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# System Requirements for the Small-K Advanced DIffractometer SANS SKADI

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## Table of Contents

# 1. INTRODUCTION

## 1.1 Purpose of the Document

This document describes the functional requirements for the Small-K Advanced DIffractometer (SKADI). The high-level scientific requirements of SKADI form the basis for the requirements specified here. It is critical that such requirements are fulfilled in order to accomplish all the demands by the science case as laid out in the Instrument proposal and the Concept of operations document, describing the expected operational use of SKADI. The subsystems requirements in this document are based on the conceptual design as laid out in the instrument proposal.

## 1.2 Definitions, Acronyms and Abbreviations

Each requirement is expressed as a natural language statement following the guidelines in the NASA Systems Engineering Handbook. Statements using the word **"shall" express a strict requirement** that has to be fulfilled for the system to be functional at all. Statements using the word **"should" express a design objective beyond which the system performance does not increase**. The requirements of this type are subject to trade or engineering studies. **It should be noted that in many cases the value given is practically impossible to achieve**, in which case the statement is equivalent to maximising or minimising the quantity in question. Statements using the word **"must" express a capability that has to be achievable**, but that is not part of the SKADI work package scope. Any design or technical solution must not preclude these requirements to be fulfilled without significant rework.

| Abbreviation | |
|---|---|
| **BTCS / BTS** | Beam Transport (and Conditioning) System |
| **CCFE** | Culham Centre for Fusion Energy |
| **CHIC** | Chopper Control System |
| **CLI** | Command Line Interface |
| **DAQ** | Data Acquisition |
| **DMSC** | Data Management and Software Centre |
| **EPICS** | Experimental Physics and Industrial Control System |
| **ESS** | European Spallation Source |
| **ESTIA** | ESS Neutron Reflectometer |
| **FRM2** | Forschungsreaktor München 2 (Research Reactor) |
| **FZJ** | Forschungszentrum Jülich (Research Center Jülich) |
| **GUI** | Graphical User Interface |
| **ICS** | Integrated Control System |
| **JCNS** | Jülich Centre for Neutron Science |
| **KWS** | KleinWinkelstreuSpektrometer (SANS instrument) |
| **LLB** | Laboratoire Léon Brillouin (Research Laboratory) |
| **Loki** | ESS SANS instrument |

| | |
|---|---|
| **MaPMT** | Multi Anode Photomultipliertube |
| **MNCP** | Monte Carlo N Particle (software) |
| **NOSG** | Neutron Optics and Shielding Group |
| **P&ID** | Process & Instrumentation Diagram |
| **PA20** | Petit-Angles 20 m (SANS Instrument) |
| **PBS** | Product Breakdown Structure |
| **PSD** | Position Sensitive Detector |
| **PSS** | Personnel Safety System |
| **SANS** | Small Angle Neutron Scattering |
| **SCS** | Scattering Characterization System |
| **SE** | Sample Environment |
| **SES** | Sample Exposure System |
| **SKF** | Svenska Kullagerfabriken (Swedish bearing manufacturer) |
| **SoNDe** | Solid-State Neutron Detector (EU Horizon2020 Project) |
| **STAP** | Scientific and Technical Advisory Panel |
| **TOF** | Time of Flight |
| **VSANS** | Very SANS |
| **ZEA** | Zentralinstitut für Engineering, Elektronik und Analytik |

## 1.3 References

1. Process for Neutron Instrument Design and Construction ESS-0051706
2. Definition of Supervised and Controlled Radiation Areas, ESS-0001786
3. Concepts of Operations (ConOps) for the SKADI Instrument
4. SKADI Instrument Proposal

# 2. SYSTEM CHARACTERISTICS

## 2.1 System Purpose

SKADI is designed to perform Small-Angle Neutron Scattering experiments, primarily on soft- and hard matter. These experiments include, but are not limited to, chemical and biological experiments, medical and pharmaceutical experiments, studies of magnetic domains as well as geological studies.

## 2.2 System Overview

SKADI consists of three main technical subsystems: The beam transport and conditioning system (BTS), the sample exposure system (SES) and the scattering characterisation system (SCS). In addition, the SKADI instrument comprises the structures that house and support these subsystems as well as the software to control the instrument and to process the recorded data as described in the instrument product breakdown structure (PBS).

# 3. SYSTEM REQUIREMENTS

The high-level requirements for SKADI make sure it will be able to meet the meet the scientific requirements by the SANS community to perform high-level research as stated in the Concept of Operations.

