Document Type:	**SKADI – Concept of Operations**
Date	22/06/2017
Version	1.0
State	TG2
Confidential level	Internal
Number of pages	30

Concept of Operations for the Small-K Advanced DIffractometer SANS SKADI

	Name (name, title, e-mail address)	Affiliation (name of institution, address)
Authors	Sebastian Jaksch, Henrich Frielinghaus Sylvain Désert Jacques Jestin Romuald Hanslik	FZJ/JCNS FZJ/JCNS LLB LLB FZJ/ZEA-1

European Spallation Source ESS AB
Visiting address: ESS, Tunavägen 24
P.O. Box 176
SE-221 00 Lund
SWEDEN

www.esss.se

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1. INTRODUCTION

1.1 Purpose of the Document

The purpose of the Concept of operations document (ConOps) is to provide a brief description of the Small-K Advanced DIffractometer (SKADI) Small-Angle Neutron Scattering (SANS) Instrument. The description includes both an introduction to the science case of the instrument as well as providing the framework and context within which the instrument will be designed, operated and maintained throughout its lifecycle.

The intended audience for this document includes everyone involved in the construction and operation of SKADI. It will also serve as a quick overview of the instrument's purpose, construction and operation for both persons familiar in the field of neutron science and those that are not.

1.2 Definitions, Acronyms and Abbreviations

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 (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] S. Jaksch, Nuclear Instruments and Methods in Physics Research A 835 (2016) 61, http://dx.doi.org/10.1016/j.nima.2016.07.041

2. HIGH LEVEL SCIENTIFIC REQUIREMENTS

The scientific areas targeted by SKADI include investigations of smart materials, biological and medical research, magnetic materials and materials for energy storage, as well as experiments on nanomaterials and nanocomposites or colloidal systems. These experiments promise a high potential impact on science and society. To maximize the societal applicability of these studies, SKADI accommodates in-situ measurements with custom-made sample environments in order to provide "real-world" conditions.

To achieve all these goals SKADI will feature the following general design properties:

- Flexibility (sample area is approx. 3x3 m^2, and versatile collimation)
- Very small Q accessible by using focusing elements
- Polarization for magnetic samples
- Good wavelength resolution, being the longest SANS instrument
- High dynamic Q-range (covering three orders of magnitude simultaneously)

The first four of these features expands the science case into areas not covered by the LoKI proposal. SKADI is envisaged as a vital part of the world leading SANS instrument suite for ESS, particularly in providing access to longer length scales and to polarized neutron measurements. The approximately 60 m long instrument allows for much space at the sample area and inside the collimation (last 8 m). It provides simple access to bulky sample environment such as high field magnets or polarization analysis units. Also large presses, load frames or other large deformation tools are possible. Most of the topics benefitting from this feature are in the hard matter field or involve magnetic particles. The large sample area also facilitates the inclusion of custom-made sample environments. Additional in-situ setups for soft matter and biological investigations such as light scattering for an expansion of Q-space, rheometers, setups for strong electric or magnetic fields or shearing setups for directed self-assembly can be accommodated.

A Q-range over three orders of magnitude is made accessible by using three detectors positions. This avoids the need to repeat the measurements at different detector distances for kinetic measurements. Apart from the kinetic measurements, fast phase transitions in soft matter or biological samples will be observable. The same holds for material science experiments during the structural failure of a material, which have gained increasing attention recently. The possibility to cover a wide Q-range in one measurement is also desirable when in-situ measurements cannot be properly replicated under the exact same conditions. Increasing stress up to the breaking point of a sample is a good example for this. Specific examples for investigations where such measurements are required are the formation of nano-foams, mixing and phase transition processes and in-situ polymerization. As all these investigations are highly applicable (nano-foams: insulation and energy saving), have a wide societal impact (mixing and phase transition in drug delivery) and are of fundamental scientific interest (following the dynamics of a polymerization/chemical reaction in real time) measurements at SKADI will contribute significantly to the early scientific success of ESS.

Polarization of the incoming beam and polarization analysis after the sample enables full analysis of the magnetic structure. In this way, all magnetic structures can be identified. These investigations are also of high interest in a wide range of fields. One example might be the ability to follow a magnetic fluid (dispersed ferromagnetic nanoparticles) under stress in real time. This has an application in car suspension setups. Here again all prerequisites for high-impact publications are met.

These features will allow SKADI to cater for the needs of a wide range of scientists, making it an ideal choice for the first day instrument. This is especially true in the light of the early success strategy by ESS, as SANS instruments have an excellent record of fast publication.

2.1 Science Case: High-Resolution

Most SANS instruments operate either with neutron selector or a in case of TOF instruments with several bandwidth choppers. Without additional measures this usually results in a wavelength resolution between $\Delta\lambda/\lambda$=10 and 20%, where the natural distribution of wavelength at TOF instruments favours long wavelengths. Leaving the rest of the configuration identical this limits the Q-resolution in the medium Q-range of 10^{-2} Å^{-1} < Q < 10^{-3} Å^{-1} to about $\Delta Q/Q$ = 10% for most current instruments and approximately 5% for SKADI.

While this is adequate for a wide range of measurements, such aspolymer melts and solutions and dispersed particles this limits the capability to analyse structures in the mesoscopic regime when ordering occurs. Here a higher resolution especially in the medium Q-range is desirable, as those intermediate structures often form on the length scale of hundreds of Angstroms, which translates directly to that Q-range. The ever more increasing purity of available proteins is another argument for resolution to keep track with the development of available samples. This is especially to also make the advantages of higher resolution in SAXS also available in SANS, which proves to be of interest for protein structure reconstruction from scattering images (A. Koutsioubas et al. *DENFERT version 2: extension* *of ab initio structural modelling of hydrated biomolecules to the case of small-angle neutron scattering data* J Appl Cryst, **49**, 690-695, 2016).

In order to illustrate the necessity for high resolution measurements an investigation of $C_{28}H_{57}$-PEO_5 micelles in solution is shown in Figure 1. The micelles start to form intermediate structures at high concentrations, which lead to pronounced peaks. However, when working with a wavelength resolution of 20% only the primary peak is visible, all higher order peaks vanish in the shoulder of that peak and therefore the possibility to analyse the structure of the lattice is limited. At a wavelength resolution of 5% however the peaks become clearly visible, and even a splitting of the primary peak can be found. This example illustrates the need for a high-resolution measurement option in a world class SANS instrument such as SKADI. The same argument is true in cases such as silica solutions or granular system where structures are formed under shearing. This also aligns well with the better availability of highly pure biological samples, such as isolated protein unimers, that have become more readily available in recent years. Therefore an extension of the wavelength resolution to well below 5% seems necessary in order to investigate such samples with greater detail in future and be able to glean new insights from that data.

The demand for higher resolutions on SANS instruments is also illustrated by the requests by users for that feature at instruments where such an option is already available today. In proposals for measurements with BILBY@ANSTO there is a consistent request for that option in all proposal cycles, making up for a third of the proposal number requested days (private communication with the instrument scientist A. Sokolova).

Taking these factors into account it seems sensible that any new world-class instrument such as SKADI should provide such an option as there are both scientific investigations that will benefit from such an option as well as there is substantial demand for that option from the

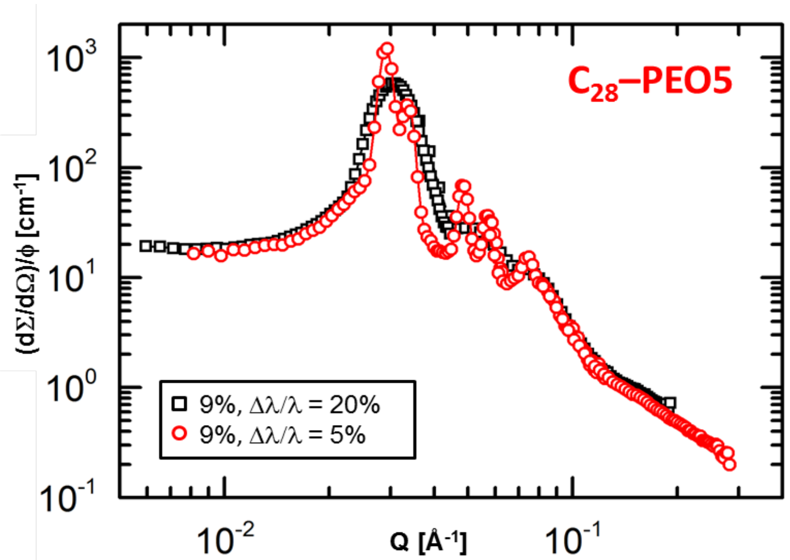

Figure 1. SANS measurement of 9 wt% $C_{28}H_{57}$-PEO_5 micelles in D_2O at KWS2, MLZ. While for a wavelength resolution of 20% the primary structure peak is visible all other peaks vanish. Only using the 5% wavelength resolution the higher order peaks become visible, also the splitting of the first peak allows an improved determination of the sample structure. (Data

scientific community. Also, in order to stay competitive for an extended period of time during operation a powerful and at the same time flexible solution for resolution selection is important.

