solved as the neutron guide is further developed and refined, but the design of the system will be based on the result of this simulation. Even though the neutron guide system is designed to not transport neutrons of high divergence, maintaining a margin when designing the system is prudent. With this in mind, oversized absorbers are beneficial.

The maximum divergence of the neutron beam is used to determine the size of the Upstream Aperture, but also the size and position of the Cleanup Apertures.

7.4.2 Pinhole Aperture Placement

The McStas model of the Beam Geometry Conditioning System is initially set up using two-dimensional slits as the Beam Defining Apertures, see Figure 23. The interesting areas are just before the two apertures as well as at the sample position. To monitor the characteristics of the beam, position sensitive detectors are created in the neutronic model at these locations. The slits are initially set up to match the smallest beam size with the largest beam divergence, as this is the most challenging set up. The distance between the Pinhole Aperture and the sample is varied to study how the FWHM of the distribution of neutrons reaching the sample plane and the beam halo changes with the distance.

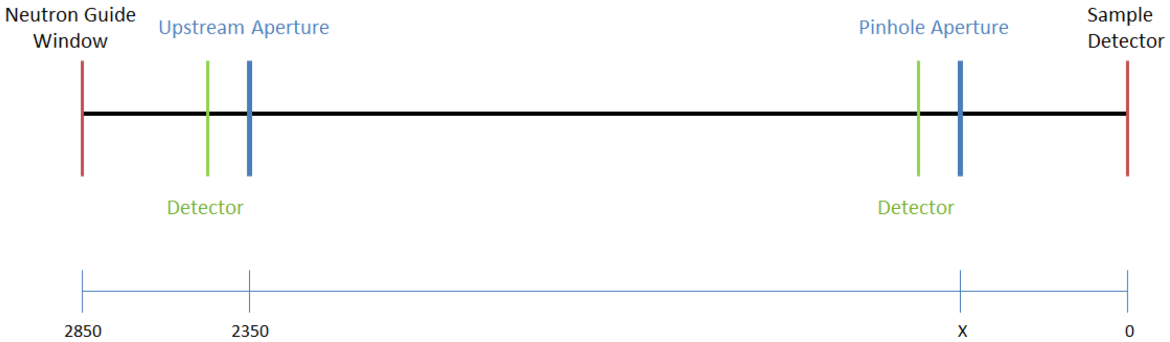

Figure 23 – Initial McStas setup

The result of the simulations shows that the optimal position of the Pinhole Aperture, to fulfill the requirements regarding beam size, beam divergence and beam halo, is just less than 2mm from the sample. The available design space at this distance is 0.5mm in the top hemisphere, which is insufficient. The conclusion is that the aperture size needs to be reduced, according to previous chapter, to be able to increase the sample-to-aperture distance.

A pattern between the aperture size and the beam size along with the beam halo was discovered while running the simulations. Due to the low beam divergence and the short distance between the sample and the aperture it may be possible to neglect the beam divergence and assume that all the neutrons are moving in line with the beam axis. This assumption means that the FWHM of the neutron beam at the sample plane and the aperture size should be equal. The aperture size depends on the distance to the sample due to the beam divergence, according to previous chapter.

It also means that the fraction of the aperture area that is covered by the beam size area should be the same as the fraction of neutrons that hit within the beam size area at the sample plane. To verify if this assumption is correct, the McStas simulations are compared with the calculated values according to the assumption, see Table 3.

Table 3 – Comparison between calculated values and result of McStas simulations

Beam size	Distance	Calculated FWHM/Beam size (aperture size)	Simulated FWHM/Beam size	Calculated halo	Simulated halo
0.2	2	0.214	0.205	12%	11%
0.2	4	0.228	0.225	23%	20%
5	15	5.11	5.15	4%	3%
5	40	5.28	5.35	10%	10%

The simulations have been performed using a detector with 200 x 200 pixels. The size of the detector is 1 x 1mm for 0.2mm beam size and 10 x 10mm for 5mm beam size, leading to a pixel size of 0.005mm and 0.05mm respectively. With this accuracy of the simulations, it is feasible to make the assumption that the beam size and aperture size is equal.

The most important beam characteristic to control is the beam size. To obtain the best result the aperture size should match the beam size, for relatively short distances to the sample. By doing this, some of the high divergence neutrons that would have otherwise hit the sample are removed, reducing the neutron flux at the sample. However, in comparison to the reduction in halo the loss in flux is negligible. In the reasonable range for the sample-to-aperture distance the loss in flux is less than 5%. The loss in flux is reduced the closer the aperture is placed to the sample.

As indicated in Table 3, the sample-to-aperture distance may be large for larger beam sizes and still fulfill the requirements. To optimize the experimental conditions, the distance should be minimized as much as possible for all beam sizes.

If only the Beam Defining Apertures are used for the Collimation System then 30 – 50% of the neutrons leaving the neutron guide window would reach the Pinhole Aperture, with a beam size of 120 x 120mm. This would result in high background due to the absorption process and the size of the absorbers would be too large, obscuring the backscattered neutrons.

The conclusion is that two apertures are not sufficient. It is necessary to clean up the beam further upstream from the sample, before it reaches the Pinhole Aperture.

7.5 Cleanup Apertures

As mentioned above, using only the Beam Defining Apertures for the collimation of the neutron beam would cause two main issues. The first issue is that there is no clearance to place absorbers sufficiently large to absorb the unwanted neutrons without obscuring backscattered neutrons. The second issue, with this setup, is that a large amount of neutrons will be absorbed very close to the sample. The radiation from the absorption would cause a lot of background noise. An illustration of the neutron beam using two apertures is shown in Figure 24.

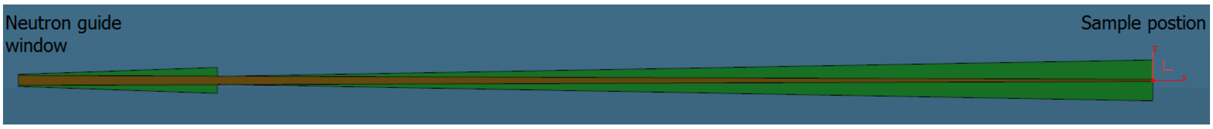

Figure 24 – Illustration of neutron beam using two slits (green is the neutron beam and brown is the useful part of the beam)

To solve these issues additional apertures are added along the neutron beam, to clean up the beam before reaching the Pinhole Aperture. The cleanup is done in two steps. The first step is to add Absorbing Baffles downstream of the Upstream Aperture, hosted by the Vacuum Tube. These Absorbing Baffles have a fixed aperture size and are designed to remove high divergence neutrons. The second step is to add an adjustable slit with absorbing blades downstream of the Vacuum Tube, removing as many neutrons as possible based on the current beam size and divergence.

7.5.1 Absorbing Baffles

The first step in cleaning up the neutron beam is the Absorbing Baffles. These are fixed absorbers mounted inside the Vacuum Tube. The purpose of the baffles is to remove high divergence neutrons. The size of the baffles and the distance between the baffles are designed to absorb all high divergence neutrons according to Figure 25. The neutrons that pass through one baffle should be absorbed by the next one.

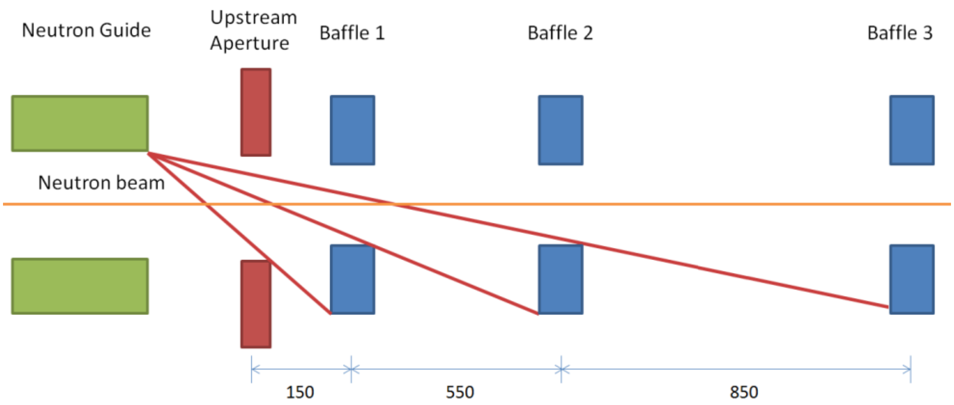

Figure 25 – The baffles are placed to absorb high divergence neutrons

The calculations to determine the position of the baffles are done based on an outer dimension of the baffles of 58mm, to match a standard dimension for vacuum tubes with clearance for a support frame for the baffles.

The inner dimensions of the baffles are tapering with the maximum beam divergence to match the secondary sample position.

7.5.2 Cleanup Slit

The Cleanup Slit should clean up the beam before reaching the Pinhole Aperture, to reduce the beam size at the Pinhole Aperture. The Cleanup Slit should be contained within the Gamma Shielding of the Vacuum System, restricting the placement of the slit. The distance between the last baffle and the Cleanup Slit is in the range of 100mm, which places the Cleanup Slit 700mm from the main sample position. With this setup, the amount of neutrons reaching the Pinhole Aperture is predicted to be reduced from 30 – 50% to roughly 5%.

7.6 Summary

This chapter has described the development of the basic architecture for the Beam Geometry Conditioning System with focus on the Collimation System. The optimal positions for the different apertures have been investigated and the result is presented in Figure 26.

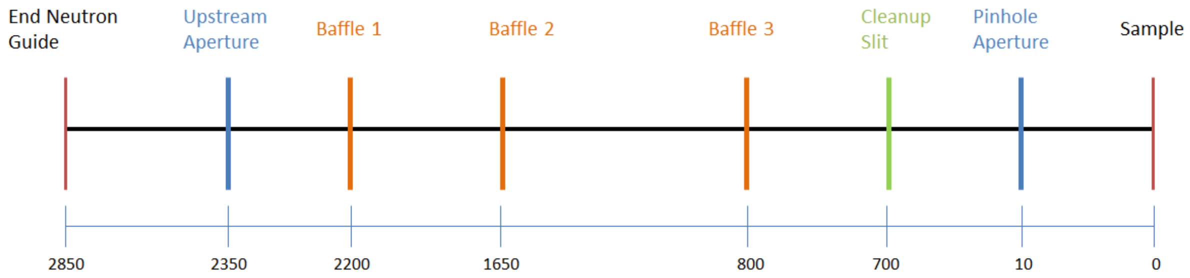

Figure 26 – Placement of the different apertures

The Upstream Aperture should be an adjustable slit with absorbing blades and so should the Cleanup slit.

The size of the Pinhole Aperture should be equal to the beam size, to allow the sample-to-aperture distance to be increased while fulfilling the requirements regarding beam size and beam halo.

The next step in the design process is to enter the concept design phase.

8. CONCEPT DESIGN OF THE BEAM GEOMETRY CONDITIONING SYSTEM

With the basic architecture defined it is possible to begin the concept design of the subsystems. This chapter describes the design of the lowest level subsystems. The completed system is presented in Figure 27.

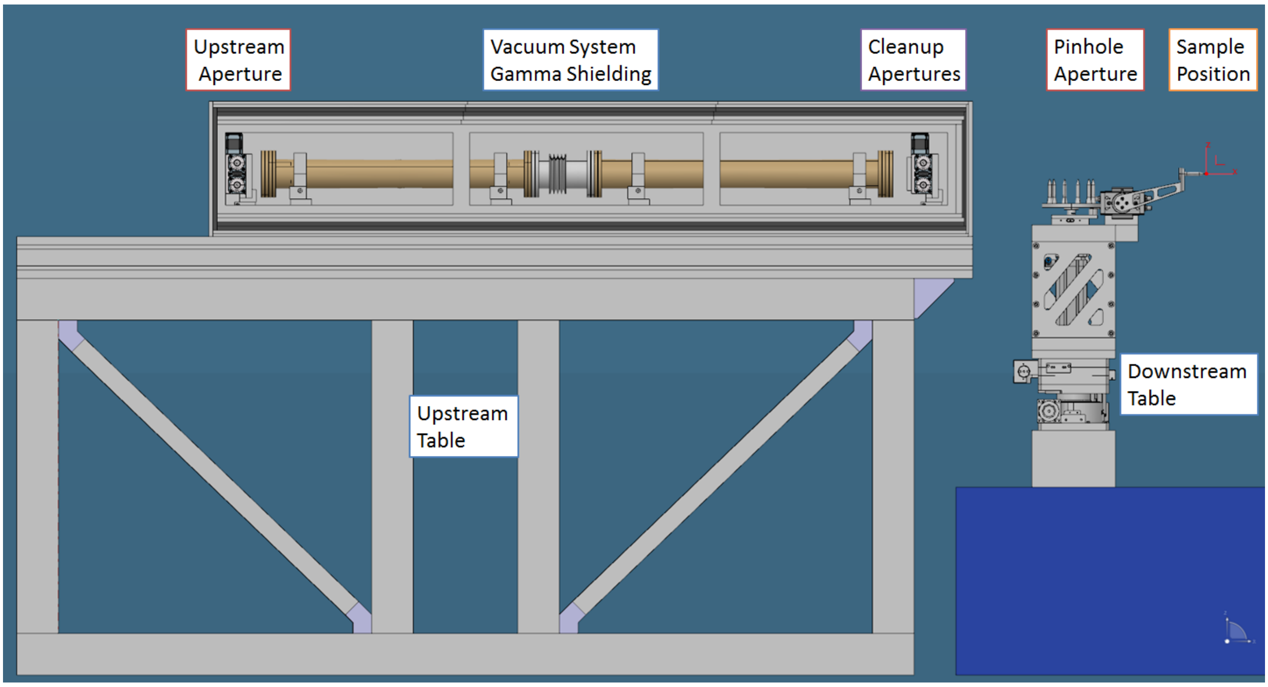

Figure 27 – Completed concept of the Beam Geometry Conditioning System

8.1 Pinhole Aperture

The design of the Pinhole Aperture is crucial for the functionality of the Beam Geometry Conditioning System. The concept design and concept selection of the Pinhole Aperture are important processes, which should be performed systematically and be well documented, to make sure that the best concept is found and developed. The concept development of the Pinhole Aperture is thoroughly described in the next chapter.