For a SANS instrument a broad Q-range and high resolution in time and space are the most important parameters. Additionally, the possibility to have a well-adapted or custom made sample environment is necessary for world-class experiments. The wide Q-range allows to explore length scales over several orders of magnitude from Angstrom to micrometre. The high flux of the ESS will allow to access very short time scales on the order of milliseconds. With the flexible sample area novel experiments will become possible, which have been unfeasible until now. For example, it will be possible to investigate the mixing kinetics between a drug and its carrier system in real time at characteristic length scales to explore new drug delivery systems. This is only one example for experiments with high potential for applications thereby having a profound impact on society.

Thus the high-level system requirements for SKADI are:

1. SKADI shall allow data collection down to a $Q_{min} = 1\times10^{-4}$ Å$^{-1}$
2. SKADI shall allow data collection up to a $Q_{max} = 1$ Å$^{-1}$
3. SKADI shall allow data to be collected simultaneously over a dynamic Q-range of $Q_{max}/Q_{min} = 1000$.
4. SKADI shall allow time resolved studies with a single shot time resolution below 200 ms.
5. SKADI shall match the size of the neutron beam to the size of the sample up to 30x30 mm$^2$.
6. SKADI shall provide polarized neutron beam with a relative polarization of >0.95.
7. SKADI shall provide a Q resolution of $dQ/Q < 15\%$ between $Q=1\times10^{-3}$ Å$^{-1}$ and $Q_{max}$
8. SKADI shall allow for custom sample environments of volumes up to at least 1.5×1.5×2 m$^3$ with masses up to 2000 kg.
9. SKADI should be optimized to a signal to noise ratio (as defined in NOSG ESS-0039408, Appendix 3) better than $10^{-4}$.

## 3.1 Functional Requirements for SKADI Subsystems

### 3.1.1 Beam Transport and Conditioning System (BTCS, 13.6.7.1)

The beam transport system transports a beam of neutrons from the moderator to the sample. The size, divergence and wavelength spectrum of the beam are tailored to the needs of the experiment.

The specification of this system defines the property of the beam and as such the achievable Q-space and resolution, which directly translates into the experimentally accessible length scales. In addition, the possibility to transport neutrons both with a high flux and a high brilliance will allow for an excellent time and spatial resolution respectively.

A proper alignment of the components is of utmost importance since a misalignment could reduce the overall performance of SKADI significantly.

Furthermore, the inherent background measured at SKADI is also determined by the beam transport and conditioning system. Therefore, the goal is to transport only useful neutrons to the sample position and avoid polluting the spectra either with neutrons of the wrong wavelength/divergence or with gamma radiation. A good signal to noise ratio also allows the investigation of weakly scattering samples that are otherwise unfeasible to be investigated.

1. **Wavelength Selection**
    1.1. The BTS shall transport neutrons with wavelengths between 3 Å to 23 Å from the moderator to the sample.
    1.2. **Rationale:** Selecting the wavelength determines the possible Q-range and thus the experimentally accessible length scales. Selecting a wavelength appropriate for the experiment being performed minimises unwanted neutrons and thus improves the signal to noise ratio.
    1.3. **Verification:** Measurement of the neutron spectrum at the sample position.
2. **Bandwidth Selection**
    2.1. The BTS shall transport neutrons from the moderator to the sample with a given, selectable wavelength bandwidth of 5 Å or 10 Å, within the wavelength range defined in requirement 3.1.1.1.
    2.2. **Rationale:** Selecting the wavelength band determines the dynamical Q-range ($Q_{max}$ - $Q_{min}$). By selecting a portion of the total available spectrum the experiment can be fine-tuned to a specific experiment.
    2.3. **Verification:** Measurement of the neutron spectrum at the sample position.
3. **Beam Size**
    3.1. The BTS shall transport the neutron beam from the moderator to the sample with a cross section between fully open (30x30 $mm^2$) and fully closed aperture.
    3.2. **Rationale:** Choosing the beam size allows to optimize the experiment with respect to the trade-off between resolution, flux and sample size.
    3.3. **Verification:** Measurement of the beam cross-section at the sample position.
4. **Maximum Beam Divergence**
    4.1. The BTS shall transport neutrons from the moderator to the sample with a maximum angular divergence of 3.75 mrad in horizontal and vertical direction.
    4.2. **Rationale:** $Q_{min} \sim \sin(div_{min})$ is linearly dependent on the divergence of the beam. This allows an optimized choice between flux and resolution, resulting in an optimized signal to noise ratio. The lower the accessible $Q_{min}$, the more versatile are the experimental possibilities.
    4.3. **Verification:** Measure beam spot size on detector at different detector positions.
5. **Beam Divergence Selection**
    5.1. The BTS shall transport neutrons from the moderator to the sample position with a selectable divergence up to a maximum of 3.75 mrad.
    5.2. **Rationale:** Matching the beam divergence to the experiment's needs optimizes resolution and signal to noise ratio.
    5.3. **Verification:** Measurement of beam profile at positions around the sample position and on detector.