3. SYSTEM CHARACTERISTICS

3.1 System Purpose

The SKADI instrument is a small-angle neutron scattering instrument. It is designed to serve a wide range of scientific fields, accommodating dedicated as well as custom-made sample environments in a versatile 3x3 m^2 sample area. This allows investigations in the fields of soft-matter and biology, over pharmaceutical and medical sciences to material science. Moreover, the possibility to include polarized neutron scattering and polarization analysis allows for the investigation of magnetic samples. For more specific information on the science case please refer to the SKADI instrument proposal and the requirements as laid out for SKADI in the SKADI system requirements document.

3.2 System Lifecycle

In Figure 2 the lifecycle of SKADI is shown. This includes the future detailed development phases. Each phase will be concluded by a tollgate review. Additionally to that review, during the construction and installation phase, there will be an intermediate design review – TRR.

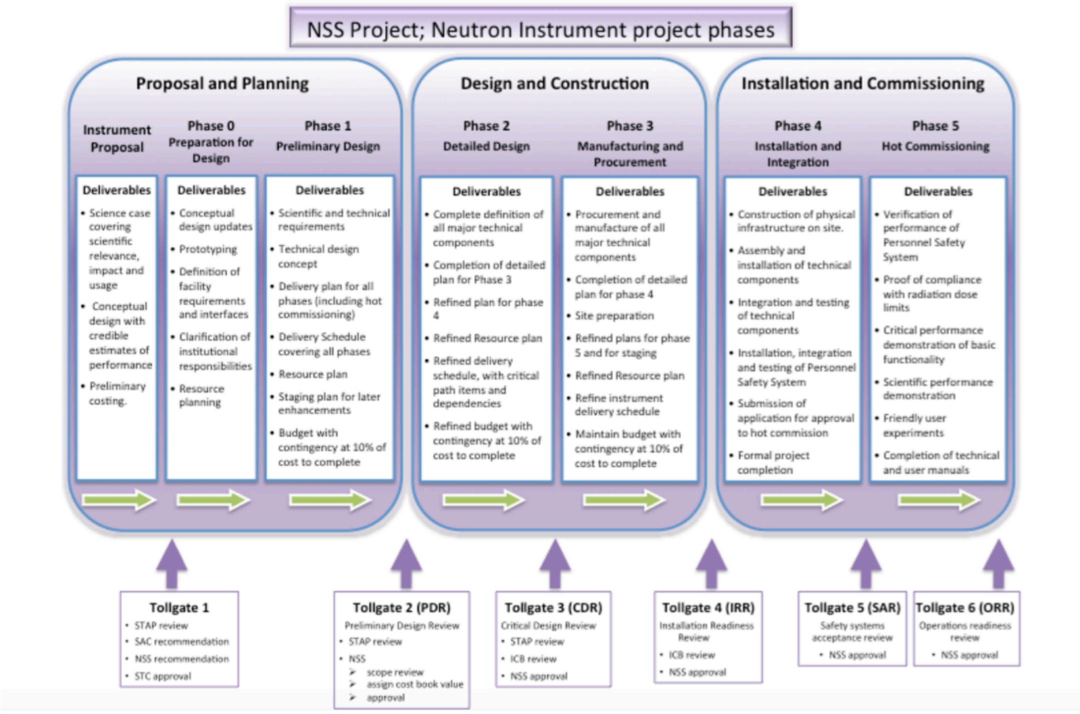

Figure 2. Life cycle of SKADI. Each phase is concluded by a tollgate review. Hot commissioning is mentioned, but not part of the construction project.

The overall life-cycles are:

- **Design Stage** – aims to develop the instrument from the proposal to a build ready state, with a majority of design drawings and component sourcing finalized, fulfilling all requirements. To ascertain that the instrument maturity progresses as planned through the tollgates (TG), accompanying design reviews are conducted. The PDR (Preliminary Design Review) and the CDR (Critical Design Review) are two of those.
- **Construction Stage** – aims to deliver a fully built, verified, tested and commissioned, ready for full operations, instrument. The stage is split into two phases; the construction and installation as well as the beam test and commissioning. Each phase is concluded with a TG and accompanying design reviews. Safety Assessment Review (SAR) and Operational Readiness Review (ORR) are two of those. For the construction and installation phase another design review is conducted, the Installation Readiness Review IRR. The IRR ensures that the instrument can proceed to and successfully complete the SAR.
- **Operations Stage** – aims to maintain an instrument with high availability and reliability for the user community to perform experiments. The operations stage will allow for scheduled maintenance as well as periods where upgrading and/or modernization of SKADI can be performed. With upgrade it is meant that additional functionality/capability is introduced into SKADI, while modernization describes an enhancement of existing functionality.
- **Decommissioning stage** – this is the period where the instrument shall be dismantled and disposed of in a safe and controlled manner, adhering to all radiation safety requirements. It is possible that SKADI will be decommissioned before ESS has reached its own end of life.

3.3 System Overview

The current concept for SKADI (see Figure 3) is a SANS machine with a maximum 20 m collimation distance and 20 m sample to detector distance with the capability of performing polarized neutron scattering and polarization analysis. SKADI uses the cold moderator with a bandwidth of 5 Å (typically 3 Å - 8 Å) in single pulse operation and a bandwidth of 10 Å (typically 3 Å -13 Å) in pulse skipping operation.

The beam delivery system consists of a curved guide to avoid a direct line of sight between sample/detector and moderator. Choppers serve to customize the wavelength band as needed for the experiment. The collimation settings with 8, 14 and 20 m provide a choice of several angular resolutions, which is further supported by collimation slits of varying size.

In the current setup SKADI is located at beam port E3. This position in the east fan of the instruments and the non-allocated beam port E4 next to SKADI allow for an easy access to the instrument. The required 3x3 m^2 sample environment staging area is planned in front of the sample area door.

SANS instruments such as SKADI are heavily oversubscribed on most neutron sources. In order to allow as many experiments on the beamline as feasible SKADI employs two strategies to have a high availability of beam time for users:

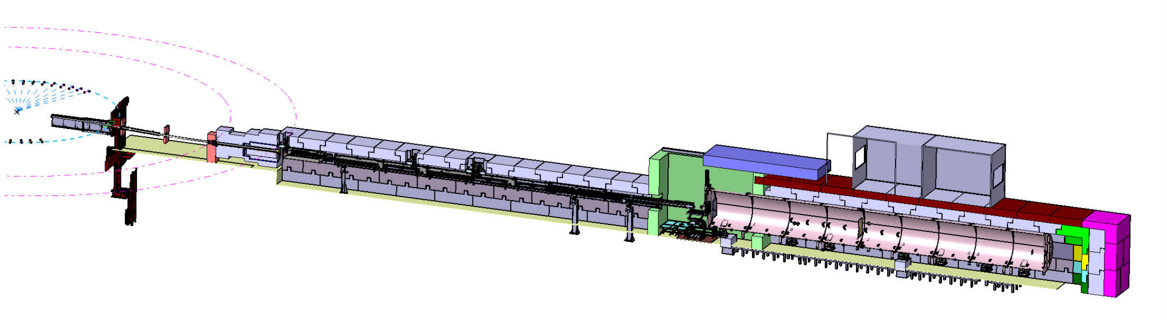

Figure 3. Overview of SKADI. The bunker wall position is marked by dashed lines.