8.2 Upstream Aperture

The Upstream Aperture is placed far away from the sample position, resulting in no limitation by the design envelope. The consequence is that a commercial off-the-shelf slit with four absorbing blades may be used. The required size of the slit and the support structure are described below.

8.2.1 Upstream Aperture Size

The maximum needed aperture size of the Upstream Aperture is calculated to match the secondary sample position, as the Upstream Aperture is a component of the secondary sample position collimation system. The distance between the secondary sample position and the Upstream Aperture is 3000mm. The maximum beam size is 5mm and the maximum beam divergence is 0.2°, resulting in a maximum needed aperture size of 26mm.

The size of the neutron beam that hits the Upstream Aperture depends on the divergence of the beam leaving the neutron guide window. As described in chapter 7.4, McStas simulations reveal that most of the neutrons have a divergence lower than 0.5°. However, a small fraction of the neutrons have a divergence up to 1.4°. With this information it is possible to calculate the size of the beam when it reaches the Upstream Aperture, 500mm from the window. Neutrons with 1.4° divergence will deviate 13mm in 500mm, resulting in a beam size of 56 x 56mm at the Upstream Aperture.

There are two different solutions to ensure that the high divergence neutrons are absorbed by the Upstream Aperture, no matter the settings of the slit. Either a slit with over dimensioned blades is used or a fixed absorber is mounted upstream of a slit with smaller blades, matching the requirements for the aperture size.

There are no advantages in being able to open the aperture more than the size of the neutron guide window at 30 x 30mm, which would be possible with a larger slit. Also, it is likely that a fixed absorber is needed, even with a slit system with large blades, to protect the mechanics of the slit and to control which materials interact with the neutron beam.

Due to the reasoning above, the Upstream Aperture should have a fixed absorber with outer dimensions of at least 60 x 60mm with an aperture of 30 x 30mm in the center. The fixed absorber should be mounted upstream of a commercially off-the-shelf slit with adjustable blades with a maximum aperture of 30 x 30mm.

According to the functional requirements, the divergence should be selectable in steps of 0.02° at the main sample position. To achieve the required divergence step size, the slit should have a step size less than 0.8mm.

8.2.2 Upstream Aperture Support Structure

The Upstream Aperture should be mounted on an adjustable support structure, to be able to align the aperture with the neutron guide window. The aperture is located close to the Vacuum System and an adaptable support structure that suits both the Vacuum Tube and the Upstream Aperture is desirable. The support structure should be adjustable in the plane perpendicular to the beam axis, the YZ-plane with the X-axis in the beam direction.

The concept for the support structure is to have a sliding block for adjustment in the Y-direction mounted on top of a screw, for adjustment in the Z-direction. The screw is locked in place using a nut. The sliding block is divided into three parts, a clamp to mount onto the screw, a plate with a groove mounted on the clamp and a plate that can slide in the groove of the first plate. The sliding plate is locked in place with two screws. The design can be seen in Figure 28.

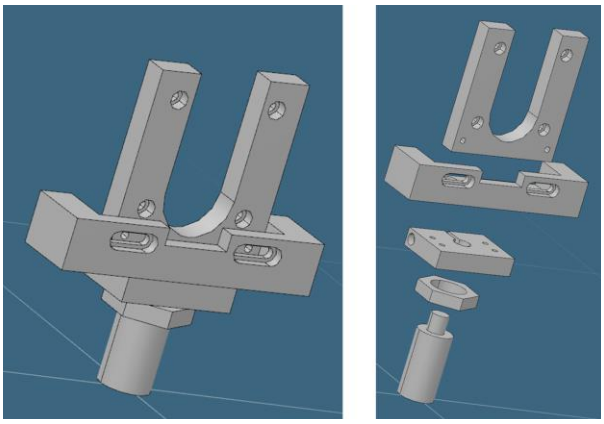

Figure 28 – Support structure for Upstream Aperture

8.2.3 Upstream Aperture COTS Slit

A commercial off-the-shelf slit that is well suited to fulfill the requirements is the IB-C30-AIR slit provided by JJ X-Ray. A brief overview of the specifications for the slit can be seen in Table 4.

Table 4 – Specifications for the slit system IB-C30-AIR

IB-C30-AIR	
Aperture size	Maximum: 30 mm x 30 mm Minimum: Full overlap
Resolution	1 micron per full step
Accuracy	± 2 micron (over 3 mm)
Mechanical dimension	150 mm x 150 mm x 64 mm 95 mm x 95 mm x 50 mm (housing only)
Blade options	2, 4, 5, 10 mm thick blades Mounted either with a 0.5 degrees knife-edge or a R16 radius edge Different materials
Common options	Motors: Custom high resolution stepping motors, including IMS motors Encoders: Back-axle rotary encoders Connector: Plate for X95 profile

The assembled subsystem is shown in Figure 29.

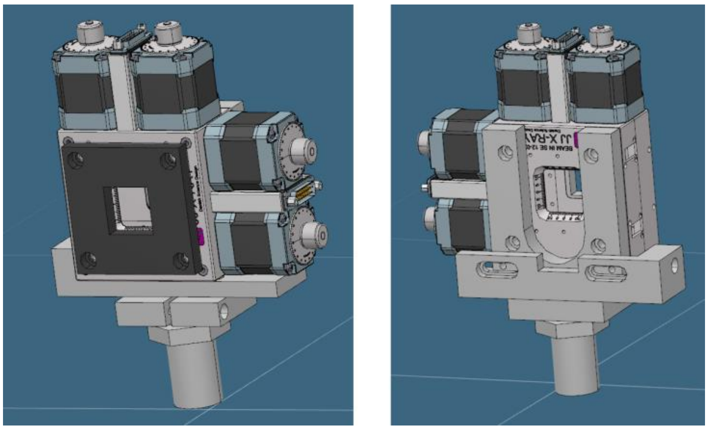

Figure 29 – Upstream Aperture with support structure, fixed absorber (shown to the left) and COTS slit

8.3 Absorbing Baffles

The design of the Absorbing Baffles is closely connected to the Vacuum Tube. To fulfill the intent of the design of the Cleanup Apertures, three baffles are needed. All three baffles are integrated within the Vacuum Tube. Different solutions for fixing the position of the baffles within the vacuum tube have been investigated. As this is not the focus of the project only the selected concept is presented.

The concept for fixing the position of the baffles is to glue each baffle to an individual aluminum frame. The frame is then inserted in the Vacuum Tube and clamped between the flange and the gasket, see Figure 30. To be able to fit the frame at the flange of the Vacuum Tube, the flange needs to be machined up to the sealing knife edge. This design requires the Vacuum Tube to be split into two tubes, see Figure 31. This is a measure that is likely to be needed regardless of the design for the Absorbing Baffles.

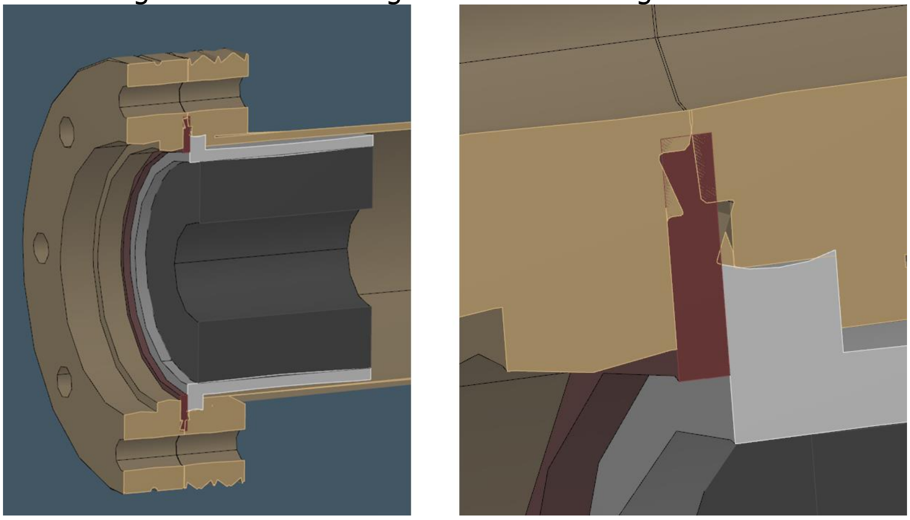

Figure 30 – The support frames are clamped between the flange and the gasket of the Vacuum Tube

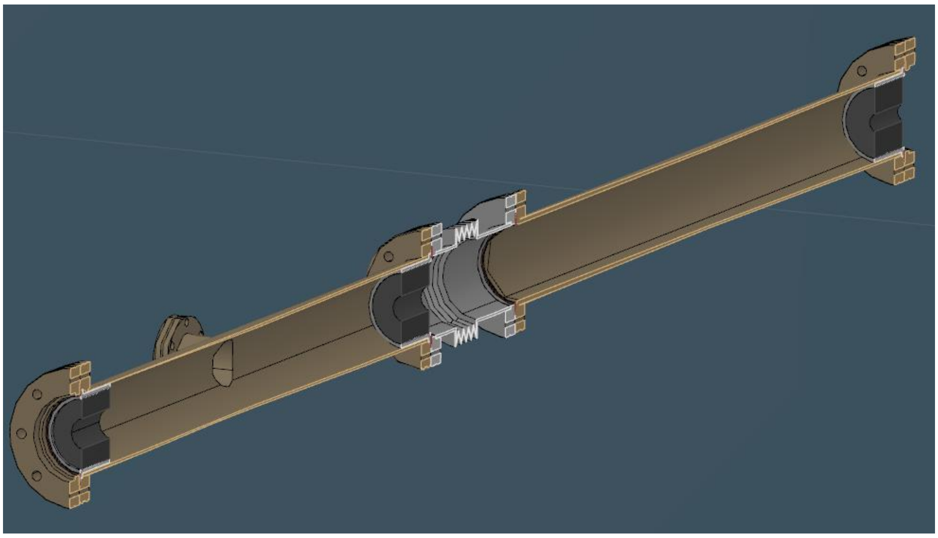

Figure 31 – Setup of the Absorbing Baffles within the Vacuum Tube

8.4 Cleanup Slit

To reduce the number of different components that need to be designed and manufactured, it would be beneficial to use the same setup and slit system for the Cleanup Slit as for the Upstream Aperture. The position of the Cleanup Slit is limited by the Gamma Shielding to 700mm upstream from the main sample position. It is not possible to place the Cleanup Slit further downstream. The impact of having the slit at this position is investigated by calculating the size of the neutron beam reaching the Pinhole Aperture. To find this size the divergence of the neutrons passing through the Cleanup Slit needs to be calculated according to Figure 32. The result is that neutrons with up to 0.5° divergence may pass the slit with the slit set to match the largest beam size and beam divergence. The neutron beam is then 22 x 22mm at the Pinhole Aperture position. To fit an absorber at the Pinhole Aperture to match this size, the distance between the absorber and the sample position must be at least 40mm to not exceed the design envelope. Whether this is an acceptable value or not depends on which concept is used for the Pinhole Aperture. If the Pinhole Aperture concept requires better control of the incoming beam size an additional cleanup slit may be added outside of the Gamma Shielding. The size of the incoming beam shall not be a limitation when selecting the concept for the Pinhole Aperture.

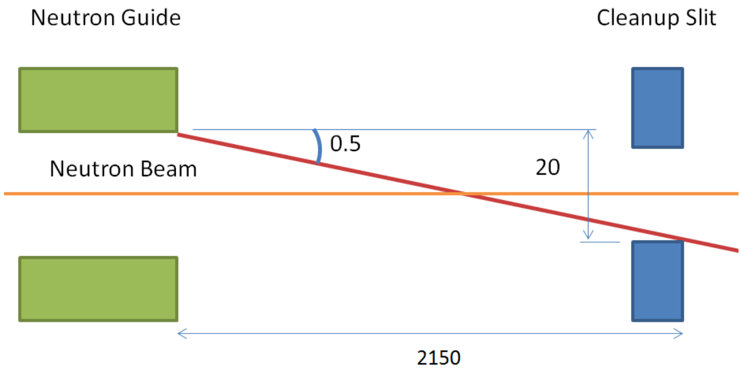

Figure 32 – Possible divergence passing through the Cleanup Slit

8.5 Upstream Table

The main objective of the Upstream Table is to support and position the Upstream Aperture and the Vacuum System in line with the neutron beam axis. However, it should also be flexible to allow installation of components that might be required in the future. To achieve this functionality the table needs to have an easily accessible interface for mounting different kinds of equipment. Such flexible interface is obtained by using aluminum profiles, see Figure 33. Aluminum profiles can easily be assembled to create rigid constructions with high flexibility.

Figure 33 – Aluminum profiles used for the Upstream Table (Bosch Rexroth)

There are many different suppliers of aluminum profiles and, in this concept design, profiles from Bosch Rexroth are used. The frame is made out of 100 x 100mm profiles with two 45° supports, see Figure 34.