6. **Line of Sight Avoidance**
    6.1. The BTS shall be constructed such that the line-of-sight between moderator and sample is closed twice before the beam geometry conditioning system.
    6.2. **Rationale:** Closing the line-of-sight reduces the transmission of unwanted neutrons/gammas improving the signal to noise ratio.
    6.3. **Verification:** Measurement of the neutron spectrum at the start of the Beam Geometry Conditioning System and comparison to simulation results.
7. **Neutron Beam Cut-off**
    7.1. The BTS shall reduce the radiation levels in the experimental cave to below 3 μSv/h as required by safety regulations (ESS-0001786) when the experimental cave is not interlocked (i.e. during sample access).
    7.2. **Rationale:** Access to the sample position has to be possible for sample change (see ConOps).
    7.3. **Verification:** Measurement of radiation levels in the experimental cave.
8. **Brilliance transfer**
    8.1. The BTS should transport neutrons from the moderator to the sample position with 100% brilliance (neutrons/(second*cm$^2$*srad*wavelength band)) transfer within the selected wavelength and divergence range.
    8.2. **Rationale:** This maximizes neutron flux at the sample, allowing either fast measurements, low concentration of samples, small samples or a combination thereof that otherwise could not be investigated.
    8.3. **Verification:** Measurement of the flux at the sample and comparison with predicted flux at the moderator surface.
9. **Intensity Profile**
    9.1. The BTS should transport the neutrons from the moderator to the sample evenly distributed and without local inhomogeneities/hotspots with a standard deviation of less than 10%.over the beam cross-section at the sample position.
    9.2. **Rationale:** This provides and even illumination of the sample and facilitates normalization of the scattered intensity (see ConOps). Weak signals from the sample can only be evaluated if the incoming beam is homogenous enough.
    9.3. **Verification:** Measurement of spectrum and beam profile at sample position.
10. **Divergence profile**
    10.1. The BTS should transport from the moderator to the sample a beam of neutrons with a smooth divergence profile with a standard deviation of less than 10%.
    10.2. **Rationale:** The beam divergence profile is convoluted with the scattering pattern, a smooth profile allows a correct normalization of the scattered intensity. If the divergence of the scattered neutrons is too inhomogeneous the Q-resolution of the instrument decreases.
    10.3. **Verification:** Measurement of the beam profile at distinct positions close to the sample position.
11. **Wavelength rejection**
    11.1. The BTS shall transport from the moderator to the sample position a beam of neutrons where the total brilliance outside the selected wavelength band is <1%.
    11.2. **Rationale:** See rationale 1.2 and 2.2
    11.3. **Verification:** Measurement of the neutron spectrum at the sample position.

12. **Accessibility**
    - 12.1. The BTS outside the bunker should be accessible for repairs while the proton beam is on target.
    - 12.2. **Rationale:** SKADI will be more robust, leading to an increased throughput of experiments.
    - 12.3. **Verification:** Measurement of the local dose rate at relevant positions.
13. **Polarization**
    - 13.1. The BTS shall transport neutrons with a polarization >95% to the sample position for the full used wavelength band.
    - 13.2. **Rationale:** In polarized neutron scattering the unpolarized part of the spectrum adds to the background. Magnetic materials or biological samples with low contrast can only be investigated if a high relative polarization is available.
    - 13.3. **Verification:** Measurement of the polarization at the sample position.
14. **Overall Accuracy**
    - 14.1. The BTS beam conditioning geometry (i.e. collimation slits and guides) shall have an accuracy of <0.1 mm.
    - 14.2. **Rationale:** Most of the other requirements rely heavily on a well-defined beam geometry. Each 3x3 $cm^2$ opening that is misaligned by 0.1 mm in x and y direction in the worst case leads to a loss in coverage of up to $(2x3 \text{ cm} \times 0.1 \text{ cm})/(3 \times 3 \text{ cm}^2) = 6\%$. This inhomogeneity is of the same order of magnitude as the inhomogeneity of the beam itself and can be accepted as a maximum misalignment.
    - 14.3. **Verification:** Measurement of slit setups.
15. **Alignment Degradation**
    - 15.1. The alignment of the BTS shall be continuously monitored via two beam monitors along the collimation distance down to the sample position.
    - 15.2. **Rationale:** Misalignment over time will lead to a decreased flux.
    - 15.3. **Verification:** Measurement of the beam parameters along the instrument.
16. **Robustness against Failure**
    - 16.1. The BTS should be robust against failure of single components.
    - 16.2. **Rationale:** In some cases operation with a limited instrument performance may be possible in the case of failure of a component. All components should be designed to meet that goal. For instance, the first chopper should be movable into an open position in case of failure.
    - 16.3. **Verification:** Test of components.
17. **Chopper Speeds**
    - 17.1. The choppers shall be designed for rotation speeds of 7 and 14 Hz (first two choppers) and between 7 and 238 Hz (last two choppers).
    - 17.2. **Rationale:** These chopper speeds are necessary to allow for all settings of wavelength selection needed for the optimization of the resolution of the experiment or the available flux.
    - 17.3. **Verification:** Test of choppers (factory acceptance test).
18. **Vacuum System Pressure**
    - 18.1. A pressure of $10^{-3}$ mbar shall be achievable throughout the BTS.
    - 18.2. **Rationale:** This is necessary for safe operation of the choppers as well as beneficial for the transmission properties of SKADI (flux).
    - 18.3. **Verification:** Vacuum measurement.