The sample environment is designed to be "Plug-and-Play". This means that the actual preparation of the setup is done off the instrument in a preparation laboratory. There the next user can prepare his experiment in advance and use an alignment system, which is identical to the one found at the instrument. Afterwards the complete setup can be moved by forklift or crane to the instrument. There the experiment can be started very rapidly as all alignment and testing has already been performed.

Even failures of single components usually do not lead to a complete breakdown. Two examples for that are: First, the chopper system, where some of the choppers (2nd, 3rd or 4th) can fail and measurements can still be performed, albeit with a slightly reduced resolution. Second, the polarizer, which automatically slides into an open position upon failure.

The following sections covers more detailed descriptions of the individual components that comprise SKADI.

3.3.1 Neutron Beam Extraction

The neutron beam extraction delivers the neutrons from the moderator into the instrument and provides a twice out of line of sight condition. This is achieved by a S-bender setup, which displaces the centre of the beam downwards by 24 cm at the bunker wall. It is located between the moderator dead area, at 2 m, and the shutter in the bunker wall, at 15 m. The neutron guides have a cross section of 3x3 cm^2 and a metal substrate (probably aluminium), coated to achieve moderate m-values (m=3). Benders with five channels allow optimal transmission. These guides will be placed in separate vacuum housings that are shielded with boron carbide. Additionally, three copper collars around the vacuum housing will minimize background based on forward scattering from the monolith.

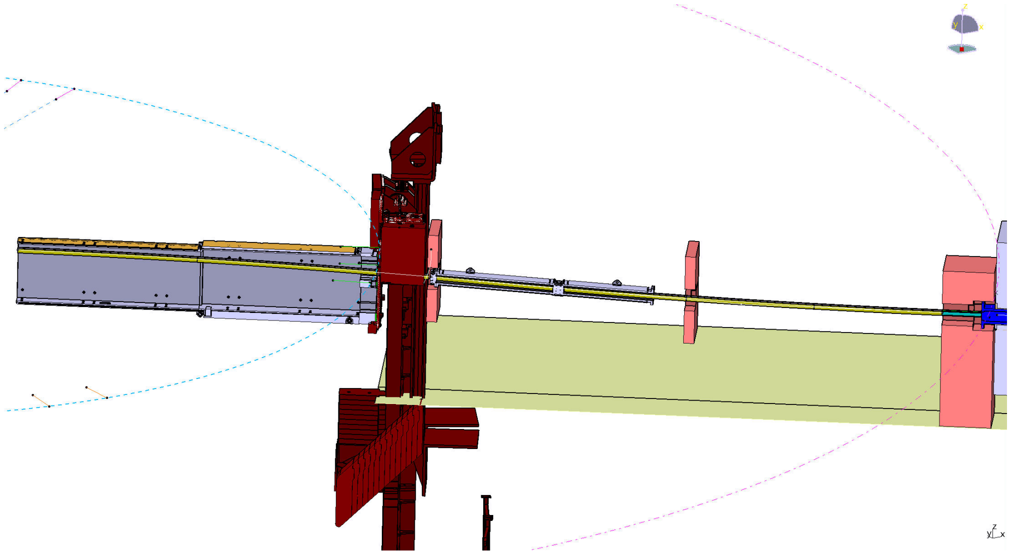

Figure 4. SKADI beam extraction and S-Bender. The neutron guide is reaching from the monolith insert to the exit at the bunker wall. The copper collars (pink) help scattering away neutrons from the bunker exit.

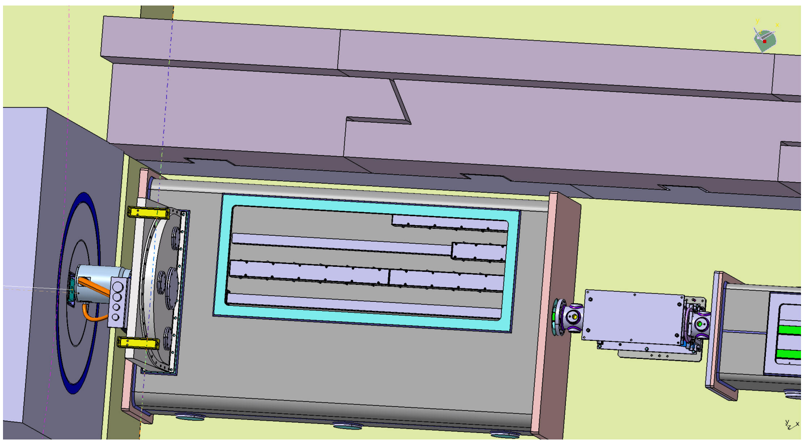

Figure 5. Polarizer with different positions for selectable wavelength bands. On the left the shutter with the motor outside the bunker can be seen, on the right the spin flipper together with the beginning of the collimation.

3.3.2 Neutron Beam Collimation

The neutron beam will be collimated choosing from various configurations of guides and absorbing slits. As a SANS instrument needs to transport mainly brilliance, and not only flux, high divergence beams are not required and moderate m-values are sufficient for the guide (m=2.5). The guides will be placed on sledges in the vacuum housing where they can be moved in and out of the beam. The slits will be fixed in position and fully opened if unused. They will thus act as an additional internal shielding inside the collimation. The setup will allow for collimation distances of 8, 14 and 20 m. The first part of the collimation stretch will house the polarizer (Figure 5). Four different positions accommodate: (i) a standard neutron guide (no polarization); a z-geometry neutron guide for wavelengths (ii) 3-10 Å; (iii) 5-20 Å respectively; as well as (iv) an empty position for later additional neutron optics.

3.3.3 Chopper Systems

The SKADI chopper system will comprise four single disk choppers that provide a maximum transmission setting, a pulse-skipping mode and a high-resolution mode. Details about the underlying calculations have been published in [1]. The choppers will be placed at 15.5, 22.85, 26.3 and 26.6 m distance from the moderator respectively, within the collimation stretch (Figure 6). It is worth noting that the first two choppers will only run in 14 and 7 Hz mode, whereas the last two will be able to run at multiples of 14 Hz for the high-resolution mode. Although it is technically possible to have non-magnetic bearings for the slower choppers we opted for using the same magnetic bearings for all the choppers. This facilitates the maintenance procedure and keeps necessary spare parts to a minimum during operation.

The proposed chopper setup fulfils the requirements of being able to select and condition neutrons of the cold spectrum ($\lambda > 3$ Å) as well being completely outside of the common bunker area, which will allow for maintenance while the beam is on target. Additionally it is failsafe in the sense that one of the choppers can fail and SKADI can still operate in a mode with reduced resolution.

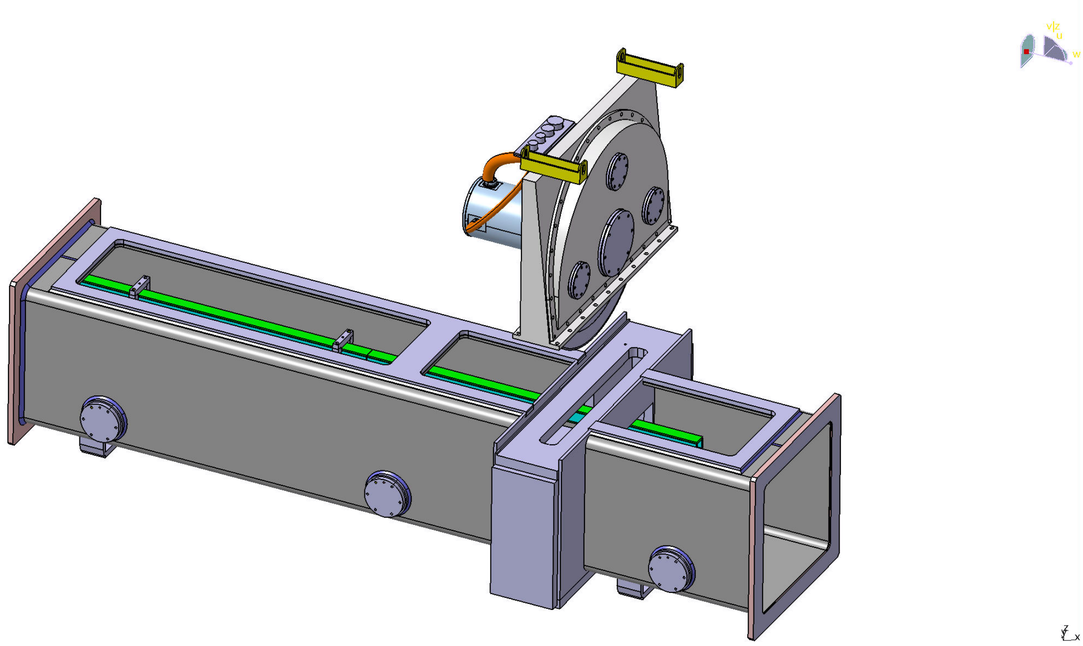

Figure 6. Positioning of a chopper inside the collimation vessel.