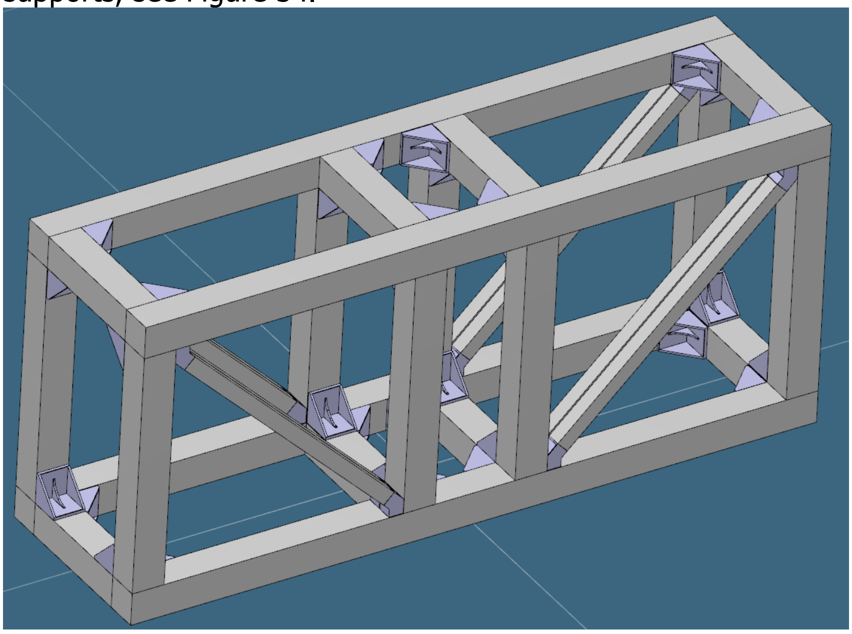

Figure 34 – Upstream Table frame structure

The top of the table consists of three 200 x 100mm profiles, see Figure 35. At this time there are no foreseen needs to place any additional equipment in between the Gamma Shielding and the Pinhole Aperture, but, if the need arises in the future, the top profiles of the table are suggested to be extended to support the equipment.

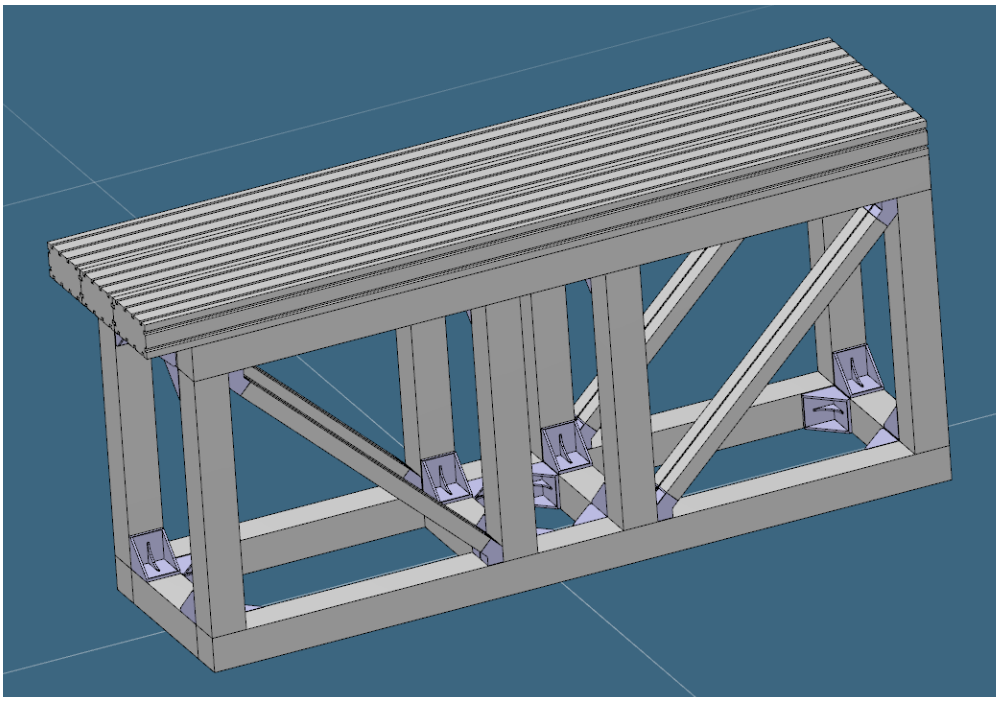

Figure 35 – Upstream Table

8.6 Downstream Table

The design of the Downstream Table depends on the design of the Pinhole Aperture. However, no matter the design of the Pinhole Aperture, the Downstream Table needs to be equipped with motorized stages to align the Pinhole Aperture with the neutron beam axis. These stages and their support may be designed decoupled from the Pinhole Aperture.

The support of the motorized stages will be mounted on the concrete base support for the experimental equipment described in the introductory chapters. The material of the support is not yet decided, but the shape of it will be a solid cube, to increase the stability of the table. The height of the support depends on the Pinhole Aperture.

The motorized stages should be able to adjust the top of the Downstream Table in three dimensions, along the X-, Y- and Z-axes. This movement is achieved by mounting a XY-stage on top of a Z-stage. As stability is a key factor when designing the Downstream Table, the stages needs to be of high quality, thus reliable stages from a renowned supplier are suggested to be used. Stages provided by Huber have been selected and are integrated in the design, which fulfills the needs of the system. The specifications for the XY-stage 5102.20 and for the Z-stage 5103.A20-40 are presented in Table 5. These two stages are designed to be mounted on top of each other.

Table 5 – Specifications for the Huber stages

	XY-stage 5102.20	Z-stage 5103.A20-40
Travel range [mm]	±15	40
Max. load [N]	2000	1500
Dimensions [mm]	170 x 170 x 62	170 x 170 x 90(130)
Accuracy [µm]	±5	±5
Repeatability (unidir.) [µm]	±2	±3
Reversal error [µm]	6	12

8.7 Vacuum Tube

The Vacuum Tube extends from the Upstream Aperture to the Cleanup Slit. Its purpose is to reduce the background noise by reducing the air scattering of the neutron beam. Another key function of the Vacuum Tube is to host the Absorbing Baffles to align them with the neutron beam axis.

The Vacuum Tube will use flanges according to a standard called the ConFlat (CF) standard. This standard uses a copper gasket and knife edges on the flanges to make the seal, see Figure 36. As the gasket is softer than the flange, the knife edges deform the gasket, creating a very tight seal. As can be seen in Figure 36, the knife edge is placed close to the outskirt of the gasket, allowing the flanges to be machined without interfering with the sealing functionality of the flange. This is used to lock the position of the baffles.

Figure 36 – The CF flange is used to lock the position of the Absorbing Baffles

As described in chapter 8.3, the Vacuum Tube must be divided into two tubes to support the center baffle. By splitting the tube, the flexibility of the alignment increases. The two tubes are connected with a flexible bellow tube that allows the two tubes be aligned individually.

The support structure for the Upstream Aperture was designed to fulfill both the requirements of the Upstream Aperture and of the Vacuum Tube. The only adjustment that needs to be done to the support structure is to replace the interface plate, which the slit is mounted on, with a clamp matching the Vacuum Tube. The clamp consists of two plates, a top and a bottom plate. The bottom plate is mounted onto the base of the support structure in the same manner as the support plate for the Upstream Aperture. The two plates are shaped as semicircles to match the tube and are connected using screws, locking the position of the Vacuum Tube. The assembly of the Vacuum Tube is shown in Figure 37. The supports will be mounted directly onto the Gamma Shielding base plate.

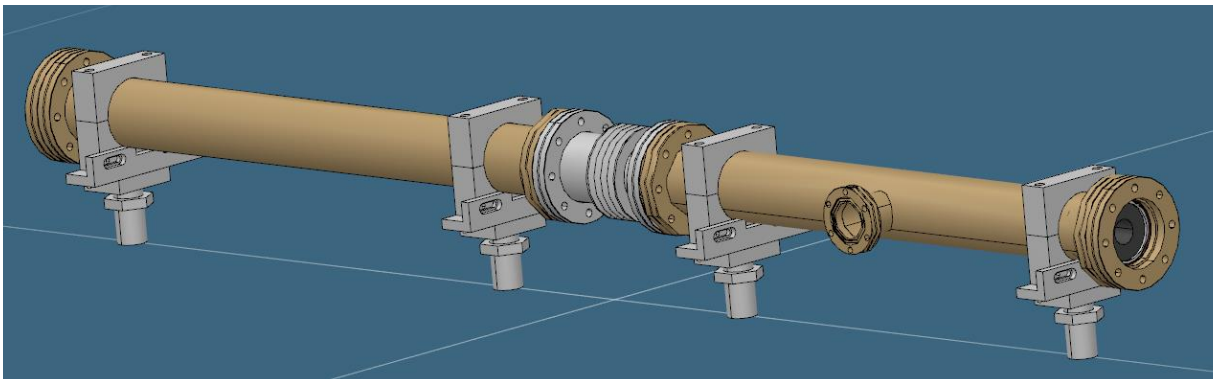

Figure 37 – Vacuum Tube with support structures

8.8 Gamma Shielding

The Neutron Optics and Shielding group at the ESS will advise on what materials to use in the different absorbers, the current assumption is that boron carbide (B_4C) will be used for the Upstream Aperture, the Cleanup Slit and the Absorbing Baffles. Different forms of radiation may be emitted when neutrons are absorbed, depending on the absorbing element. When boron carbide absorbs neutrons gamma radiation is emitted. The design of the Beam Geometry Conditioning System allows at least 90% of the neutrons leaving the neutron guide window to be absorbed by these apertures, depending on the desired beam size. To stop the gamma radiation created in this absorption process from reaching the detector system the apertures are enclosed by the Gamma Shielding.

As the requirements of the shielding are uncertain and the Neutron Optics and Shielding group do not yet have definite guidelines on how to design the shielding, only a basic concept is presented in this project. The Gamma Shielding system will have to be updated in the future when the understanding of the requirements is clearer.

The concept for the Gamma Shielding is to encapsulate the Upstream Aperture, the Cleanup Slit and the Absorbing Baffles in a box of shielding material. The walls of the box have a sandwich structure with aluminum and lead. Lead is not a suitable material for construction due to its soft properties. However, lead absorbs gamma radiation effectively. Adding the aluminum increases the construction properties.

The box consists of a series of plates connected to a support structure. The walls and roof of the box are divided into segments for easier access to the Vacuum Tube. It might be necessary to have the lead plates overlapping to not have a straight line-of-sight path for the gammas to leak from the box. It is suggested that the plates are locked in placed to avoid unauthorized personnel to access the shielding components.

The base plate of the box has threaded holes matching the support structures for the Upstream Aperture, the Cleanup Slit and the Vacuum Tube. The Gamma Shielding is shown with one wall removed in Figure 38.

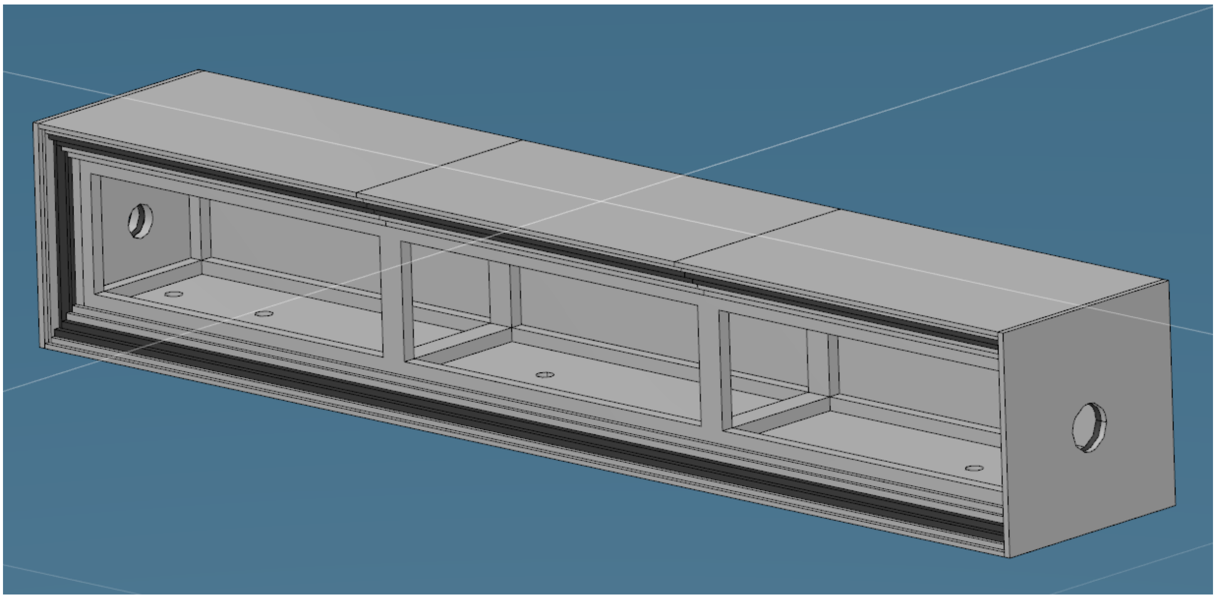

Figure 38 – The Gamma Shielding

9. CONCEPT DEVELOPMENT OF PINHOLE APERTURE

The Pinhole Aperture is the last aperture of the collimating system, defining the size of the neutron beam reaching the sample. The Pinhole Aperture should be placed as close to the sample as possible, while remaining within the design envelope. The size of the aperture should be adjustable in the range of 0.2 – 5mm, depending on the experiment needs.