19. **Vacuum Pumping time**
    19.1. The final pressure shall be achievable within a pumping time < 1h starting from atmospheric pressure.
    19.2. **Rationale:** Start of experiment has to wait until a sufficient vacuum is reached.
    19.3. **Verification:** Measurement of vacuum.

### 3.1.2 Sample Exposure Systems (SES, 13.6.7.2)

The sample exposure system positions the sample into the beam and controls the environmental parameters of the sample as dictated by the needs of the experiment. For simple conduction of an experiment on a set of samples a sample changer is necessary.

For most users the sample environment is where they are in closest contact with the instrument. Therefore, only a good control of the sample environment and a reliable repeatability will allow high-quality experiments.

1. **Horizontal and Vertical Positioning**
    1.1. The SES shall position the sample in the beam of neutrons with an accuracy of +/- 0.1 mm and a precision of +/- 0.05 mm in horizontal and vertical direction respectively.
    1.2. **Rationale:** The sample needs to be in the beam of neutrons and correctly illuminated (See ConOps). It is also worth noting that repeatability of this positioning allows for a more reliable comparison between different samples.
    1.3. **Verification:** Test of positioning system.
2. **Rotational Positioning**
    2.1. The SES shall position the sample in the beam of neutrons with an accuracy of +/- 0.1 degree and a precision of +/- 0.05 degrees in horizontal and vertical direction respectively.
    2.2. **Rationale:** Many experiments rely on a precise determination of the sample orientation. (see ConOps, similar to requirement 1).
    2.3. **Verification:** Test of positioning system
3. **Sample Environment Equipment**
    3.1. The SES shall permit the installation and positioning of a sample environment equipment with volumes up to at least $1.5\times1.5\times2$ m$^3$ with masses up to 2000 kg.
    3.2. **Rationale:** The experiment may require equipment to control the environmental parameters of the samples (see ConOps). Users that bring their own custom-made sample environment should not be constrained by space restrictions of the instrument. Often these custom-made sample environments contribute greatly to high-profile research.
    3.3. **Verification:** Test of mounting system.

4. **Change of Sample Environment**
    4.1. The SES shall allow a preparation of the sample environment outside the experimental cave of SKADI with a setup identical to the on-instrument sample area.
    4.2. **Rationale:** Off-instrument sample preparation allows for a higher throughput of experiments. Also some preliminary investigations may work without neutrons and it is beneficial to keep the sample environment the same for comparability.
    4.3. **Verification:** Test of sample environment
5. **Change of Setups**
    5.1. The SES should allow the change of setups for different sample environments in 30 min.
    5.2. **Rationale:** A fast change of sample environments increases the throughput of experiments.
    5.3. **Verification:** Test of sample environment.
6. **Automatic Sample Change**
    6.1. The SES shall allow changing the sample without manual user intervention.
    6.2. **Rationale:** Automated sample change is required in order to optimize the use of the available beam time (see ConOps). Often large series of samples have to be investigated to screen a parameter space of a sample.
    6.3. **Verification:** Test of sample environment.
7. **Magnetic materials**
    7.1. As far as possible magnetic materials shall be avoided in the SES.
    7.2. **Rationale:** Polarized neutron scattering may be influenced by magnetic materials.
    7.3. **Verification:** Test of sample environment.

### 3.1.3 Scattering characterisation systems (SCS, 13.6.7.3)

The scattering characterization system detects the scattered and transmitted neutrons after interaction with the sample to produce meaningful experimental data.