3.3.4 Shutters

Apart from the light shutter at the monolith, which will be under control of the target group, SKADI will feature a heavy shutter at the exit of the bunker, as well as a sample shutter after the polarizer. The heavy shutter will be placed in the bunker wall in an insert at the exit of the beam path through the bunker wall (Figure 7). That specific location was selected for the reasons that (i) this allows work on the collimation stretch while beam is on target and (ii) it allows operating the motor outside the common bunker area where radiation hardness is less of an issue.

The shutter will be attached to the bunker wall from the inside with additional collimation shielding to prevent streaming and have two positions, open and close. In the open position a piece of the neutron guide will be in the beam, whereas in the closed case a sandwich of B4C, iron, boron-epoxy and lead over the complete length of the shutter will allow for blocking the direct beam. In case of loss of current in the motor due to a failure the shutter will slide in the closed position under its own weight.

The sample shutter on the other hand will be located directly after the bunker and be designed to close on its own in case of a failure. This shutter is used for fast access and sample change in the sample area but does not necessarily provide sufficient shielding to access the collimation stretch.

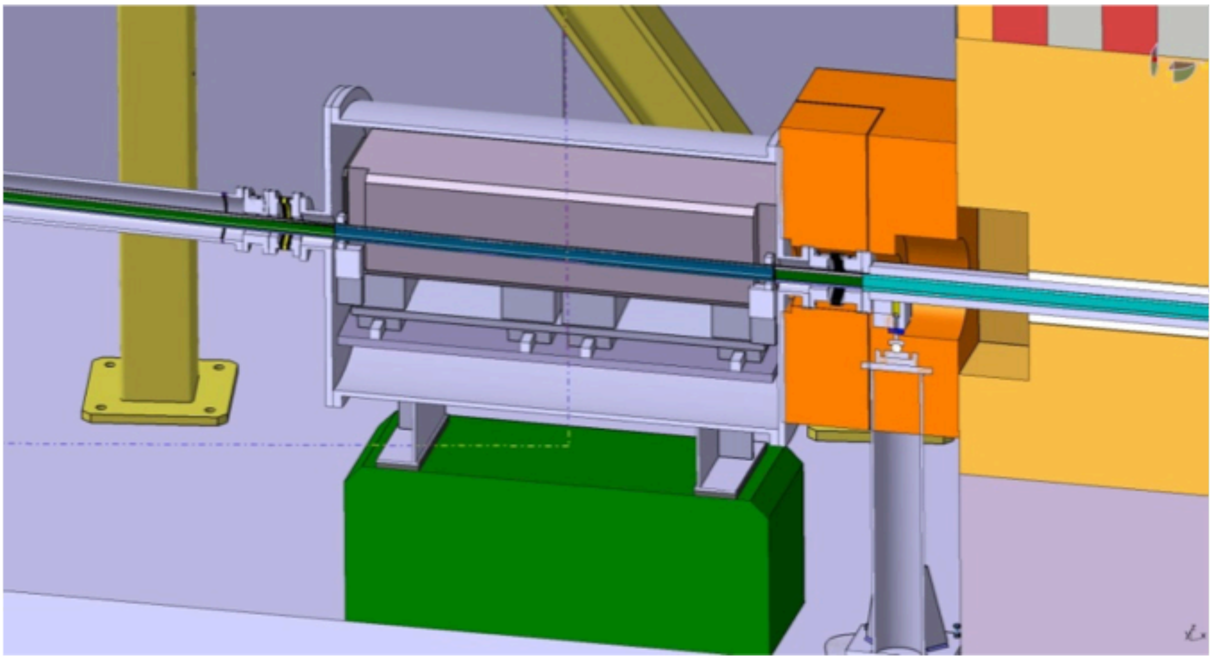

Figure 7. Heavy shutter inside the bunker wall. The neutron guide inside the bunker wall can be aligned from outside the bunker, so misalignment due to creeping of the concrete can be corrected. There is only one vacuum for the whole flight tube, so no windows are necessary.

3.3.5 Shielding

In any operational stage, the shielding will provide a safe working environment at SKADI. In terms of operation, only the sample area will have a shielding that is accessible through doors/roof hatches.

Shielding at other positions has to be craned out, which is detailed in the maintenance section.

3.3.6 Sample Area

The 3x3 m^2 sample area (Figure 8) will provide ample space to conduct experiments also with bulky equipment at the sample position. The free height over the beam in the sample area will be 2 m to allow for cryostats or other equipment standing over the beam. As the beam height of 1.9 m does not allow for safe and easy work at the sample position, there will be a platform with a hollow floor in such a way that the beam height above floor level is 1.5 m. This hollow floor will also allow for media distribution below the actual working area, minimizing possible safety hazards and facilitating the work.

Inside the sample area there will be a standard mounting setup on a carrier. This will allow off-instrument preparation of the sample environment and subsequent fast switching of the thusly-prepared sample environment. Using this approach the change between different users and hence setups will be possible within half an hour.

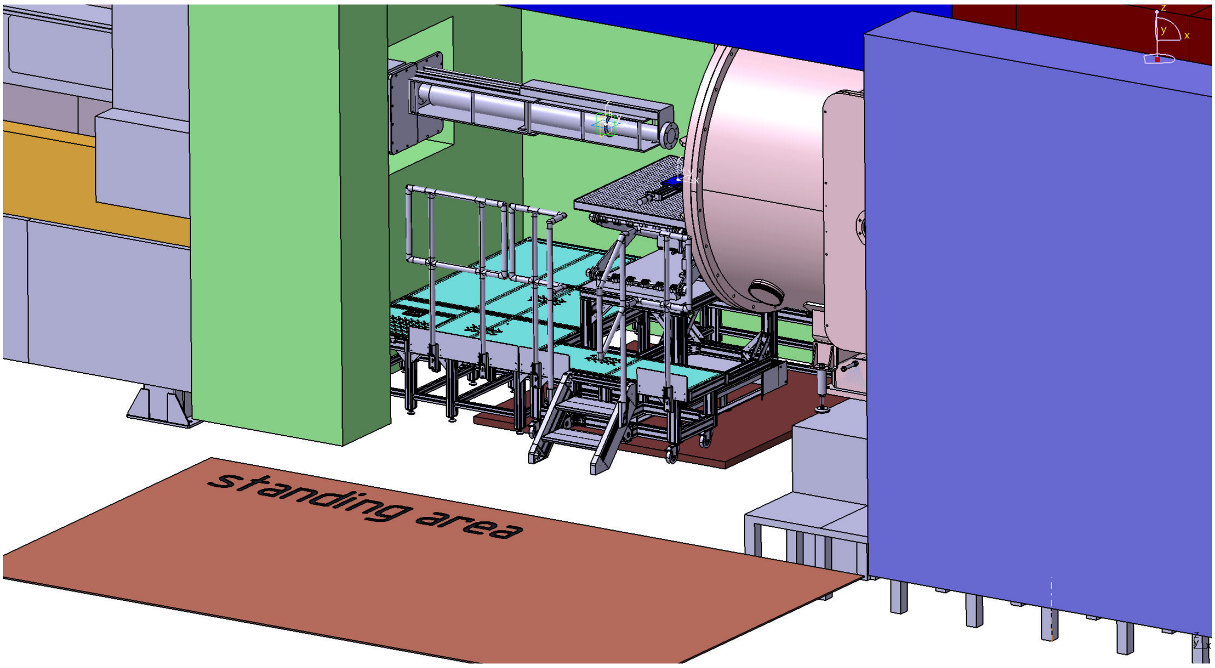

Figure 8. SKADI sample area. The false floor part with the stairs can be removed easily, so a pallet jack can be used to exchange the sample setup. The nose at the end of the collimation can extend the vacuum close to the sample.