The concept selection process described in this chapter has been reviewed and approved by the instrument lead engineer and the instrument scientific project leader and is published as a separate document in the ESS document managing system CHESS.

9.1 Existing Systems

All beam line instruments have a collimation system, regardless of using neutrons or X-rays. One of the most common collimation methods is to use a collimation system with apertures, as described in the initial chapters. This kind of collimation system uses a pinhole aperture close to the sample to define the beam size. Depending on the field of science studied at the instrument, the pinhole aperture is designed in two different fashions, based on the interest in backscattered neutrons. Many instruments are not interested in the backscattered neutron and therefore do not take the footprint of the system into account. In this case, the aperture is adjusted using a slit system or selecting an aperture size from a revolver. Both solutions have a high profile and large footprint.

If the backscattered neutrons are of interest, the high profile solutions are not feasible. The pinhole aperture in these cases is usually designed as an aperture with fixed size. If the aperture size needs to be adjusted this is done by manually changing the pinhole aperture. An example of an instrument using such a fixed pinhole aperture is the iBIX at J-PARC, see Figure 39.

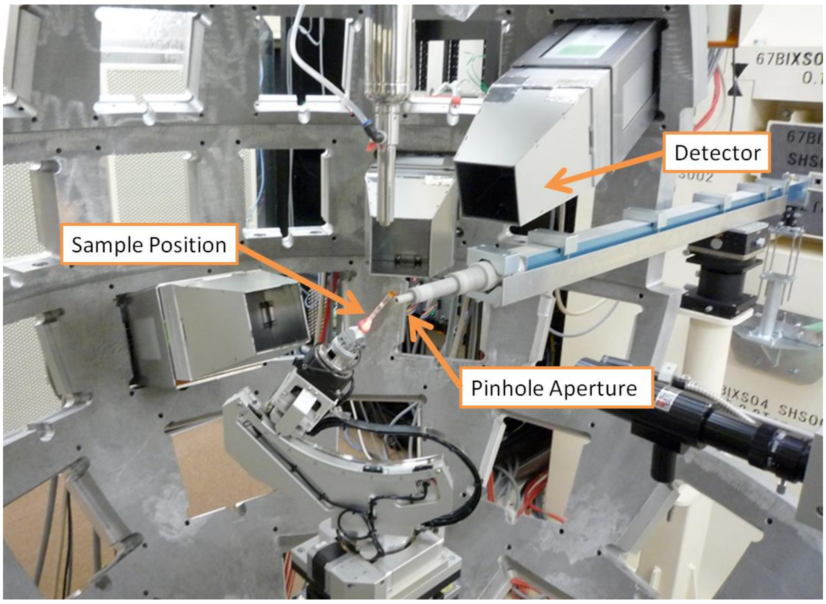

Figure 39 – End station of iBIX, J-PARC (iBIX, J-PARC, 2009)

There are exceptions to fixed pinhole aperture when backscattered neutrons are of interest. An example of a pinhole aperture with low profile but with motorized adjustment of the aperture size is the slit system Vakuum Tube Cross Slit Screen 3002.60M, provided by Huber. This slit system is used by the instrument XMaS at the ESRF. The size of the jaws is 4mm and each jaw may be individually positioned, see Figure 40.

Figure 40 – Commercially available slit system provided by Huber, Vakuum Tube Cross Slit Screen 3002.60M (XMaS, ESRF)

The Beam Geometry Conditioning System at NMX requires the beam size to be adjustable in the range of 0.2mm up to 5mm, while allowing backscattered neutrons to be observed up to 165° from the beam axis. The distance between the Pinhole Aperture and the sample should be as small as possible. Adjustment of the aperture size should not require manual operation, but be motorized. Due to these reasons, it is likely that none of the existing systems for the Pinhole Aperture can be used at NMX. To find the best concept for the Pinhole Aperture a concept selection process is performed.

9.2 Identified Concepts

There are many different solutions on how to design the Pinhole Aperture. The five most feasible concepts have been selected and are briefly presented in this chapter.

9.2.1 Deck of Blades

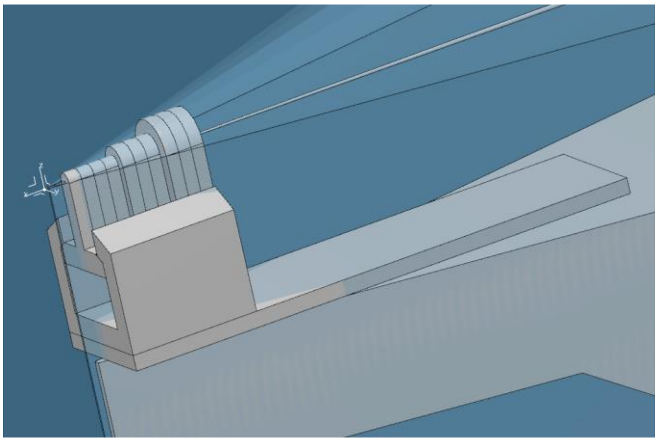

Figure 41 – Deck of blades

A number of absorbing blades are stacked in line with the neutron beam axis, see Figure 41. Each blade has a specific aperture size. The blades are supported by a frame below the neutron beam axis. The blades can slide along the z-axis to be placed in the neutron beam, defining the beam size.

9.2.2 Double Slit Jaws

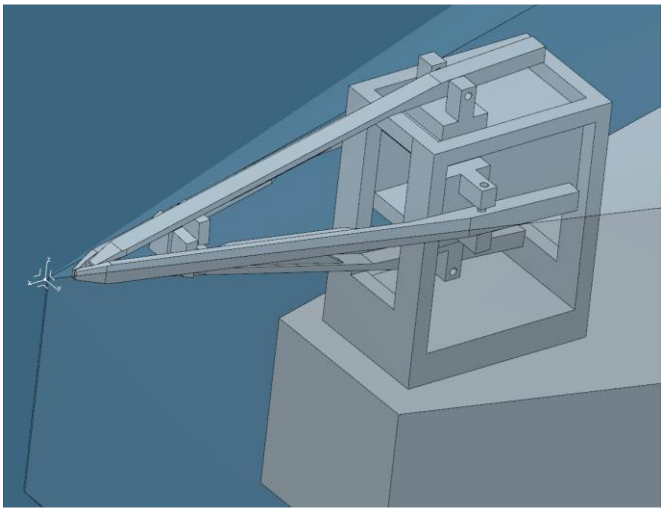

Figure 42 – Double slit jaws

Four separated jaws are mounted on a support frame using hinges, see Figure 42. The jaws are rotated by actuators. The jaws are made of absorbing material. To be able to have narrow jaws, additional absorbing blades are mounted on them 30mm upstream. These blades will clean up the beam before it reaches the tip of the jaws. For larger beam sizes these will be the main absorbers. In the case of large beam sizes, the tip of the jaws will reduce over illumination. For small beam sizes the upstream absorbing blades will clean up the beam and the tips will define the beam size.

9.2.3 Extendable Arms

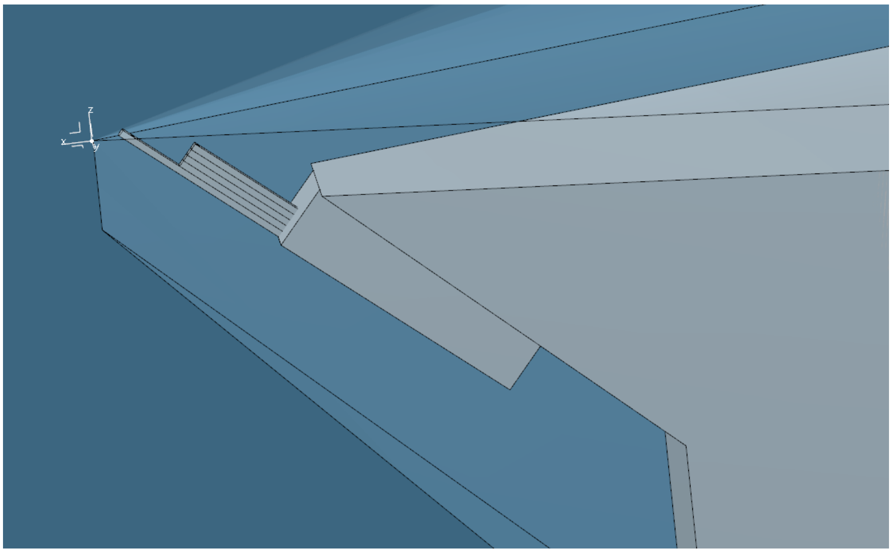

Figure 43 – Extendable arms

A number of extendable arms are mounted on the front table, see Figure 43. Each arm is carrying a fixed absorber with a specific aperture size. The arms can be individually placed in the neutron beam. The arms may be operated by linear stages, pneumatics or other mechanic solutions.

9.2.4 Exchangeable Cartridges Using a Rotating Arm

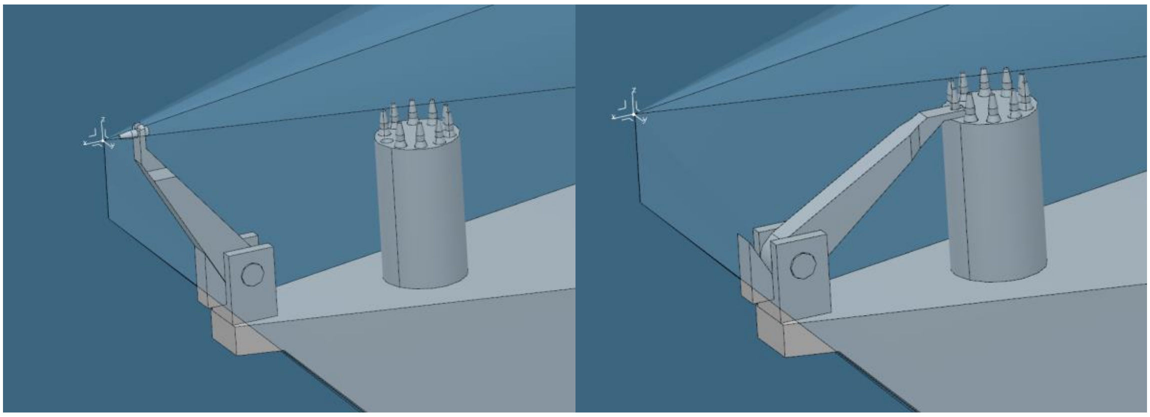

Figure 44 – Exchangeable cartridges using a rotating arm

An arm is mounted on a rotary stage, see Figure 44. The tip of the arm has a slot to carry absorbing cartridges. The cartridges are conical to match the shape of the slot in the arm and to secure a repeatable positioning of the cartridge during cartridge exchange. The active absorbing cartridge is kept in place on the arm using permanent magnets. A number of cartridges are stored in a rotating carousel, also using permanent magnets. A solenoid is placed under the carousel in correspondence of the cartridge exchange position, used to release the cartridge from the arm during the unloading phase. To change the active cartridge, the arm rotates 90° to come in contact with the carousel. The solenoid is activated to attract the cartridge towards the carousel body. The arm rotates away from the carousel and the carousel turns to place the new bullet the exchange position. The arm rotates in the loading/unloading position by the carousel and the solenoid is deactivated. The cartridge will now latch to the arm. To optimize the functionality the carousel is mounted on a linear stage to be able to move it out of the beam axis.

9.2.5 Revolver

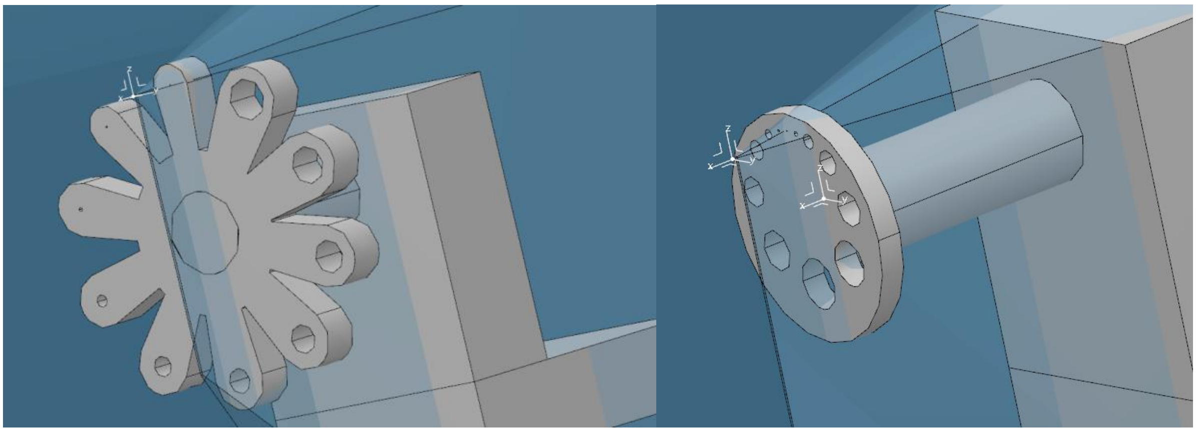

Figure 45 – Revolver

A revolver with a fixed number of fixed apertures is mounted on a rotatory stage, see Figure 45. The revolver is turned to select the wanted aperture size. Either the revolver is a solid circular plate or it has a number of outgoing arms with the apertures. This is a standard solution for pinhole collimation systems.