The SCS therefore has to be both able to handle a high flux, but also to determine minute differences in the homogeneity of the neutron flux both in time and space.

1. **Detection Efficiency**
    1.1. The SCS shall detect transmitted neutrons in the selected wavelength band with an efficiency of >80% over the complete wavelength band.
    1.2. **Rational:** Neutron detection efficiency should be equivalent to current state-of-the-art technology (see ConOps). This allows either for fast measurements or small and/or diluted samples.
    1.3. **Verification:** Measurement of detection efficiency
2. **Angular resolution**
    2.1. The SCS shall have an angular resolution <=0.15 mrad at the longest sample-detector distance of 20 m.
    2.2. **Rationale:** The angular resolution contributes to the precision with which the sample structure can be determined.
    2.3. **Verification:** Test of SCS with a reference sample.

3. **TOF resolution**
   - 3.1. The SCS shall record neutrons with a time-of-flight resolution <0.05 ms.
   - 3.2. **Rationale:** The time-of-flight resolution contributes to the precision with which the sample structure can be determined.
   - 3.3. **Verification:** Measurement (TBD).
4. **Neutron Selectivity**
   - 4.1. The SCS should detect neutrons incident to the detector system other than cold neutrons with a 0% efficiency.
   - 4.2. **Rationale:** Radiation other than cold neutrons decreases signal to noise ratio.
   - 4.3. **Verification:** Measurement of spectrum for hot neutrons and gammas at the sample and detector position.
5. **Accessible solid angle**
   - 5.1. The SCS shall be able to detect neutrons scattered by the sample within a polar angular range of ±26 degrees and an azimuthal angular range of 360 degrees.
   - 5.2. **Rationale:** Reaching high Q and measure a full scattering circle contributes to both the detection efficiency as well as to the determination of the sample structure.
   - 5.3. **Verification:** Test of detector system.
6. **Detector positioning**
   - 6.1. The SCS shall position the detectors with an accuracy and precision of <1 mm along the beam axis.
   - 6.2. **Rationale:** An accurate positioning of the detector is required for the calculation of the correct Q values. A high Q resolution is necessary for a good reconstruction of the sample structure.
   - 6.3. **Verification:** Test of detector system.
7. **Detector positioning**
   - 7.1. The SCS shall position the detectors with an accuracy and precision of <1 mm on both axes perpendicular to the beam axis. Only a good Q resolution allows for a good reconstruction of the sample structure.
   - 7.2. **Rationale:** Exact Q calculation requires exact positioning.
   - 7.3. **Verification:** Test of detector positioning system.
8. **Detector Noise**
   - 8.1. The SCS should record <1 neutron/(s $m^2$) on the full detector system in the absence of incoming radiation, i.e. a blocked beam.
   - 8.2. **Rationale:** Dark current decreases signal to noise ratio.
   - 8.3. **Verification:** Test of detector system with a blocked beam.
9. **Achievable counting rate**
   - 9.1. The SCS shall be able to handle counting rates of >20MHz/$m^2$ of detector area.
   - 9.2. **Rationale:** To use the high flux of the ESS to full capacity, the detector needs to be able to achieve high count-rates. These high count-rates allow for fast measurements.
   - 9.3. **Verification:** Test of detector.

10. **Spatial Detector resolution**
    10.1. The SKADI detector shall have two resolution areas with a spatial resolution of 3 mm (inner detector, 20x20cm$^2$ at 20m, ±5 mrad) and 6 mm (rest of detector area).
    10.2. **Rationale:** These resolutions are needed to fulfil all Q resolution related requirements. The detector resolution directly translates to Q-resolution and therefore the accuracy with which the sample structure can be measured.
    10.3. **Verification:** Test of detector.
11. **Vacuum System Pressure**
    11.1. A pressure of $10^{-3}$ mbar throughout the SCS shall be realized.
    11.2. **Rationale:** This is necessary for safe operation of the choppers as well as beneficial for the transmission properties of SKADI. Scattering in air after the sample inhibits an accurate determination of the sample structure.
    11.3. **Verification:** Vacuum measurement.
12. **Vacuum Pumping time**
    12.1. The final pressure shall be achievable within a pumping time < 1h starting from atmospheric pressure.
    12.2. **Rationale:** Start of experiment has to wait until a sufficient vacuum is reached.
    12.3. **Verification:** Measurement of vacuum.
13. **Positioning time**
    13.1. Movement of the detector shall not be slower than 2 m/min.
    13.2. **Rationale:** Slow moving detectors create both a dead time for measurement as well as require samples to be stable over longer times.
    13.3. **Verification:** Measurement of positioning system.