3.3.7 Detectors

SKADI will feature 1 m^2 of active detector area with a resolution of 6x6 mm^2 in general and a small 20x20 cm^2 detector at 20 m sample-detector distance with a resolution of 3x3 mm^2. The SoNDe project will deliver the detector technology and part of the detector modules for SKADI. The detector area will be balanced at three positions (Figure 9 and Figure 10) to cover a Q-range of three orders of magnitude. The two front detector positions will be mobile, while the rear detector position will be fixed at 20 m sample-detector distance.

This setup will allow a constant high resolution at low Q while allowing covering a Q-range adapted to the experimental problem. Each moving detector will be located on its carrier with 1 m^2 capacity. Both detectors will have a 20x20 cm^2 aperture in order to let the neutrons scattered at the smaller angles to pass through and reach the rear detector. Initially, the 1 m^2 coverage will be balanced between the three detectors so that every detector will not be fully equipped. The rear detector will be fully equipped at a size of 20x20 cm^2. This will lead to an over illumination when the two forward detectors are not at the rearmost position. However, there will be no gap in Q-space due to the TOF capability of SKADI and the spread of wavelengths.

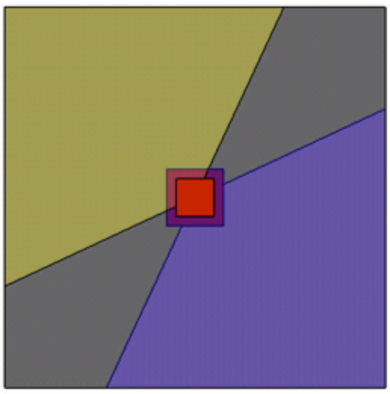

Figure 9. Detector coverage of the active area as seen from the sample position. All three detectors standing behind each other are superimposed. Blue area is from the front detector, yellow area is from the centre detector, red area is from the back detector. Grey areas are overlapping areas of both front and centre detector.

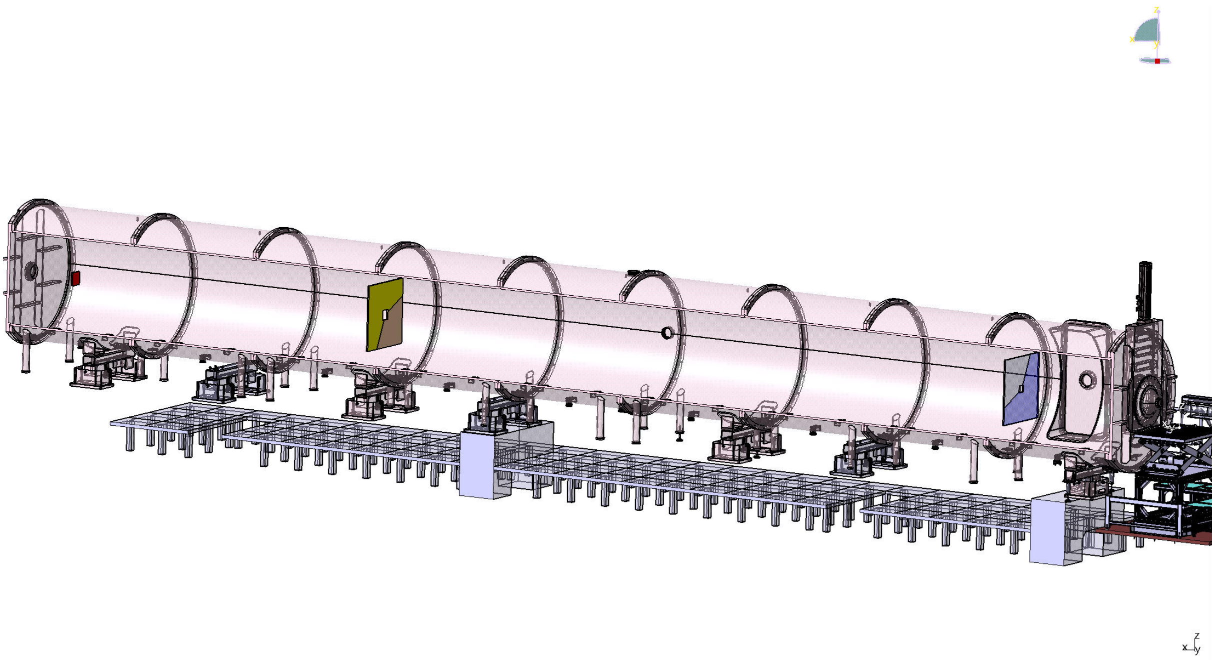

Figure 10. SKADI detector setup for a collimation setting of 14m. As in the figure above all three detectors are shown (same colour coding). Seen from the sample position (right), a full square meter of active detector area is seen. The two larger detectors can be moved within the detector tube to achieve optimized coverage/resolution to meet specific experimental requirements.

3.3.8 Beam stop

Instead of a traditional fully blocking beam stop SKADI will feature an absorber system (3 multi-grid systems adapted to the wavelength bandwidth and flux) that allows for the rear detector to detect and withstand the directly transmitted beam during a scattering experiment. Such a system will be of a nearly conical shape and also serve as a beam attenuator for scattering normalization using the centre detector at 20 m SDD (transmission measurements). These beam stops will be done as full absorbers with an appropriate amount of drillings to allow for transmission to the detector behind.

3.3.9 Personnel Safety System (PSS)

PSS will mitigate the risks associated with running a user program at the instrument. The risks assessment and PSS requirements for operating SKADI will be provided by the ESS.

3.3.10 Control Hutch

The experimental team will be able to control the sample environment remotely from the control hutch. There will be dedicated computers for controlling operational parameters of SKADI, of the sample environment as well as for data collection and reduction/initial analysis.

3.3.11 Sample Preparation Area

Preparation of the sample right before and during the experiment will be performed here. This includes simple sample preparations that can safely be performed without a dedicated laboratory, such as adding solvent to a sample and cutting a solid sample. Also the preparation of the sample environment as such before a user change can be performed here. For work requiring a laboratory with safety measures, such as a fume hood, the central ESS laboratories have to be used.

3.3.12 Instrument Control

The instrument control will allow remote control of most of the components of SKADI from the control hutch. This includes systems such as the chopper system, slit positions and the detector system which are necessary to change during the course of an experiment. Control from computers at other locations should be available for the instrument team. Software solutions to achieve these goals will be worked out in cooperation between the instrument team, the ESS integrated control systems group and the ESS Data Management and Software Centre (DMSC).

3.3.13 Future Upgrade Possibilities

The future upgrades of SKADI comprise three main features:

- Detector area
- Sample environment
- Polarization analysis

Each of these upgrade paths is necessary to operate an instrument that continually performs at world class and can use the high performance of the ESS source to capacity.

Concerning the **detector area** SKADI is capable of housing 2 m^2 of active detector area in order to allow for extremely low measurement times to investigate fast structural changes. Increasing from the projected 1 m^2 to the full coverage will considerably improve the performance of SKADI concerning fast measurements such as the polymerization of nano-foams or crack formation in natural rock.

The **sample environment** of SKADI is currently projected to be one cuvette changer with and one without temperature control with at least 5x10 positions each. Additional sample environment setups will be coming from the sample environment pool. Upgrading this sample environment pool, in collaboration with Loki in a small SANS specific pool, would benefit the scientific breadth of experiments that can be performed at SKADI. The most requested specific sample environments at other SANS facilities are stopped-flow setups for mixing of liquids and temperature jumps, rheometers to allow for in-situ rheology and stress strain rigs. Any of these sample environments caters to a specific target group, however they are vital in their overall sum to fully exploit the potential of SKADI.