9.3 Concept Screening

Concept screening is a quick method to compare different concepts based on requirements and general criteria, to find the most promising concepts. The general criteria are described in Table 6. A more detailed and in-depth comparison of the most promising concepts is then performed, called concept scoring.
Table 7 shows a concept screening matrix for the different identified concepts, presented above. Concept 1, the Deck of blades, is arbitrarily selected as the reference concept, which the other concepts are compared to.

Table 6 – Criteria description

	Description
Contained within the envelope	How well the assembly is contained within the envelope, especially in the top hemisphere.
Aperture flexibility	How well the size and shape of the aperture can be changed.
Goniometer positioning flexibility	How much space is available for the goniometer below the sample, corresponds to the size and placement of the support table
Aperture-to-sample distance	How close the aperture can be to the sample, without exceeding the envelope.
Adaptable for changes	How easy it is to implement any future changes in the requirements, e.g. regarding absorbing material.
Robustness	How robust the solution is, in terms of likelihood of jamming and stability

Table 7 – Concept screening matrix

	Concept 1 **Deck of blades**	Concept 2 **Jaws**	Concept 3 **Extendable arms**	Concept 4 **Rotating arm**	Concept 5 **Revolver**
Contained within the envelope	0	+	+	+	-
Aperture flexibility	0	+	-	+	-
Goniometer positioning flexibility	0	+	-	+	-
Aperture-to-sample distance	0	+	0	+	-
Adaptable for changes	0	-	0	+	-
Robustness	0	0	+	0	+
sum	**0**	**+3**	**0**	**+5**	**-4**
Continue develop	**No**	**Yes**	**No**	**Yes**	**No**

Concepts 1, 3 and 5 have the lowest score and will not be further investigated. Concepts 2 and 4 have the best score and will proceed to the next selection stage, concept scoring.

9.4 Concept Breakdown

The result of the concept screening is that the *Double Slit Jaws* and the *Exchangeable Cartridges Using a Rotating Arm* are the best and most feasible concepts. In this chapter the concepts are broken down into the required components. The specifications plus the pros and the cons of each concept are also identified, preparing for the concept scoring described in the next chapter.

9.4.1 Components

Table 8 – Identified components

Double slit jaws	Exchangeable Cartridges Using a Rotating Arm
4 picomotor actuators with encoders	Al fork
8 bearings	Pneumatic rotatory stage
4 springs	Rotatory support
4 shafts	Pneumatic linear stage
4 rotatory supports	Carousel support
4 arms out of absorbing material/coated	Stepper motor with encoder
4 larger absorbing plates mounted on the arms	Carousel
Al support frame	10 cartridges
Al/concrete tube	Solenoid
	Many small magnets

9.4.2 Specifications

Table 9 – General specifications

Double slit jaws	Exchangeable Cartridges Using a Rotating Arm
Assembly length: ~200mm	Assembly length: ~350mm
Aperture size: 0-~10mm	Aperture size: 0.2-5mm
Step size: ~0.06-0.1mm	Step size: Varies/To be decided, 10 discrete steps
Sample-to-absorber distance: o 0.2-2,5mm sample: ~5-15mm o 2,5-5mm sample: partly ~15-20mm, secondary absorber at 30mm upstream	Sample-to-absorber distance: ~5-15mm
Beam shape: o 0.2-2,5mm sample: Square o 2,5-5mm sample: semi-square	Beam shape: Arbitrary
Manually operable: coarsely/inaccurately by turning the Picomotor	Manually operable: Yes
Goniometer clearance: o Arm angle: ~15deg o Table distance: ~100mm	Goniometer clearance: o Arm angle: 20deg o Table distance: ~150mm
Width-height absorbers distance: 6mm	

9.4.3 Pros and Cons

Table 10 – Identified pros

Pros	
Double slit jaws	**Exchangeable Cartridges Using a Rotating Arm**
High flexibility in beam size, small step size	Possible to match the aperture size and shape to specific experimental conditions
Low complexity	Small sample-to-absorber distance for all beam sizes
Short assembly along beam axis	High stability
The tips of the arms will reduce over-illumination with large sample size	Adaptable to future changes
High reliability/unlikely to jam	

Table 11 – Identified cons

Cons	
Double slit jaws	**Exchangeable Cartridges Using a Rotating Arm**
Large sample-to-absorber distance for large sample sizes	Discrete beam sizes/Many cartridges might be needed
The arms, springs and picomotor might not be sufficiently stable	New bullets may have to be manufactured to fulfill specific requirements regarding beam size/shape, planning needed
Absorption in four different planes, hard to define where the absorption occurs	Long assembly along the beam axis
Beam shape depends on beam size	Complex process to change beam size
Uneven sample-to-absorber distance between height and width	Less reliable/More likely to jam

9.5 Concept scoring

In this chapter the two concepts are evaluated to find the best solution. This is done using a concept scoring matrix with criteria based on the specifications and the pros and cons identified in the previous chapter. The different criteria in the concept scoring matrix are described in Table 12. The criteria will be weighted depending on how critical that specific criterion is to the design. The concepts will get a score in the range of 1 to 5 for each criterion, where 1 is very bad and 5 is very good. The weight values are set based on advice of the instrument lead engineer and the instrument scientific project leader. The given score is then multiplied by the weight to give the final score for that criterion. The concept with the highest total score is the best concept, which will be further developed.

Table 12 – Criteria description

	Description
Expected reliability	How likely the system is to jam or fail
Adaptive to future requirement changes	How easy it is to implement any future changes in the requirements, e.g. regarding used materials or thickness of the absorbing material
Sample-to-absorber distance	How close the aperture can be to the sample, without exceeding the envelope.
Flexibility in absorbing material	How easy it is to change the used absorbing material and what materials that could be used with the solution
Complexity	How complex the mechanism for changing aperture size is, corresponding to motorized axes
Beam size adjustability	How freely it is possible to select the beam size
Consistent beam shape	How well the beam shape keeps it shape for different sample-to-aperture distances
Flexible width/height	How freely the shape of the beam can be selected, mainly in terms of width and height
Manually operable	How well the system can be manually operated, e.g. if a motor fails
Footprint	How large the footprint of the assembly is within the envelope, it is preferable to have a small assembly that doesn't fill the entire envelope
Goniometer position flexibility	How much space is available for the goniometer below the sample, corresponds to the size and placement of the support table

Table 13 – Concept scoring matrix

	Weight	**Double slit jaws**		**Rotating arm**	
		Score	Weighted score	Score	Weighted score
Expected reliability	3	4	12	3	9
Adaptive to future requirement changes	3	2	6	4	12
Sample-to-absorber distance	3	3	9	5	15
Flexibility in absorbing material	2	2	4	5	10
Complexity	2	4	8	2	4
Accessible solid angle	2	3	6	4	8
Assembly length	1	4	4	3	3
Beam size adjustability	1	5	5	5	5
Consistent beam shape	1	2	2	4	4
Flexible width/height	1	4	4	4	4
Manually operable	1	3	3	4	4
Footprint	1	2	2	4	4
Goniometer position flexibility	1	4	4	3	3
Total weighted score		69		85	

9.6 Conclusions

The *Double Slit Jaws* concept is the most flexible solution regarding beam size, as it can select the beam size continuously with high precision instead of having a fixed set of beam sizes to choose from. However, it is not as crucial to be able to select the beam size in fine steps for large beam sizes as when dealing with small sizes. It is sufficient to have ten specific beam sizes in the range of 0.2 – 5mm to fulfill the needs of the instrument. Hence, the criteria regarding beam size have low priority and a low weight in the scoring matrix. Instead it is the flexibility of the assembly that decides which concept is most suitable.

Many critical parameters have not yet been decided for the instrument, such as what materials should be used for the absorber and how thick they have to be. The requirements may also change in the future and the Beam Geometry Conditioning System has to easily be adjusted to these changes. The *Exchangeable Cartridges Using a Rotating Arm* concept can easily be upgraded with new cartridges to match the potential new requirements, whereas to upgrade the *Double Slit Jaws* concept new jaws will have to be manufactured.

The most important parameter from a scientific standpoint is the sample-to-aperture distance. The shorter the distance, the higher the flux and the lower the halo is. The *Exchangeable Cartridges Using a Rotating Arm* concept can be placed very close to the sample for all the beam sizes, while the *Double Slit Jaws* needs a larger distance for larger beam sizes.

The *Exchangeable Cartridges Using a Rotating Arm* is the best concept as it fulfills the requirements regarding beam size and shape while allowing high flexibility for adjusting the system for future needs. This concept is the only concept entering the detailed design phase.

10. DETAIL DESIGN OF PINHOLE APERTURE

The best concept for the Pinhole Aperture according to the concept selection process is the *Exchangeable Cartridges Using a Rotating Arm* concept. This concept consists of three main components, the cartridge, the rotating arm and the carousel. The design of these three components has to ensure reliable functionality of the system. This chapter describes the design of the components along with the design of the Downstream Table that supports the Pinhole Aperture. The complete Pinhole Aperture with the Downstream Table is presented in Figure 46.

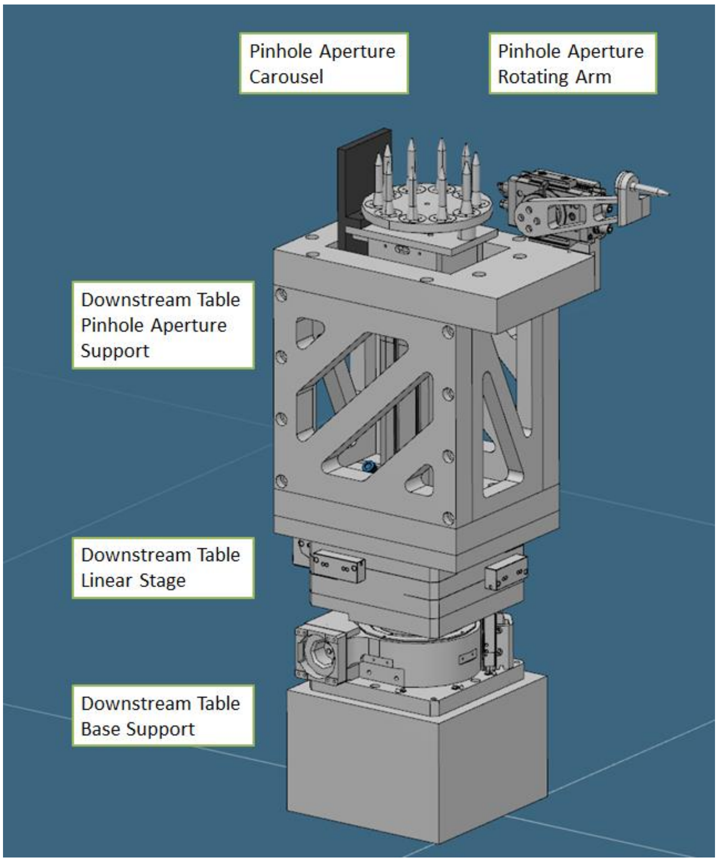

Figure 46 – Complete Pinhole Aperture including the Downstream Table

10.1 Pinhole Aperture Functionality

An absorbing cartridge with a fixed aperture is positioned in line with the neutron beam by an arm. The cartridge is kept in place on the arm using permanent magnets. A number of passive cartridges are stored in a rotating carousel, keeping them out of the neutron beam. The passive cartridges are kept in place on the carousel using magnets. To change the aperture size, the active cartridge is replaced according to the following procedure.

The first step in the sequence to change the active cartridge is to rotate the arm with the active cartridge to the exchange position. The carousel should already be at the position with the empty slot at the correct location. If not, the carousel is turned to place the empty slot straight below the active cartridge. The linear stage is raised to place the carousel at the exchange position at the arm, see Figure 47. The magnetic force towards the arm is stronger than the force towards the carousel plate, allowing the cartridge to remain on the arm. To release the cartridge from the arm a solenoid is activated. The cartridge is then attached to the carousel plate instead of to the arm. While the solenoid is activated the linear stage is lowered removing the carousel from the arm. At the bottom position of the linear stage the solenoid is deactivated. The carousel is rotated to select the cartridge corresponding to the desired beam size. The solenoid is activated again to lock the cartridge to the carousel plate. The linear stage is raised again to place the new cartridge at the arm. By deactivating the solenoid the cartridge is released from the carousel and latches to the arm. The linear stage is lowered again and finally the arm is rotated back to place the cartridge in line with the neutron beam.