### 3.1.4 Experimental cave (13.6.7.5)

The experimental cave houses the final beam-defining elements of the BTS, the SES and the SCS. It shields the surrounding hall from the radiation generated by these systems as well as shielding the detector from external radiation.

The experimental cave shall be equipped with an access control system following the safety standards provided by the ESS PSS group. Part of the system will be a radiation safe entrance door, oxygen deficiency warning system and motion control emergency switches. Necessary vacuum, cryogenic liquids and magnetic field safety measures shall be taken to ensure ESS safety regulations (ESS-0002381, ESS-0034035 and ESS-0001786).

1. **Mounting Components**
    1.1. The experimental cave shall allow the mounting of technical components required for the BTS, SES and SCS with the required precision and stability.
    1.2. **Rationale:** The technical components have to be housed in the experimental have on a suitable support structure.
    1.3. **Verification:** Metrology and test of function.

2. **Utilities**
    2.1. The experimental cave shall provide the required utilities to the elements of the BTS, SES and SCS systems.
    2.2. **Rationale:** The components housed in the experimental cave need access to the respective utilities in order to function.
    2.3. **Verification:** Test of equipment
3. **Biological Shielding**
    3.1. The experimental cave shall shield its surroundings against the radiation produced by the neutron beam to safe levels according to ESS radiation and safety regulations (<3 µSv/h).
    3.2. **Rational:** Radiation shielding is necessary for a safe operation of SKADI.
    3.3. **Verification:** Measurement of dose rate around the experimental cave.
4. **Sample Environment footprint**
    4.1. The experimental cave should allow the mounting of sample environments with dimensions of volumes up to at least 1.5×1.5×2 $m^3$ with masses up to 2000 kg.
    4.2. **Rationale:** Some experiments may require bulky and/or heavy sample environment.
    4.3. **Verification:** Test of sample environment.
5. **Detector Shielding**
    5.1. The experimental cave should shield the detectors from radiation to below 1 count/(s $m^2$) detected on the complete detector system.
    5.2. **Rationale:** External radiation decreases signal to noise ratio.
    5.3. **Verification:** Measurement with a blocked beam.
6. **Load Access**
    6.1. The experimental cave shall allow access to the sample environment for loads of up to 2000 kg.
    6.2. **Rationale:** Heavy sample environment has to be brought into the experimental cave.
    6.3. **Verification:** Test of sample environment.
7. **Activated sample storage**
    7.1. Storage of activated samples shall be possible in the experimental cave.
    7.2. **Rationale:** Activated samples need to be stored in a shielded area to cool down.
    7.3. **Verification:** Test of experimental cave.

### 3.1.5 Control hutch (13.6.7.6)

The control hutch houses the experiment control and data processing terminals. During an experiment the user team spends most of their time in the control hutch.

Experiments will be controlled remotely from this control hutch. The hutch needs to provide ample space to coordinate the experiments and perform initial data analysis for one full experimental team (users and beamline personal). For short amounts of time an overlap of two experimental teams shall be considered in the layout procedure. Enough computing infrastructure needs to be provided within this area to perform the mentioned tasks.

1. **Instrument control terminal**
   1.1. The terminal in the control hutch shall allow the user to control the technical components of SKADI, including the sample environment, from a single dedicated computer system.
   1.2. **Rationale:** The instrument control should be possible using a single computer system.
   1.3. **Verification:** Test of the instrument control system.
2. **Data reduction terminal**
   2.1. The terminal in the control hutch shall allow the user to process the recorded data to corrected intensities as a function of momentum transfer at a dedicated computer system (see ConOps).
   2.2. **Rationale:** Data reduction must be possible from at least one computer system in the immediate vicinity of the instrument control.
   2.3. **Verification:** Test of the data reduction system.
3. **Working space**
   3.1. The control hutch shall allow the user to have sufficient working space for two 4 person user teams.
   3.2. **Rationale:** A user system typically consists of up to 4 persons and there needs to be space for the coming and departing user team simultaneously.
   3.3. **Verification:** User feedback.
4. **Comfort**
   4.1. The control hutch should be a comfortable working environment for the users. Here national and industry standard regulations should be applied (such as ISO 9241).
   4.2. **Rationale:** Users work long hours and a comfortable working environment improves the productivity of the user team.
   4.3. **Verification:** User feedback.
5. **Access to the instrument**
   5.1. The control hutch should be located close (<30 m) to the experimental cave door.
   5.2. **Rationale:** Users need to mount and change samples during their experiments and hence need fast and easy access (see ConOps).
   5.3. **Verification:** Test of instrument access.
6. **Sample Preparation**
   6.1. Either inside or immediately adjoining the control hutch there should be the possibility for simple sample preparation.
   6.2. **Rationale:** Samples may need fast treatment just before being mounted.
   6.3. **Verification:** Test of sample preparation.