Polarization analysis allows for both the investigation of magnetic samples as well as incoherent background suppression for soft matter samples. While it is vital for a fully-fledged analysis of magnetic samples (which comprises about 10-15% of the scientific proposals at other facilities) for the suppression of incoherent background in hydrogen rich samples often it is more successful to exchange the hydrogen vs. deuterium. However this is not always possible, which leaves a small portion of the soft-matter users that will benefit from a polarization analysis at SKADI. Overall this accounts for about 20% of the potential users of SKADI.

4. SYSTEM STAKEHOLDERS

We consider the users (SH-1) as major stakeholders. The scientific scope of SANS machines caters for the needs of a huge user base (SH-1.1) and addresses a broad range of scientific fields, including biology, chemistry, physics and materials science, as well as medical sciences. Additionally, there is also an ever-growing group of potential users (SH-1.2) from research areas that have to date little or no experience in neutron scattering such as food sciences. It is important to cater for the needs of both groups in order to use SKADI to its full scientific capacity. This in turn requires a very adaptable instrument, which takes into account the very specific needs of the respective communities.

As the ESS is a multinational effort, most of the instruments are constructed in a concerted effort of multiple partner labs (SH-2). Their mission to serve the European user community with world-class instruments is supported by their respective funding agencies (SH-3).

The coordination of the international contributions is a challenge that is accomplished the ESS Neutron Scattering Systems Division (SH-4) and the ESS organization (SH-5) as a whole.

A special case for SKADI is the integration of the EU funded SoNDe project (SH-6).

Table 1 shows a detailed list of stakeholders within these groups. For each stakeholder group we identify a representative and indicate their interest and or involvement in SKADI.

Table 1. SKADI stakeholders.

Group ID	Stakeholder Group	Individual ID	Stakeholder	Representative	Interest/Involvement
SH-1	User community	SH-1.1	Users of SANS instruments	STAP	Provides Science Case, Expect access to a world-leading instrument
SH-1	Potential Users	SH-1.2	Potential Future Users	STAP	
SH-2	FZJ/LLB	SH-2.1	Instrument Core Team, LIS	Sebastian Jaksch/ Jacques Jestin	Deliver SKADI in Schedule and in Budget, participate in the project beyond construction phase
SH-2	FZJ/LLB	SH-2.2	Instrument Core Team, LE	Romuald Hanslik/Sylvain	

				Désert	
SH-3	BMBF	SH-3.1	National Funding Body (Germany)		Provide Resources for SKADI, aim to maximise In-Kind contributions, Represent the Member States in ESS ERIC Council
SH-3	CNRS/CEA	SH-3.2	National Funding Bodies (France)		
SH-4	ESS-NSS	SH-4.1	Instrument Construction Subproject	CIPE (Gabor Lazlo) CIPS (Ken Andersen)	Early Scientific Success of ESS, Deliver world-class Instrument Suite in Time and Budget, Track project progress and decide about progress at Tollgate Reviews, Change Management
SH-4	ESS-NSS	SH-4.2	Neutron Scattering Systems Project	NSS PM(Shane Kennedy)	
SH-4	ESS-NSS	SH-4.3	Science Directorate	DS (Andreas Schreyer)	
SH-4	ESS-NSS	SH-4.4	Neutron Optics and Shielding Group	GL (Phillip Bentley)	Compliance to ESS standards, facilitate budget savings by "horizontal contributions", Provide resources for integration work
SH-4	ESS-NSS	SH-4.5	Neutron Chopper Group	GL (Nikolaos Tsapatsaris)	
SH-4	ESS-NSS	SH-4.6	Detector Group	GL (Richard Hall-Wilton)	
SH-4	ESS-NSS	SH-4.7	Motion Control and Automation Group	GL (Thomas Gahl)	
SH-4	ESS-NSS	SH-4.8	Data Management and Software Centre	GL (Mark Hagen)	

SH-4	ESS-NSS	SH-4.9	Integrated Control Systems	GL (David Brodrick)	
SH-4	Related instrument projects	SH-4.10	Loki Instrument Team	Andrew Jackson	
SH-4	Related instrument projects	SH-4.11	ESTIA Instrument Team	Artur Glavic	
SH-5	ESS	SH-5.1	IKRC	Dr. Marco Marazzi (Chair)	Final accreditation of contributions, Assess and evaluation of deliverables of the Work Packages.
SH-5	ESS	SH-5.2	SAC	N.N. (Chair)	Provides independent advice, on scientific and technical issues related to the instrument suite and the facility and its scientific operation.
SH-6	SoNDe	SH-5.1	SoNDe Consortium (FZJ, LLB, ESS, IDEAS AS)	Sebastian Jaksch	Delivery of Detector Prototype in Time and Budget, Patent owners for new developments of the project
SH-6	SoNDe	SH-5.2	Funding Body (European Union)	Project Officer	

5. OPERATIONAL CONCEPTS

5.1 Operational Environment

It is envisioned that the beam port allocation for SKADI is to be E3. SKADI will therefore extend from the bunker into the east hall, which means there is potential strain at the crossing from the base plate of the bunker into the east hall. This strain is mitigated by not having any active components in this area, as well as beam windows.

SKADI will be operated under ambient conditions in the hall, which means a controlled environment of 22±2 °C will be maintained all around the year. The floor height will be approximately 2 m below the beam height. Floor loading in the east guide hall will not exceed 20 t/m^2. Floor underneath the bunker can accommodate 30 t/m^2. The stability of the floor in the east hall has a specified maximum of 3 mm w.r.t. elastic movement and another maximum 3 mm due to creep/deformation.

Utilities and media are brought to the instrument from the gallery in case of the east experimental hall. For the bunker area we will adhere to the standards set forward by the ESS.

Media for the east hall include: DIH2O, N2, instrument grade compressed air, cooling water low. Utilities include: office IT, office communications, power supply, MPS, PSS, DMSC and ICS. For detailed and updated listing of requirements and/or specifications related to operational environment see the System Requirements Document. Details for e.g. maintaining the stable temperature in the experimental hall are still in development but one suggested solution could be to place ventilation hoods directly above instrument equipment generating most heat.

The ESS has five different operating modes: Shutdown, Studies, Studies on Target, Startup and Production. These modes have various impacts on instrument operations. Pure experimental work can only be conducted in Production mode. Access to instrument equipment for maintenance, calibration, cold commissioning is mainly done during shutdown, studies and studies on target – naturally after due safety assessment and still possibly with some restrictions. During start-up instrument operations is limited to alignment, commissioning and calibration runs.

- When the ESS has entered into steady-state operations the following principal schedule will apply: 200 day/year of neutron production for the ESS users after 2026
- Proton beams will be on target for 225 days/year
- Two long shutdowns, one in winter (~6 weeks) and the other in summer (~10 weeks) followed by Studies and Studies on Target periods
- Three optional Studies days every second week to avoid long down time of instruments due to failures of activated components, followed by two days for Studies and Studies on Target
- A series of Studies days to allow for fine-tuning of accelerator and target systems

One goal of the ESS is to ensure that at least 90 % of the production time is available for neutron experiments on the instruments, allowing the full scope of experiments for which the instruments were designed. This is in accordance with the availability and reliability assessments made by the ESS [ESS-0017709 and ESS-0008886].

SKADI is foreseen to be operated by a team of 3-4 scientists, one engineer and one technician, where a portion of their work time can be dedicated to other instruments. While the scientific staff will be mostly dedicated to SKADI (at least 3 full-time equivalent - FTE), the technical staff can also support other instruments than SKADI (0.75 FTE technician, 0.5 FTE engineer). ESS will be manned 24/7, so this manning should allow for flexibility for users when conducting experiments and making preparations or analyzing results. The tools provided by DMSC, physically located in Copenhagen, are at the instrument team's and users' disposal for data collection, storage and analysis.

5.2 Operational Scenarios

It is crucial for the long-term scientific productivity of SKADI that conducting experiments is as streamlined as possible. This includes preparation and installation of a sample environment, configuring the experiment, performing the experiment and unmounting the sample environment after the experiment has been performed.