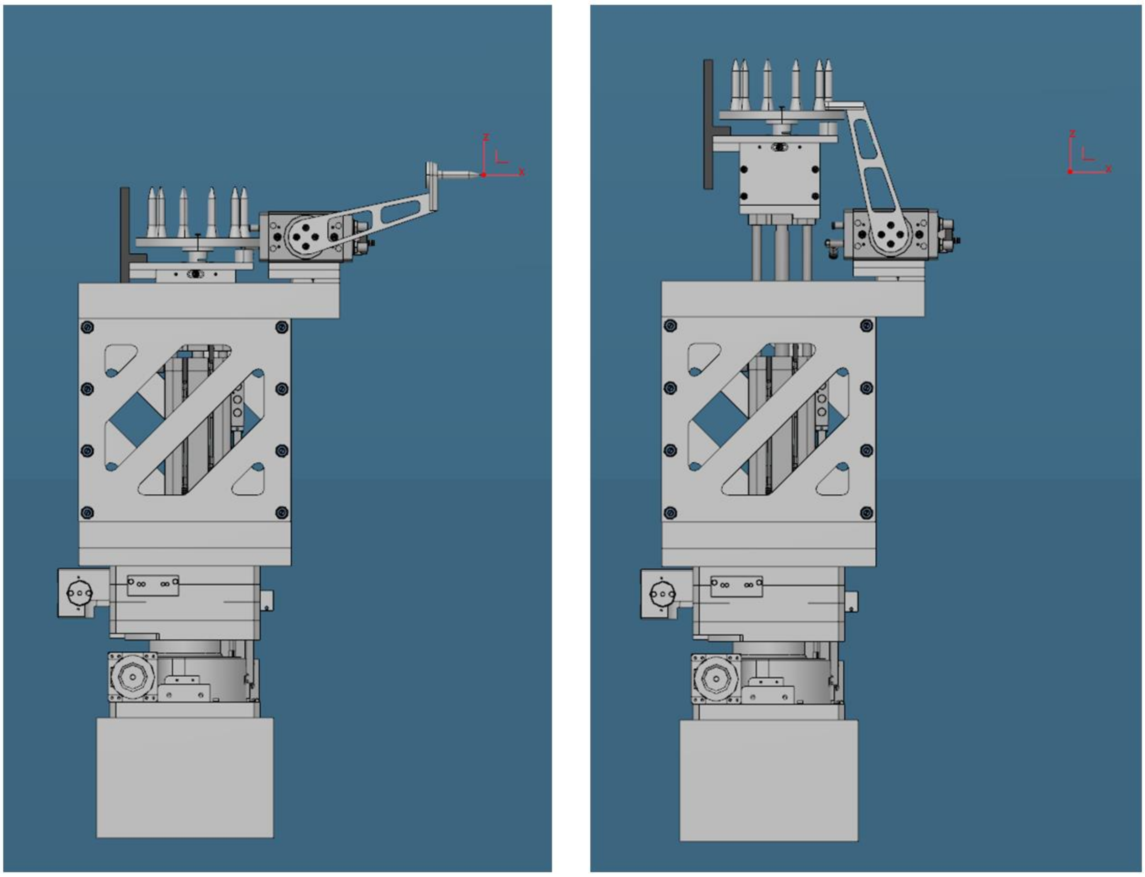

Figure 47 – Illustration of the operational settings of the pneumatic stages (to the left) compared with the exchange position (to the right)

10.2 Pinhole Aperture Cartridges

The first and the most important component of the Pinhole Aperture is the cartridge. The shape of the cartridge is important for the functionality of the system. Depending on the absorbing material used the design may vary slightly. The design described below is assuming that the cartridge can be manufactured as one solid part by turning. The cartridge may be made out of a neutron absorbing material or be made out of aluminum and then be coated with an absorbing material after manufacturing. Possible coatings are gadolinium or lithium.

The cartridge design can be divided into three critical areas, the base, the contact cone and the tip, see Figure 48.

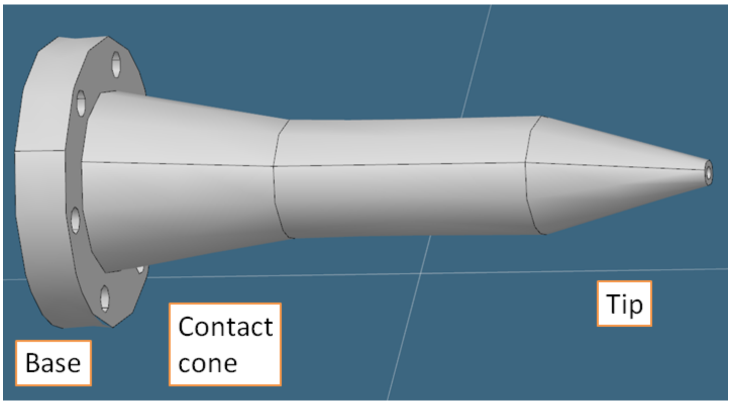

Figure 48 – Cartridge divided into three design areas

The base absorbs most of the unusable neutrons that reach the Pinhole Aperture. As described in the concept design of the Cleanup Slit, the size of the neutron beam reaching the Pinhole Aperture is roughly 22 x 22mm for a beam size of 5mm. To ensure that all unusable neutrons are absorbed the base need to have a diameter of 30mm. This requires the cartridge to be at least 60mm long. The base has another function as well, as it carries the permanent magnets to latch the cartridge to either the arm or the carousel. The magnets are glued in place inside holes in the base. The holes are placed on the downstream side of the base, by the rotating arm, to ensure that neutrons do not hit the magnets directly. The magnetic forces should be stronger towards the rotating arm than towards the carousel, so the cartridge latches to the arm in the exchange position while the solenoid is deactivated. This action is aided by having the magnets mounted on the arm side of the base.

The contact cone positions the cartridge on the arm in a repeatable fashion. The diameter of the cone at the base is slightly larger than the diameter of the slot in the arm, creating a small gap between the base and the arm. The reason for this is that only the contact cone should be in contact with the arm, while placing the magnets close to the arm. The diameter of the end of the contact cone is 2mm smaller than the slot in the arm. This will guide the cartridge in place when the arm and carousel are moved into the exchange position. Using small disc magnets in both the cartridge and the arm will reduce the likelihood that the cartridge rotates in the exchange procedure, as the magnets will aim to be as close as possible to their counterparts in the mating part.

The shape of the tip of the cartridge defines the minimum distance to the sample without exceeding the design envelope. Having a 15° chamfer centered on the sample position is the optimal shape of the tip. The limiting parameters to the distance are then the beam size and the wall thickness of the tip. Assuming a wall thickness of 0.5mm the minimal sample-to-aperture distance is then 3mm for a beam size of 0.2mm and 12mm for 5mm.

10.3 Pinhole Aperture Rotating Arm

The second component is the rotating arm which supports the active cartridge and places it in line with the neutron beam, see Figure 49.

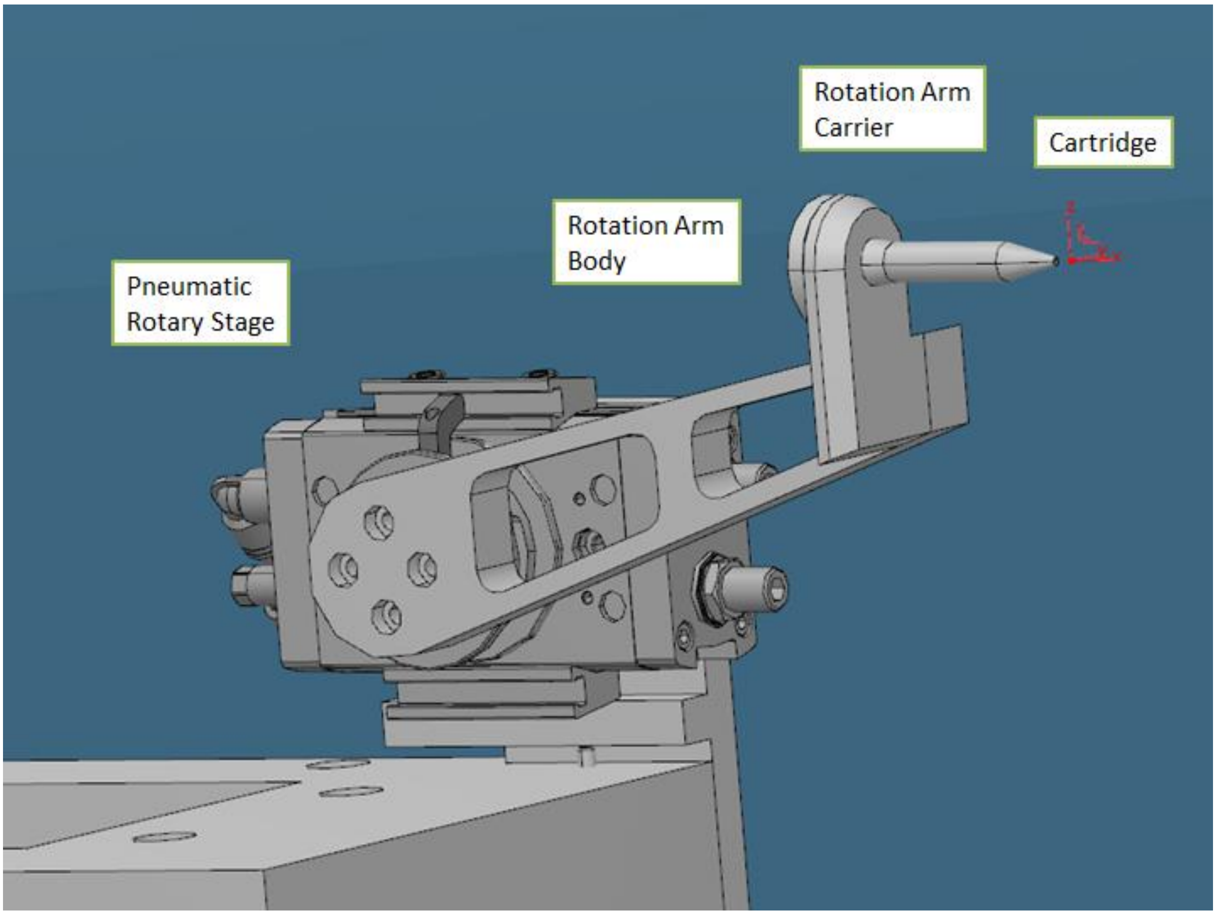

Figure 49 – The rotating arm mounted on the pneumatic stage

The arm is mounted on a rotary stage, with two end positions separated by 90°. One end position places the cartridge in line with the beam axis and the other places the arm in the exchange position. The rotary stage only needs these two end positions and being able to place the arm in any intermediate position does not add to the functionality of the system. The solution selected for implementing the movement is to use a pneumatic rotary stage. A pneumatic rotary stage which fulfills the requirements for the system is the Semi-rotary drive DRRD (DRRD-16-180-FH-PA-R) provided by Festo. The most important requirement for the rotary stage is its repeatability. The selected stage has a repetition accuracy of <0.05°. As the rotating arm is 160mm a 0.05° rotation would move the tip about 0.15mm. The contact cone of the cartridge will guide the components in place up to 1mm offset. The angular positions of the end positions are flexible by adjusting two screws.

The rotary stage exceeds the envelope on one side of the beam axis in the lower hemisphere. Due to this the arm can be shaped like an L, as the angle obscured by the arm already is obscured by the stage, see Figure 50.

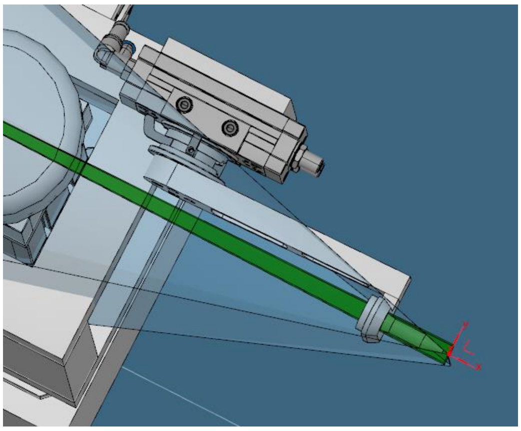

Figure 50 – Arm and rotary stage exceeding the design envelope (light blue), obscuring the same angle in the lower hemisphere

The arm is divided into two parts, the body and the carrier. This increases the flexibility for future updates, as only the carrier has to be replaced in case a new design of the interface between the cartridge and the carrier is needed. One possible future change might be to mount the beam-stop onto the rotating arm. The connection between the body and the carrier consists of a screw and two pins. Having two pins allows the carrier to be mounted with high repeatability on the body.

The body of the arm is not centered directly below the neutron beam axis. To perform experiments at the secondary sample position the arm is placed in the exchange position allowing the neutron beam to pass the arm, see Figure 51.

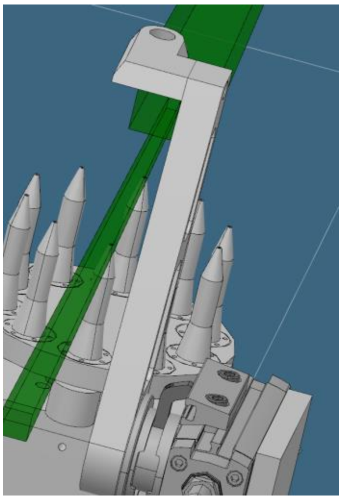

Figure 51 – Neutron beam (green) passing by the arm when the arm is placed in the exchange position

10.4 Pinhole Aperture carousel

The last component of the Pinhole Aperture is the carousel. The purpose of the carousel is to store the passive cartridges. The carousel consists of a circular plate mounted directly onto a stepper motor to be able to select cartridge. The stepper motor is connected to a support frame mounted onto a linear stage. Just as in the case of the rotary stage for the rotating arm, the linear stage only needs two end positions and a pneumatic linear stage is therefore used. The pneumatic linear stage used is the Compact cylinder ADNGF, metric (ADNGF-63-140-P-A) provided by Festo.

As described in chapter 10.1, the cartridge should latch to the rotating arm instead of the carousel disk at the exchange position. To release the cartridge from the rotating arm to the carousel disk a solenoid is used. The used solenoid is a Stephenson Gobin 58 - 0125 12 VDC Electromagnet, type 58, which has a holding force of 90N. The solenoid is mounted on the support frame, just beneath the exchange position for the cartridges, see Figure 52.