### 3.1.6 Experimental hall

Experimental hall infrastructure includes all the shielding, infrastructure and support systems for the BTS, SES and SCS in the neutron guide hall.

Access to the gallery housing the media (such cooling water and vacuum) has to be provided.

1. **Mounting Components**
   1.1. The experimental hall shall allow the mounting of technical components of the BTS, SES and SCS with the required precision and stability.
   1.2. **Rationale:** The technical components have to be physically mounted on a suitable support structure.
   1.3. **Verification:** Metrology and acceleration measurements.
2. **Utilities**
   2.1. The required utilities to the components of the BTS, SES and SCS shall be made accessible within the experimental hall.
   2.2. **Rationale:** The components within the experimental hall need their respective utilities to function.
   2.3. **Verification:** Test of the respective components.
3. **Access**
   3.1. The experimental hall shall allow access for personnel when the proton beam is on target.
   3.2. **Rationale:** Access for personnel is necessary for operation, maintenance and repair.
   3.3. **Verification:** Test of components.
4. **Biological Shielding**
   4.1. The experimental hall shall allow for radiation shielding of the components of the BTS, SES and SCS to safe levels according to ESS radiation safety regulations (<3 µSv/h).
   4.2. **Rationale:** The surroundings of SKADI need to be safe for personnel access.
   4.3. **Verification:** Measurement of dose rates in affected areas.
5. **Access to SKADI sample position**
   5.1. The layout of SKADI and equipment in the experimental hall shall permit access to the sample area of SKADI many times per day for personnel and equipment according to the sample environment requirements.
   5.2. **Rationale:** Operation of SKADI is only possible if the sample position is accessible in a manner suitable to perform an experiment.
   5.3. **Verification:** Test of access to sample position.

### 3.1.7 Sample preparation area (13.6.7.7)

The sample preparation area contains all the necessary equipment for sample handling, mounting and storage between experiments, as well as the simple sample preparation facilities.

To allow for a simple and reliable performance of the experiments, this area also needs to be as close to SKADI as possible. In order to account for safety requirements only safe to handle substances can be stored there, but access to dedicated laboratories is necessary. The sample can then be stored here before being measured.

1. **Sample mounting**
    1.1. The sample preparation area shall allow the user to mount sample environments with the dimensions of volumes up to at least 1.5×1.5×2 $m^3$ with masses up to 2000 kg.
    1.2. **Rationale:** The sample environments needed for the experiments need to be mounted on SKADI.
    1.3. **Verification:** Test of mounting of sample environment.
2. **Sample Storage**
    2.1. The sample preparation area shall allow the storage of samples in the required environments during the experiments.
    2.2. **Rationale:** A large amount of samples may be required for some experiments.
    2.3. **Verification:** Test of sample storage units.
3. **Sample preparation**
    3.1. The sample preparation area shall allow for simple sample preparation steps (e.g. adding of solvent, cooling/heating)
    3.2. **Rational:** Samples may require preparation immediately before being put into the sample environment.
    3.3. **Verification:** Test of sample preparation.
4. **Access to laboratories**
    4.1. Access to laboratories for sample handling shall be close (less than 5 min. walking distance).
    4.2. **Rationale:** Samples to be handled and works that have to be performed in a dedicated laboratory (such as chemistry laboratories) need to be fast to reach for sensitive samples.
    4.3. **Verification:** Check distance between instrument and support laboratories.
5. **Access to laboratories**
    5.1. Access to laboratories for sample handling shall be safe and easy (no stairs, or elevators in case of elevations).
    5.2. **Rationale:** Tripping hazards or other transport accidents may pose a severe security risk with hazardous samples or sensitive samples may be destroyed.
    5.3. **Verification:** Check way between instrument and preparation laboratories.

### 3.1.8 Integrated control and monitoring systems (13.6.7.11)

The integrated control and monitoring system allows the user to control the experimental parameters and process the neutron data. It also contains the control and monitoring systems needed for the safe operation of the instrument.

Computers for this control system will be in the control hutch, but the control itself will also be accessible from other computers for remote control.