As a prerequisite to perform this in a streamlined manner, preparation off the instrument has to be possible, so as not to lose operation time for preparing a setup. These installations will also be standardized as far as possible in order to share with other instruments, most notably Loki. This allows for a helpful exchange of knowledge and possible spare parts for operation.

The basic concept follows the ideas outlined below:

- A mounting setup will be below a carrier for the sample environment, which can be placed in as many instruments as possible
- Onto that mounting setup, users and instrument staff will be able mount and configure sample environment in a preparation laboratory
- In that preparation laboratory, there will be an alignment system exactly as is on the sample area of SKADI, where in place of the neutrons there will be a safe to operate laser beam, thus allowing for exact alignment
- As soon as the preparation is completed and the assigned beam time started, the sample can be moved by forklift or crane to the sample area of SKADI and be mounted there

This procedure considerably cuts down preparation time of neutron experiments as it is done nowadays.

The beam time for user experiments is allocated in a peer-review process based on scientific merit and feasibility. Proprietary access for industry may also be possible.

Regarding the possible users of SKADI there can roughly be made a distinction into three groups with distinctive needs

- Fully trained and experienced SANS users. This group usually requires very specific preparation of the instrument, however often can perform their experiments in an efficient manner with limited help from the beamline scientist during and after the beam time. This group usually consists of STEM scientists with a strong technological background. Here also full access to any setting SKADI may offer should be accessible through the controls.
- Intermediate users with some experience. Here some settings may be hidden, as they would not serve an improved conduction of the experiment and pose a potential risk to both users and experiment.
- Users with little to no experience. This group requires both a very detailed preparation, help during the beam time and help evaluating the recorded data. They

often come from fields which have in the past started using neutron scattering as a method, but did not receive the technological training or that are in a field which has not used neutron scattering previously. Here only a limited set of settings should be available. Essentially operation should be a plug and play for this group.

The users team will need to consist of at least 4 persons, with two of PhD or PhD student level, so that a 24 h operation with always at least one experienced experimenter (not necessarily experienced in performing an experiment at a SANS machine, but with the ability to independently work at a large scale facility) on site can be maintained. The samples will be brought along or shipped, some simple preparation work for the samples themselves can be done in the preparation laboratories. In order to complete safety and radiation training and prepare their setup as needed, the experimental team will need to be on site for the ESS at least one day in advance, depending on the complexity of the experiment.

The users will process the data at the ESS at least up to a point where it can be input into third party software (usually intensity vs. q reduction). One part of the measurement software will be available as a live view of the data collection. This simple life view should enable the experimentalist to a limited overview of the sample behaviour, i.e. peaks at certain q, slopes of the intensity vs scattering angle plots. This is not to be confused with the final data evolution, but rather as a tool to perform the experiment as intended.

5.2.1 Preparatory Measurement

In order to perform a proper data reduction on an absolute scale preparatory measurements will be needed on SKADI. These measurements include recording the dark current detector image, recording the empty sample holder for transmission calculation and recording a near perfect incoherent scatterer or near perfect glass to calibrate the detector sensitivity.

On today's SANS instruments such as the KWS1/2, D11, D22 and D33 this is done by measuring with the beam blocked by a piece of boron carbide. The sample cell will be measured alone, as an additional measure the solvent might be measured in dissolved samples, to separate sample from solvent scattering. For the measurement of an incoherent scatterer or a perfect glass either H_2O or poly(methyl methacrylate) is used.

Also exact measurements of the instrument as such, namely resolution functions with appropriate samples should be measured. These datasets can later be used to distinguish between experimental influence and properties of the sample.

These three datasets will then later be used for data reduction during data treatment.

5.2.2 Soft Matter Experiments

Soft matter experiments have over the last decades become a domain of the SANS community. Therefore it is hard to pinpoint the commonalities as there is a multitude of possible experimental questions to be answered that all in turn need specific conditions for the sample, time resolution or settings of the experiment.

Still it is possible to point out some general conditions for soft-matter experiments. Usually the needed temperature range is at or around the temperature where water is still fluid. Outside that area the experiments rarely exceed temperatures of 700 K where most polymers, plastics and other soft matter materials disintegrate or below 250 K where most soft matter materials lose their viscoelastic properties. Also regarding other properties of the environment most soft matter samples range around ambient conditions.

One very typical example is the measurement of a solution of a sample dispersed in a solvent that will be presented here. After the preparatory measurements have been done a (quartz glass) cuvette with a free path of a few millimetres will be filled with the sample. The short free path is used to avoid multiple scattering within the sample. This may also be achieved by diluting the sample further down. Additionally most experimenters try to avoid hydrogenated solvents and prefer deuterated solvents in order to minimize the incoherent background. The cuvette is then placed into the sample holder, which serves to create the intended conditions (e.g. temperature) and the sample will be exposed to neutrons. The exact settings of SKADI at this point determine resolution, flux and covered q-range by the collimations settings. Therefore they have to be adjusted to the exact parameters. The recorded data are then reduced which essentially means getting an intensity vs. q dataset for each sample and sample condition. Here, as an example, the scattering of latex spheres dispersed in heavy water is shown (Figure 11). After reduction, depending on the complexity of the sample, a model function is derived that is then fitted to the dataset, in this case homogeneous spheres. Depending on the chosen model function parameters of the sample behaviour can be determined.

Here then, in order to separate the resolution of the instrument from the distribution of particle sizes, the model function can be convoluted with the resolution of SKADI. Any remaining distribution is then attributed to the distribution of particle sizes.

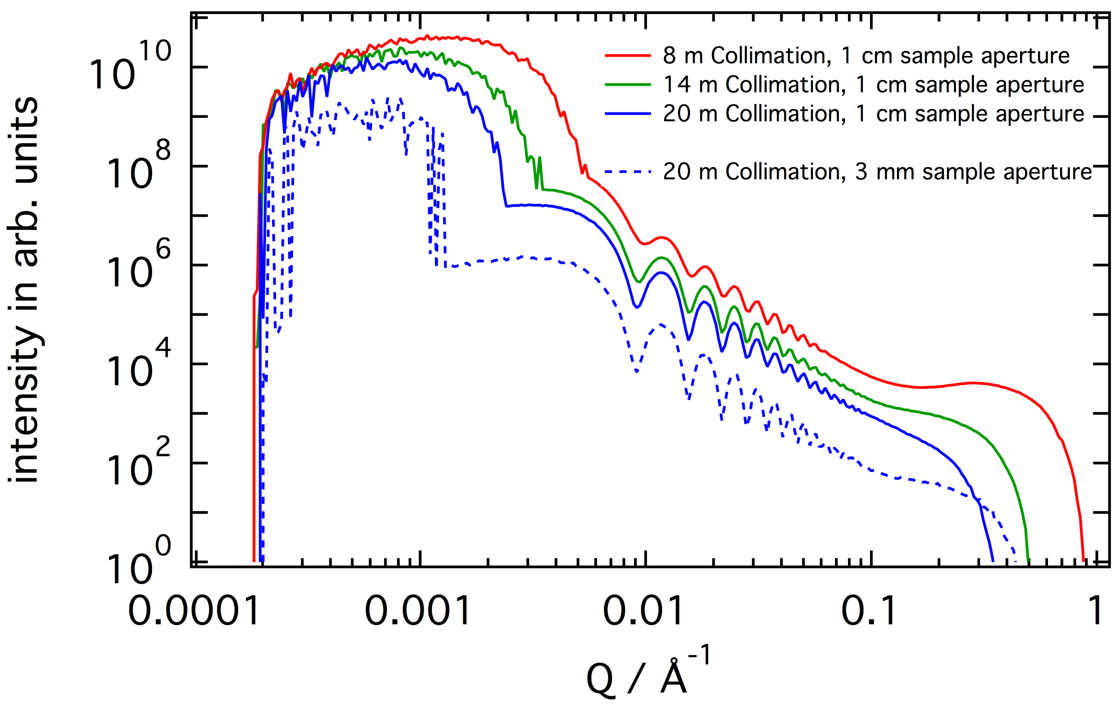

Figure 11. McStas simulation of 50 nm suspended particles in D_2O.