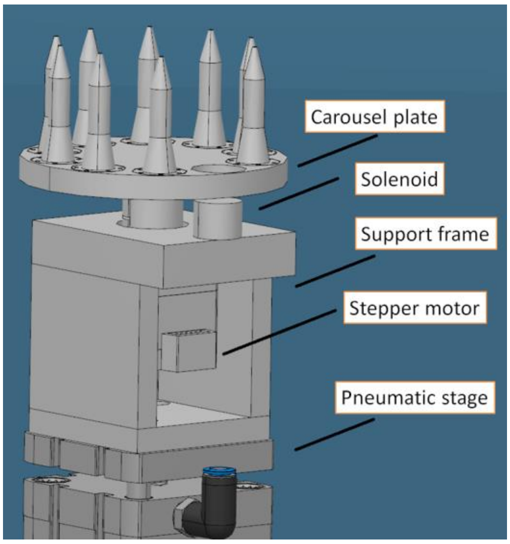

Figure 52 – Carousel assembly

The carousel plate carries up to ten cartridges. The entire carousel plate should be replaced to change the cartridges stored at the Pinhole Aperture. The carousel plates should have indexes to keep track of which set of cartridges is mounted in the carousel. To be able to change the carousel plate in a quick and repeatable fashion the interface to the rigid coupling needs to be carefully designed.

The solution used for the interface is to have a circular slot with a groove in the carousel plate and adding a threaded ball spring plunger to the rigid coupling, see Figure 53. The carousel plate is snapped in place at the correct angle and then fixed in place with a screw from the top.

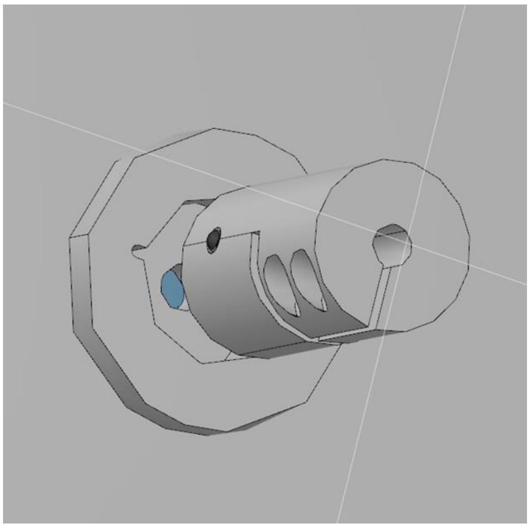

Figure 53 – Interface between the rigid coupling and the carousel plate

The passive cartridges are kept in place on the carousel plate using permanent magnets. Slots are added for each cartridge position to have an additional mechanism to keep the cartridges in place, see Figure 54. A lid should be mounted to protect the cartridges when a carousel plate is removed from the carousel, see Figure 55.

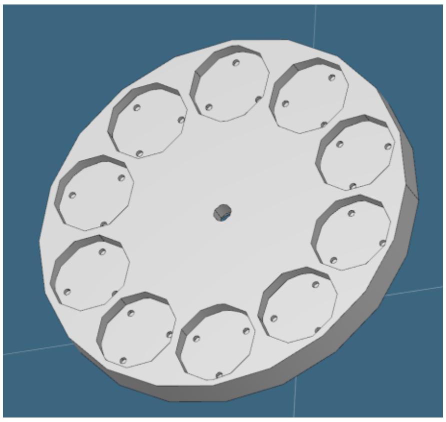

Figure 54 – Carousel plate

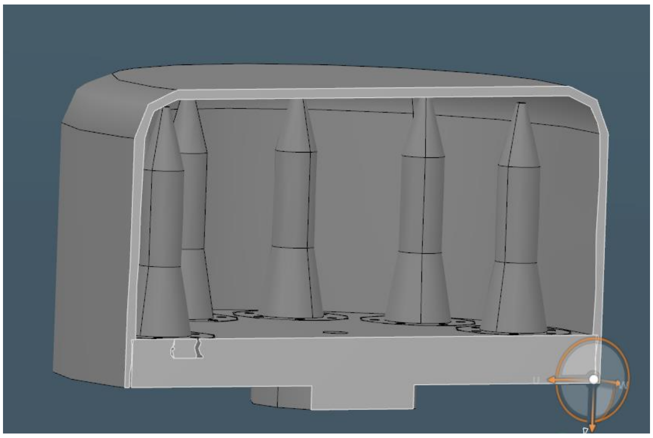

Figure 55 – Protective lid

The support frame for the stepper motor is a key component for aligning the rotating arm with the carousel at the exchange position. The support frame is designed as a box to fit the stepper motor. The stepper motor is mounted on the lid of the box. The position of the lid on the box is adjustable using grub screws. To be able to mount the box on the pneumatic stage in a repeatable fashion the bottom plate has a groove, see Figure 56.

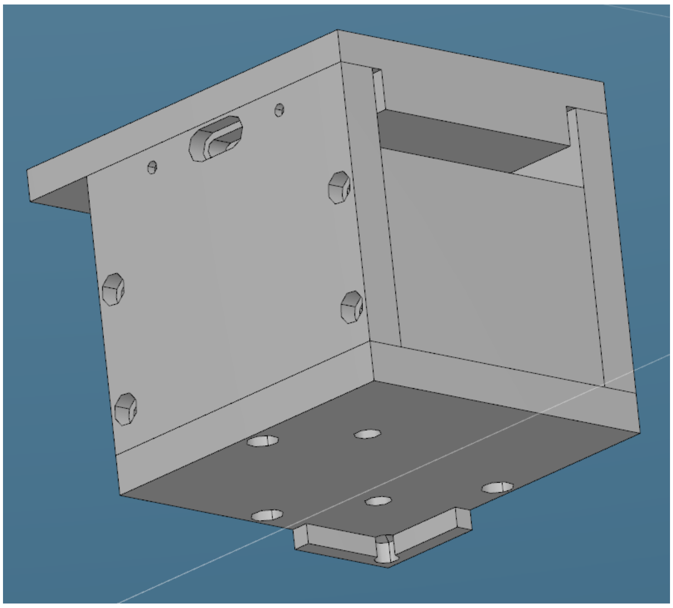

Figure 56 – Support frame for the stepper motor

During the cartridge exchange process the support frame is placed in the neutron beam. To protect the stepper motor and prevent the neutrons to interact with materials with unwanted neutron interaction properties an absorber is mounted on the lid of the support frame, see Figure 57.

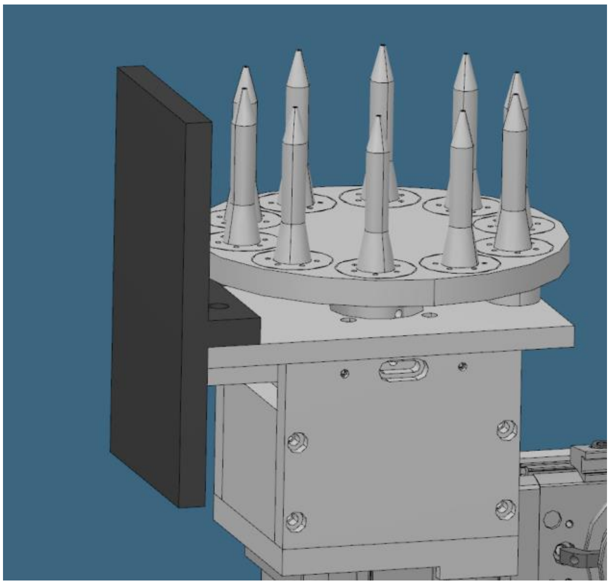

Figure 57 – Absorbing plate mounted on the support frame to absorb the neutron beam while the linear stage is raised

10.5 Pinhole Aperture Support

The support for the Pinhole Aperture is the top part of the Downstream Table. The support is designed as a box to fit the linear stage, mounted on top of the XY-stage. The top plate of the box supports the rotary stage for the arm and the bottom plate supports the linear stage and thus the carousel. Both the top and the bottom plate have grooves in them to be able to mount the stages in a repeatable fashion. The position of the rotary stage is adjustable in the Z-direction using an adjustment screw, while pushing the mounting plate against the groove. The complete Downstream Table with the Pinhole Aperture mounted is shown in Figure 58.

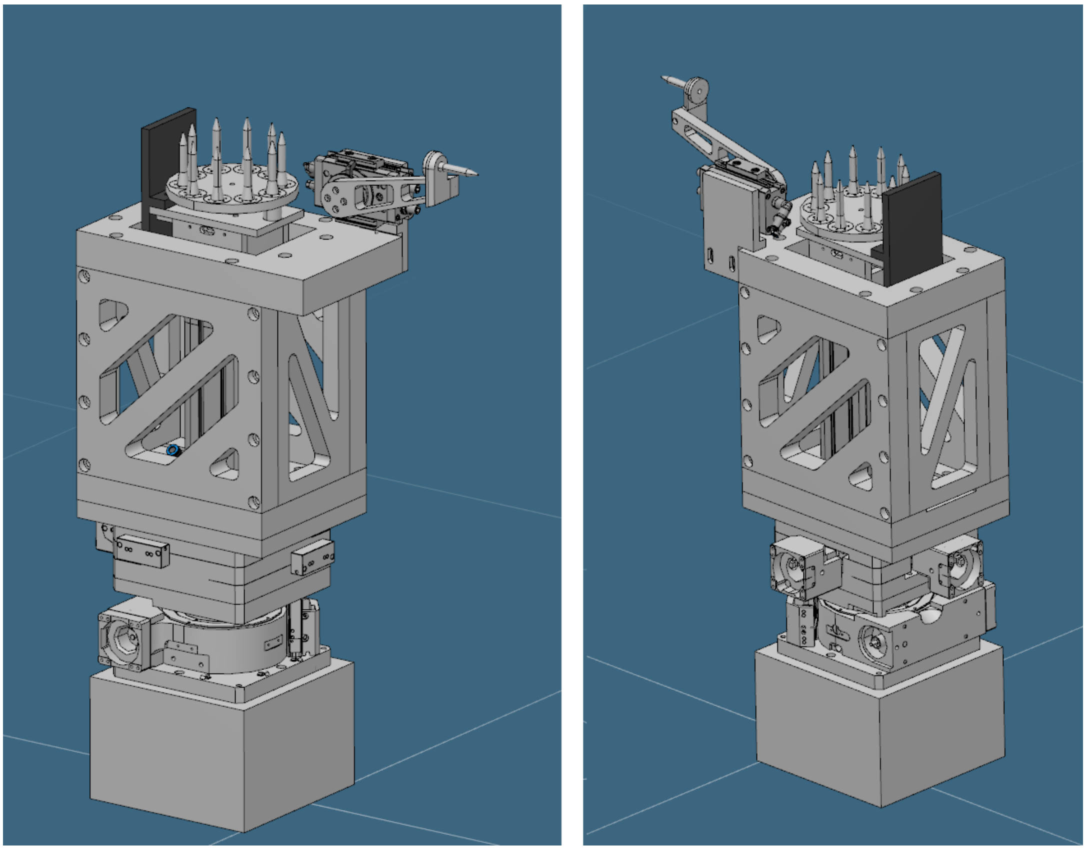

Figure 58 – Complete Downstream Table, including the Pinhole Aperture

10.6 Pinhole Aperture Alignment

One of the challenges of the *Exchangeable Cartridges Using a Rotating Arm* concept is the reliability of the system. To reduce the risk of jamming of failure the rotating arm and the carousel needs to be aligned to each other at the exchange position. The alignment for the different degrees of freedom is presented in Table 14. All components are mounted using pins, grooves or adjustment screws. This makes it possible to mount and dismount the different components of the Pinhole Aperture with high repeatability, ensuring the functionality of the system.

Table 14 – Possible adjustment in the different degrees of freedom

Degree of freedom	Adjustment method	Range
X-direction	Adjustment screws on the stepper motor support plate	±3mm
Y-direction	Adjustment screws on the stepper motor support plate	±3mm
Z-direction	Adjustment screw on the rotary stage mounting plate	±3mm
XY-rotation	Stepper motor	Freely
XZ-rotation	Adjusting the end positions of the rotary stage	Freely
YZ-rotation	Shims at both the linear stage and the mounting plate of the rotary stage	±5°

11. COMPLETE DESIGN OF THE BEAM GEOMETRY CONDITIONING SYSTEM

The conceptual design of the Beam Geometry Conditioning System is now completed within the scope of this project. The system is assembled into the model of the End station, presented in Figure 59. The validation plan states that the system shall be validated in two steps. The first step in validating the design is to perform McStas simulations to validate the neutronic performance of the system. The second step is to evaluate the requirements, by scoring each requirement in terms of their fulfillment.