1. **Instrument Control GUI**
   1.1. The integrated control and monitoring system shall allow the user to control the experimental parameters through a graphical user interface.
   1.2. **Rationale:** A good GUI makes instrument control fast, easy and reliable (See ConOps).
   1.3. **Verification:** Test of control system.
2. **Instrument control CLI**
   2.1. The integrated control and monitoring system shall allow the user to control the experimental parameters through a scriptable command line interface.
   2.2. **Rationale:** A good scriptable CLI allows for flexibility and repeatability for more experienced users and ESS staff.
   2.3. **Verification:** Test of CLI.
3. **Preliminary Data Visualization**
   3.1. The integrated control and monitoring system shall allow for the visualization of selected important parameters of the scattered data (see ConOps).
   3.2. **Rationale:** Preliminary data visualization helps the user to better monitor the progress and success of the experiment.
   3.3. **Verification:** Test of data visualization.
4. **Saving the instrument and sample environment status**
   4.1. The integrated control and monitoring systems shall allow to save the status of both SKADI as well as the sample environment to replicate the settings at a later time.
   4.2. **Rationale:** Users having multiple beam times with the same or a very similar experiment will want to reproduce the settings of any given experiment.
   4.3. **Verification:** Test of saved instrument/sample environment status.
5. **Data Processing GUI**
   5.1. The integrated control and monitoring system shall allow the user to process the recorded data with a GUI to corrected intensities as a function of momentum transfer.
   5.2. **Rationale:** A good GUI simplifies data treatment (see ConOps).
   5.3. **Verification:** Test of data treatment GUI.
6. **Data Processing CLI**
   6.1. The integrated control and monitoring system shall allow the user to process the recorded data with a CLI to corrected intensities as a function of momentum transfer.
   6.2. **Rationale:** A good CLI simplifies the treatment of large amounts of data for experienced users and ESS staff.
   6.3. **Verification:** Test of CLI
7. **Role Based User Access**
   7.1. The integrated control and monitoring system shall allow the discrimination of users and thus the accessible instrument controls.
   7.2. **Rationale:** Depending on the users experience more or less privileges regarding instrument control may facilitate the experiment.
   7.3. **Verification:** Test of user control system.

8. **Hazard Detection PSS**
   8.1. The integrated control and monitoring system shall detect hazards that may compromise safety for personnel.
   8.2. **Rationale:** Detection of hazards such as fire, radiation, flooding or asphyxiating atmosphere can prevent injury to personnel.
   8.3. **Verification:** Test of safety system.
9. **Hazard Detection Instrument Protection**
   9.1. The integrated control and monitoring system shall detect hazards that may comprise protection of the instrument.
   9.2. **Rationale:** Detection of hazards such as fire, radiation, flooding or asphyxiating atmosphere can prevent damage to SKADI.
   9.3. **Verification:** Test of safety systems.

## 3.2 Operational Requirements for SKADI

The operational requirements are statements that concern either the instrument team or the user team. In order to allow for an efficient operation and optimal scientific output the teams working on SKADI should heed the specified requirements.

### 3.2.1 Team Requirements

1. **Operation Hours**
   1.1. During operation of the neutron source SKADI shall operate 24/7.
   1.2. **Rationale:** This allows for the best use of beam time.
   1.3. **Verification:** Feedback from users/instrument team.
2. **Team Size**
   2.1. SKADI shall be operated by a team of four scientists (at least 3 FTE).
   2.2. **Rationale:** The high flux allows for short beam times. In order to allow for a good user support with beam times of 2 days (plus at least 1-2 days for data evaluation support) enough personnel has to be available to perform all the necessary tasks.
   2.3. **Verification:** Feedback from users/instrument team.

### 3.2.2 User Requirements

1. **Arrival**
   1.1. Users shall arrive at least 24h prior to the start of the experiment.
   1.2. **Rationale:** Setting up the sample setup requires time, as well as all organisational issues with access to the facilities of the ESS. Only by an early arrival a timely start and thus good use of the beam time is possible.
   1.3. **Verification:** Feedback from users/instrument team.
2. **Departure**
   2.1. Users shall have at least 1 working day at ESS before leaving.
   2.2. **Rationale:** Data reduction and preliminary discussion with the instrument team significantly improves the scientific output of SKADI.
   2.3. **Verification:** Feedback from users/instrument team.

3. **Team size**
    3.1. User teams for beam times longer than 24 h shall consist of at least 4 persons.
    3.2. **Rationale:** In order to allow for 24h operation of the instrument, several shifts are necessary.
    3.3. **Verification:** Feedback from users/instrument team.
4. **Experience**
    4.1. While experience specifically at ESS or a neutron scattering instrument in general is not required, there should be at least one researcher per shift capable of independent work in a large scale facility.
    4.2. **Rationale:** Safety of operation for the user team.
    4.3. **Verification:** Feedback from users/instrument team.