5.2.3 Hard Matter Experiments

Hard matter experiments cover a much wider parameter range than most soft matter experiments, however they more often do not require a container for liquid samples. Usual examples are measurements of transitions between super conduction phases at a few 10 K or transitions between different metal/alloy lattices at temperatures of 700 K and above. Additionally to that, often strong magnet fields or high pressures are required for the experiment.

The data collection process in itself is similar to the one used for soft matter experiments. After the preparatory measurements, the sample is put into the sample holder and the experiment is performed as described above. Also the general process of data reduction and data analysis is similar, albeit that other model functions have to be used, which are adapted to the physical parameters of the sample.

5.2.4 Engineering Experiments

Although SKADI is not a dedicated engineering instrument, some questions in engineering can also be investigated by SANS and the huge sample area for custom made sample environments offer themselves for engineering sample environments, such as heavy load rigs or heating furnaces.

In general these experiments will have a lot in common with the hard matter experiments. For this user group more support during the data evaluation might be needed in order to gain the most of the collected data.

5.3 Maintenance Concepts

5.3.1 Levels of Maintenance

Within the ESS there are three defines levels of maintenance [ESS-0003640]:

- Organizational maintenance: Maintenance performed on site where the element is normally being operated.
- Intermediate maintenance: Maintenance performed on site at a dedicated workshop
- Supplier Maintenance: Maintenance performed off-site at the supplier. This supplier may also be an in-Kind partner

5.3.2 Maintenance Categories

Maintenance can either be corrective or preventive. By using condition based monitoring we aim to keep preventive maintenance during scheduled shutdown periods of the ESS in order to keep the production phases available for experiments on the instrument as the main mode of maintenance. Corrective maintenance may server to either correct an error which occurred during the operation or be used to maximize reliability and availability of SKADI.

Preventive maintenance is part of scheduled maintenance which also includes maintenance work to be conducted on components where condition based monitoring is not feasible. This may however also include maintenance on parts that cannot be reached under production conditions of the ESS, in order to maximize their availability, such as components in the bunker. The specific schedule will be subject both to component reliability and severity of errors on SKADI as well as coordination with other instruments on use of limited resources during shutdown times.

During scheduled maintenance access to components that are placed within the common shielding bunker is limited by a cooling down period. After the cooling down period the components can be handled safely from a radiological perspective.

Some components, such as detectors, can be maintained without being removed from their operational environment, whereas other components, such as choppers have to be removed from their surrounding shielding in order to be accessible for maintenance. This removal usually requires also the removal of the shielding itself, which can be very heavy and thus require the use of the hall crane or a local crane. The time necessary for this is in itself often a major part of the time needed for the complete maintenance, particularly in the case of the common bunker shielding which is additionally subject to a cooling down policy after the proton beam has been switched off. The removed shielding components will have to be stored inside the guide hall, which also makes storage space a limited resource, that has to be coordinated between the instruments. After maintenance and reassembly of the shielding operational safety has to be verified again, e.g. by an interlock procedure.

Removal of components for maintenance off site is both limited by restrictions of the time needed and available for maintenance as well as radiological safety.

Some components will require more frequent maintenance, for instance constantly moving parts such as choppers and vacuum pumps. The maintenance schedule will be developed to ensure a minimal need for unscheduled maintenance (see paragraph below) and consequent loss of user beam time. As the lead-time for maintenance varies strongly depending on the position of the component, the components in less easily accessible locations have less frequent maintenance.

Corrective maintenance will mainly apply when an event happens forcing maintenance to be done unscheduled. This occurs when either a component failure or detection of an issue that requires immediate action arise during user operation. The instrument will have to stop user operations for the duration of repairs or maintenance. The unscheduled maintenance of components that are not accessible when the proton beam is on target will have to wait for the next facility shutdown, which may cause significant loss of beam time. To minimize this type of maintenance a great deal of consideration needs to go into the design of each piece of equipment of the instrument to facilitate for swift and safe corrective measures to be made, to the greatest extent possible. Most notable here is to keep as few components that might require maintenance in those areas.

5.3.3 Maintenance Philosophy

The maintenance philosophy of SKADI aims to utilize condition based monitoring in order to have scheduled, preventive, maintenance be the norm, and unscheduled corrective maintenance be the exception. In order to achieve that goal, survey and accessibility are two key features in design considerations of any component.

Access to components inside the common shielding bunker will as a rule be from the top through the roof of the bunker. There also specially designed remote handling tools will be needed in order to safely perform a maintenance. Outside the bunker the components that do not have to be removed from their operational environment will be accessible when the shielding is removed, where parts of the shielding will be used to facilitate access, e.g. as walking gangways.

6. CONSEQUENCES OF THE CONCEPTS

6.1 General Design Considerations

6.1.1 Upgrade Options

Possible upgrade options identified during the development of SKADI shall be considered and catered for if possible.

6.1.2 Robust Design

The general design goal of SKADI was to minimize the complexity of the overall system while maintaining full scientific and operational capability. The major design decisions towards that end were to avoid any active components within the bunker (anything in need of electronic control or movement by a motor) as well as using the same chopper concept as several other instruments in order to facilitate maintenance and spare part handling.

Due to the harsh environment along the beamline, in particular inside the target monolith and the common shielding bunker area, design solutions have to be as robust as possible to minimize unscheduled downtime of SKADI. Robust should be regarded in terms of minimizing the number of components and moving parts, increasing structural strength and having predetermined failure stages. This failure stages will allow for an operation with decreased performance after the failure of the corresponding component. These considerations include

- Optics in the extraction system. Here especially the front part, close to the moderator will be subject to heavy beam damage that not only may degrade high m coating but will also prevent easy handling during maintenance.
- Shutter systems
- Neutron guides and their alignment
- Chopper design solutions

Any additional measures to increase the robustness of SKADI, that present themselves during the design will be taken into account.

6.2 Coordination with Other Systems

Close monitoring and continuous coordination with the following interfacing systems is critical:

- Neighbouring beamlines - especially inside the first 15 m, i.e. monolith and common shielding bunker where crosstalk might occur. Any compromises there could potentially affect the performance of SKADI negatively. This should be kept in mind and possible mitigation scenarios have to be developed. Outside the bunker mainly spatial restrictions are of concern. This especially involves close collaboration with ESTIA.
- Target monolith insert – alignment with the S-Bender of the neutron extraction system.
- Shutter systems – alignment and repeatability of alignment together with surrounding components
- Systems inside the bunker – to prevent unintended downtimes in an area that is often not accessible for extended periods of time.

This coordination also includes, but it not limited to the coordination with other instruments all over the ESS concerning common solutions for

- Sample Environment: Here already the development of a common sample environment setup for fast change is in full progress
- Choppers: A similar chopper system to Loki is planned. The use of SKF spindles is foreseen for a wide range of instruments and the SKADI team is participating in the effort to develop such a solution.
- Detector: The SoNDe project, in which the SKADI team is heavily involved, is providing a detector technology that is usable also for other instruments.
- ICS: The SKADI team is coordinating with the Loki team in order to have a close resemblance in their control systems in order to facilitate maintenance.
- DMSC: An effort with all instruments employing small angle scattering is made to have both a commonly readable data format as well as a data evaluation software that is meeting the requirements of the user community. To that end, together with the Loki team, a workshop is already planned to coordinate for future development efforts.

6.3 Training of personnel

The organization for the operational phase of the ESS is not yet determined. The team will need to comprise at least one instrument scientist experienced in soft-matter experiments and one with experience in hard matter experience. Both scientists should retain a research profile and dedicate time to scientific research of their own in order to better understand the needs of the user community at present and also those that may arise in the future. They should be augmented by Postdoc-level researchers engaging both in method development and participating in user support. Here also PhD students may be a sensible addition to the team, which makes involvement of the instrument scientist with universities desirable.

The technical support of the instrument will include mechanical, electrical, software and other instrument specific engineer and technician personnel. Here it is desirable that one technician is part of the instrument team, in order to always have a technician familiar with the specific instrument.

The users arriving at SKADI to perform experiments will be supported by a local contact, such as one of the instrument scientists. More experienced users should be able to operate the instrument independently after a short introduction by the local contact. Less experienced users will require more constant support. This should be taken into account for feasibility checks of the proposed experiments.