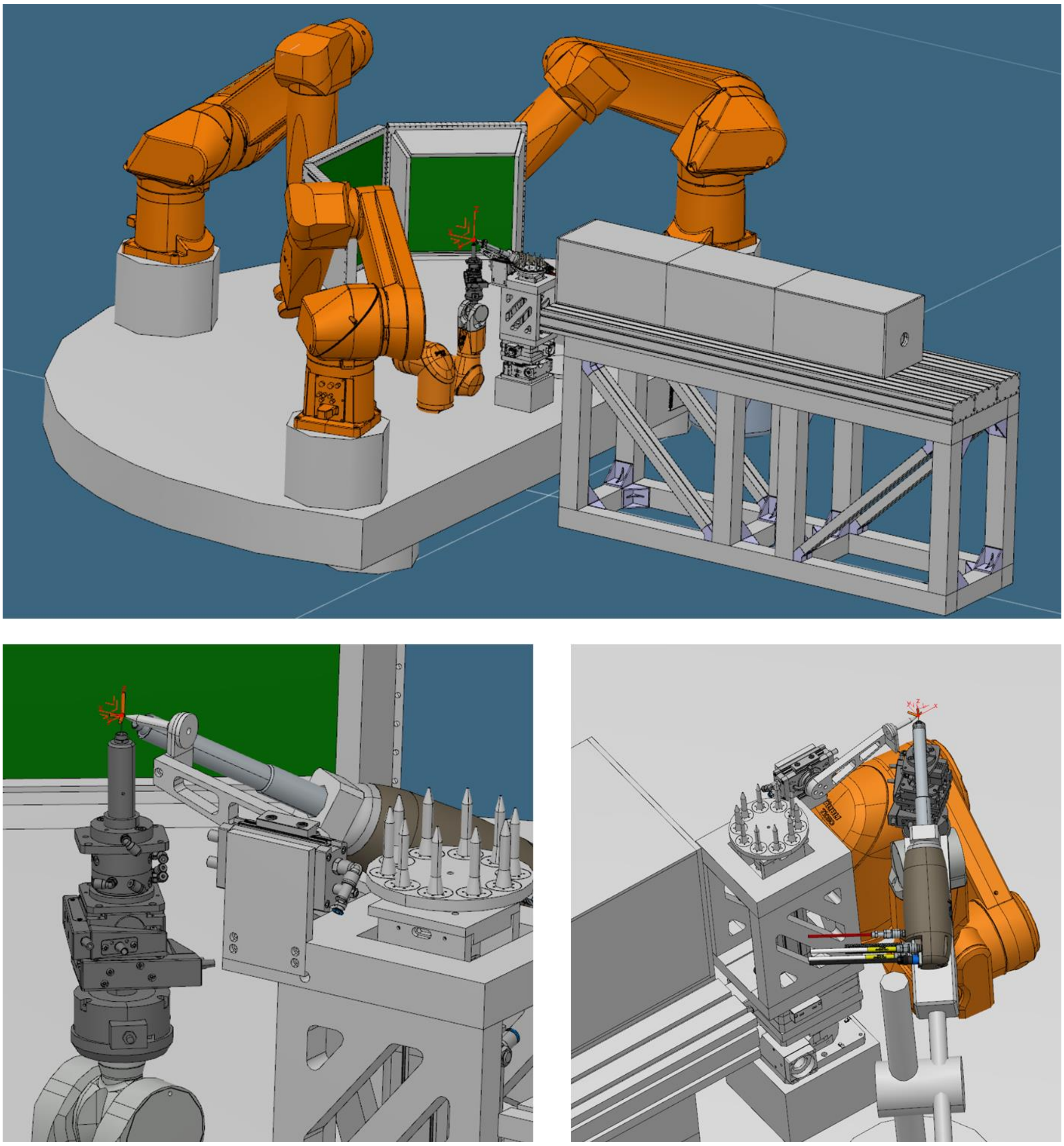

Figure 59 – Completed Beam Geometry Conditioning System assembled with the NMX End station

11.1 Simulated Validation

To validate the neutronic performance of the system, McStas simulations are performed according to the validation plan. Position sensitive detectors are implemented at every component of the system to ensure that the intent of the design is fulfilled. The result of the simulations matches the expected values for the beam characteristics in a satisfying manner. The characteristics of the neutron beam reaching the sample position of the validation simulation for 0.2mm beam size and 0.2° beam divergence are shown with a logarithmic scale in Figure 60.

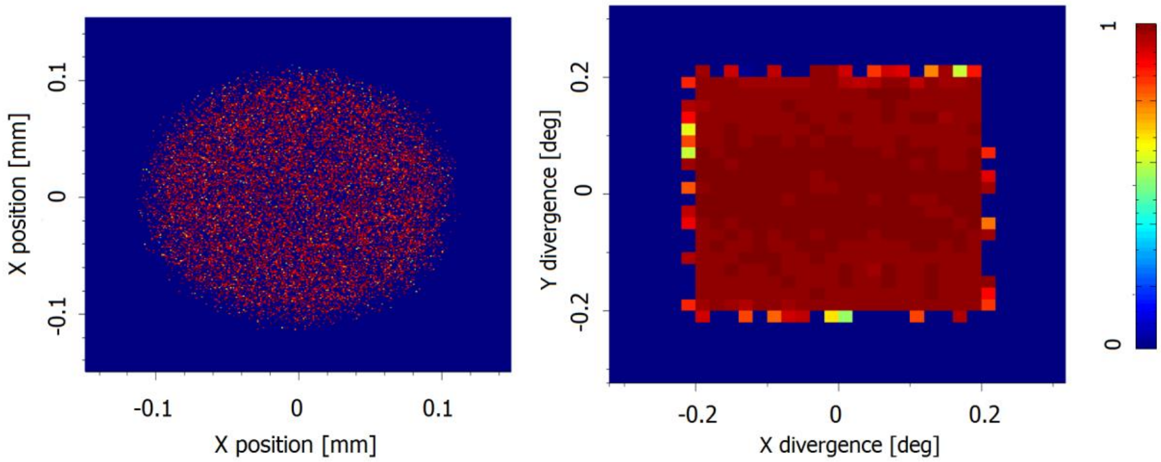

Figure 60 – Beam characteristics at the sample position of the validation simulation

The simulations show that roughly 90% to 97% of the neutron beam leaving the neutron guide window is absorbed by the Upstream Aperture and the Cleanup Apertures, depending on the desired beam size. These components are placed within the Gamma Shielding, preventing the generated gamma rays to reach the detector system. A maximum of roughly 8% of the neutrons leaving the window are absorbed by the Pinhole Aperture.

11.2 Requirement Fulfillment

To evaluate the design each requirement is marked based on how well it is fulfilled. The requirements that are left unmarked cannot be evaluated at this stage of the design, as they require more information regarding either used materials or other systems of the instrument which are not yet designed.

Table 15 – Evaluation of the functional requirements

Functional Requirement	Fulfillment
Beam maximum size The BGCS shall define at the sample a beam of neutrons with a maximum size (full width half maximum) of 5 x 5 ± 0.1 mm.	*Fully fulfilled*
Beam minimum size The BGCS shall define at the sample a beam of neutrons with a minimum size (full width half maximum) of 0.2 x 0.2 ± 0.02 mm.	*Fully fulfilled*
Beam maximum divergence The BGCS should define at the sample a beam of neutrons with a maximum divergence of ±0.2°.	*Fully fulfilled*
Beam minimum divergence The BGCS shall define at the sample a beam of neutrons with a minimum divergence of ±0.02°.	*Fully fulfilled*
Beam size selection The BGCS should allow the beam size to be selected in 0.05 ± 0.02 mm steps in both height and width independently.	*Fully fulfilled* Specific beam sizes and beam shapes may be acquired by creating matching cartridges
Beam divergence selection The BGCS shall allow the beam divergence to be selected in 0.02° steps.	*Fully fulfilled*
Neutron background The BGCS should absorb 99.9% of the thermal and cold neutrons outside the selected beam size and divergence	
Gamma ray background The BGCS should not expose the detector system to radiation that detector system cannot distinguish from thermal neutrons.	*Partly fulfilled* 90% to 97% of the neutrons leaving the neutron guide window are absorbed with the Gamma Shielding. The material of the absorber at the Pinhole Aperture should be selected in a sense that the emitted radiation is not detectable by the detector system
Accessible solid angle The BGCS should not obscure neutrons scattered by the sample within an angular range of ±165° from the neutron beam axis in the top hemisphere.	*Fully fulfilled*
Beam halo The BGCS should define at the sample a beam of neutrons with a distribution such that more than 90% of the neutrons are within the beam size area.	*Fully fulfilled*

Table 16 – Evaluation of the constraint requirements

Constraint Requirement	Fulfillment
Design space The system shall be contained within the envelope model ESS-0052092	*Partly fulfilled* Fulfilled in the top hemisphere, which is the critical area of the design
Support areas The system shall be supported on the areas identified in the envelope model ESS-0052092	*Fully fulfilled*
Stability The centroid of the collimated beam shall remain within 10% of the beam size from the effective sample position (as identified by the goniometer)	
Structural materials Structural materials shall be agreed with NOSG	
Centring cameras The BGCS should provide support for the sample centring cameras	*Not fulfilled* Too many uncertainties, support can be added on the Downstream Table
Cryostream The BGCS should provide support to the cryostream and other possible equipment to install at the side	*Not fulfilled* Too many uncertainties, support can be added on the Downstream Table
Air travel The neutrons should not travel more than 1000 mm in air from the neutron guide window up to the sample.	*Partially fulfilled* The neutrons travel 1300mm in air, including the 500mm required clearance after the neutron guide window
Axis All axis should be motorized, encoded and manually operable via knob on the motor	*Fully fulfilled*
Maintenance It should be possible to maintain the system (including installation) using the experimental cave overhead crane	
Upgrades The system should allow upgrades by installation of future components	*Fully fulfilled*
Shielding accessibility The system should avoid unauthorized personnel to access the shielding components of the BGCS	
Secondary shutter The BGCS should leave 500mm of free space after the guide window	*Fully fulfilled*
Beam diagnostic The pinhole should be adjustable ±15mm in y and z (x is along the beam) and should allow to diagnose the beam profile	*Fully fulfilled*
Repairs The BGCS should be accessible for repairs while the *proton beam is on target,* from within the experimental cave.	*Fully fulfilled*

11.3 Project Purpose and Objective Fulfillment

The purpose of the project was to perform the conceptual development and design of the Beam Geometry Conditioning System for NMX. The system was designed to minimize the footprint on the backscattered neutrons. The design of the Pinhole Aperture allows neutrons to be collected up to 165° from the neutron beam axis, in the top hemisphere. Another key objective of the system was to minimize the gamma radiation reaching the detector system. 90 – 95% of the neutrons leaving the neutron guide window are absorbed within the Gamma Shielding, preventing the radiation to reach the detectors.

The neutronic performance of the system should be optimized. The most important parameter for the Beam Geometry Conditioning System in terms of neutronic performance is the distance between the Pinhole Aperture and the sample position. The design of the Pinhole Aperture was performed to minimize this distance. The limiting parameter with the selected Pinhole Aperture design is the thickness of the wall at the tip of the cartridge.

A concept for the Beam Geometry Conditioning System has been presented at the end of the project, along with a detail design of the pinhole collimation system. Drawings of the Pinhole Aperture have been made, both construction and assembly. With the completion of the drawings, the pinhole collimation system is ready for prototyping.

12. DISCUSSION

The used methods and results are discussed in this chapter.

12.1 Design Process

The design of the system has been done according to the ESS standard for the design process. The standard describes the different phases of the design process and the milestones that should be checked. The initial steps of the design are to define the functional requirements for the system and of the constraints of the design. This information is collected in the Engineering Design Specification (EDS). What information should be included in the EDS is clearly specified in the standard, but has to be adjusted for each individual design project. The next step is the initial design phase, which should be done based on the EDS. The different decisions that are made during the initial design phase should be added into a design folder. The design folder tracks the development of the system from initial designs to the detailed design. A suggested list of documents that should be produced during the design is presented in the standards. The benefit of presenting a generic list of documents that should be produced is that all design projects have documents with the same name, facilitates finding information. The initial design should be reviewed and approved before the detailed design phase is initialized. The detailed design should be reviewed and approved before the detailed drawings are made.

The standard presents a highly logical chain of design steps and reviews for the design process. What are missing in the standard are guidelines on how the design should be performed. Concept generation and the concept selection are not discussed in the standard. These are important steps in all design projects, to ensure the correct and most feasible solution is found. There is no suggested document presenting the concept selection process either. It is important to have the concept selection process documented and easily accessible to find the reason a specific concept was selected, or more importantly not selected, in case the requirements for the system changes as the system develops.

12.2 Requirements

One of the most important constraint requirements was that the design should be contained within the design envelope model. However, the design envelope model used in this project did not contain as much information as it could have. The envelope model consisted of a homogenous surface model. Different areas of the envelope had, in reality, different priorities on how important it was that the design did not exceed the envelope. This could have been implemented in the beginning of the project using different colors based on priority.

Another discussed requirement is the beam size selection. According to the requirements the beam size should be selectable in 0.05 ± 0.02 mm steps in both height and width independently. This requirement was implemented to describe the requirement on the stability of the beam size selection system. Initially the design of the Pinhole Aperture had continuously adjustable absorbers for selecting the aperture size. With this design the adjustment for the absorbers needs high stability, which the requirement is referring to. It is not necessary to be able to select the beam size with such high precision, as mentioned in the concept selection chapter.

12.3 Future work

There are areas of the design that can be further investigated and developed, which have been briefly discussed during the project.

The first potential improvement is to add tapering flight tubes in between the Gamma Shielding and the Pinhole Aperture. By adding a flight tube it is possible to reduce the number of neutrons absorbed by the Pinhole Aperture even further then what was achieved by the Cleanup Apertures. The flight tube may be coated with gamma absorbing material to reduce the background noise caused by the absorption. Implementing the flight tube requires an investigation on how to align the tube with the Pinhole Aperture and with the neutron beam axis. Other questions that need to be answered are how to adapt it to the secondary sample position and how it interacts with the carousel of the Pinhole Aperture during the cartridge exchange sequence.

The second potential improvement is to add external end stops to the rotary stage of the rotating arm, to increase the repeatability of the movement. Whether the end stops are needed or not depends on the actual functionality of the system. The rotary stage has a repeatability of <0.05° which cause the cartridge to be placed ±0.15mm from the nominal position. According to the theoretical calculations this should not cause any issues, but how the interaction between the arm and the carousel works in reality is hard to predict. External end stops may be added to the Downstream Table, using two grub screws to adjust the position.

A third improvement that may be investigated is to add a cover to the carousel, to protect the passive cartridges while stored at the Pinhole Aperture. The cover should only allow the position of the active cartridge to be accessed or the cover should be removed when the cartridge exchange process is commenced.

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