LoKI Small Angle Neutron Scattering Instrument (LoKI) System Requirement Document

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1. INTRODUCTION

1.1 Purpose of the document

This document describes the functional requirements for the subsystems of the LoKI Small Angle Scattering Instrument (LoKI) and defines a functional baseline as outlined in the ESS Systems Engineering Management Plan and the underlying ISO/IEC 15288:2008 standard. The requirements are based on the high level scientific requirements derived from the scientific case of the instrument as outlined in the instrument proposal as well as the Concept of Operations (ConOps) document that describes the expected operational use of the instrument. The subsystem requirements in this document are based on the conceptual design presented in the instrument proposal.

1.2 Definitions, acronyms and abbreviations

Each requirement is expressed as a natural language statement following the ESS Requirement Development Guidelines as well as 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 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 LoKI work package scope. Any design or technical solution must not preclude these requirements to be fulfilled without significant rework.

Abbreviation	Explanation of abbreviation
SANS	Small Angle Neutron Scattering
PBS	Product breakdown structure
BTS	Beam transport and conditioning system
SES	Sample exposure system
SCS	Scattering characterisation system
STAP	Scientific and technical advisory panel
SPL	Scientific project leader
LE	Lead engineer
CIPE	Chief instrument project engineer
CIPS	Chief instrument project scientist
NSS	Neutron scattering systems
PM	Project manager
DS	Director for Science
DH	Division Head
GL	Group leader
CLI	Command line interface
GUI	Graphical user interface

1.3 References

1. Systems Engineering Management Plan
2. LOKI Instrument proposal
3. LOKI Concept of Operations document
4. ESS Requirement Development Guidelines
5. NASA Systems Engineering Handbook, Washington, DC, USA: National Aeronautics and Space Administration (NASA). NASA/SP-2007-6105

2. SYSTEM CHARACTERISTICS

2.1 System purpose

The instrument allows the collection of SANS data from a wide variety of samples. See LOKI Concept of Operations document and LOKI instrument proposal as well as references therein for more details.

2.2 System overview

The instrument 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 instrument includes the structures that house and support these subsystems and the software to control the instrument and process the data as described in the instrument product breakdown structure (PBS).

3. SYSTEM STAKEHOLDERS

Group ID	Stakeholder Group	Individual ID	Stakeholder	Surrogate
SH-1	User community	SH-1	Existing users of small angle neutron scattering	STAP
SH-2	ESS	SH-2.1	Instrument core team	SPL (Andrew Jackson) LE (Clara Lopez)
SH-2	ESS	SH-2.2	Instrument construction subproject	CIPE (Robert Connatser) CIPS (Ken

Group ID	Stakeholder Group	Individual ID	Stakeholder	Surrogate
				Andersen)
SH-2	ESS	SH-1.3	Neutron scattering systems project	NSS PM (Oliver Kirstein)
SH-2	ESS	SH-2.4	Science Directorate	DS (Dimitri Argyriou)
SH-2	ESS	SH-2.5	Neutron Optics Group	GL (Phillip Bentley)
SH-2	ESS	SH-1.6	Neutron Chopper Group	GL (Iain Sutton)
SH-2	ESS	SH-2.7	Detector Group	GL (Richard Hall-Wilton)
SH-2	ESS	SH-2.8	Electrical Engineering Group	GL (Thomas Gahl)
SH-2	ESS	SH-2.9	Data Management and Software Centre	DH (Mark Hagen)

4. SYSTEM REQUIREMENTS

High-level scientific requirements for the instrument (13.6.3)

1. The instrument shall allow data to be collected to a Q_{min} of < 0.001 $Å^{-1}$.
2. The instrument shall allow data to be collected to a Q_{max} of > 1 $Å^{-1}$.
3. The instrument shall allow data to be collected simultaneously over a continuous Q range with Q_{max}/Q_{min} > 1000.
4. The instrument shall match the size of the neutron beam to the size of the sample.
5. The instrument should allow the Q resolution (dQ/Q) to be optimised for the experiment.
6. The instrument should be capable of providing a Q resolution < 10% dQ/Q over the whole Q range.
7. The instrument should allow data collection from samples < 9 mm^3 volume
8. The instrument should maximise the signal-to-background (S/B) ratio of the small angle scattering.

General notes

Instrument parameters that are defined as user selectable should be selectable with < 5 min delay (see ConOps).

4.1 Functional Requirements for LOKI subsystems

4.1.1 Beam transport and conditioning system (BTS) (13.6.3.1)

Initial function statement

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

Functional requirements

1. **Bandwidth Selection**
   1.1. The BTS shall transport from the moderator a *beam of neutrons* to the *sample* with a wavelength bandwidth selectable between 0.4 Å and 20 Å.
   1.2. **Rationale**: Selecting the bandwidth determines the measured Q range (see 13.6.3 (3)). Selecting a bandwidth appropriate for the experiment being performed minimises unwanted neutrons and thus contributes to maximising S/B (see 13.6.3 (7))
   1.3. **Verification**: Measurement of the neutron spectrum at the sample
2. **Wavelength Selection**
   2.1. The BTS shall transport from the moderator to the sample a beam of neutrons of a given bandwidth (see 13.6.3.1 (1)) with wavelengths that lie in the range 1.8 Å to 22.0 Å.
   2.2. **Rationale**: The selection of wavelength determines the Q range that is accessible (see 13.6.3 (1-3))
   2.3. **Verification**: Measurement of the neutron spectrum at sample
3. **Beam size**
   3.1. The BTS shall transport from the moderator to the sample a beam of neutrons with maximum size (full width) of 20 ± 0.1 mm and minimum size of 3 ± 0.05 mm.
   3.2. **Rationale**: Matching the beam size to the sample size maximises the S/B (see 13.6.3 (4,6,7))
   3.3. **Verification**: Measurement of the beam intensity profile at sample
4. **Beam divergence**
   4.1. The BTS shall transport from the moderator to the sample a beam of neutrons with maximum *divergence* of ±0.6° and minimum *divergence* of ±0.02°.
   4.2. **Rationale**: Varying the divergence allows the resolution to be optimised and contributes to maximising the S/B by not delivering unwanted neutrons. (see 13.6.3 (4,5,8))
   4.3. **Verification**: Measurement of the beam divergence at sample
5. **Beam size selection**
   5.1. The BTS shall transport from the moderator to the sample a beam of neutrons with a *selectable* size.
   5.2. **Rationale**: Matching the beam size to the sample size maximises the S/B (see 13.6.3 (4,7,8))
   5.3. **Verification**: Measurement of the *beam intensity profile* at sample
6. **Beam divergence selection**
   6.1. The BTS shall transport from the moderator to the sample a beam of neutrons with a selectable divergence.

6.2. **Rationale**: Matching the beam divergence to the experiment optimised the resolution and maximises S/B (see 13.6.3 (4,5,8))
6.3. **Verification**: Measurement of the beam divergence at sample

7. **Line-of-sight avoidance**
   7.1. When the experimental cave is not *interlocked* the BTS shall block radiation from the target to a level required by safety regulations.
   7.2. **Rationale**: The user must be able to change a sample (see ConOps)
   7.3. **Verification**: Measurement of the dose rate in the experimental cave
8. **Brilliance transfer**
   8.1. The BTS should transport from the moderator to the sample a beam of neutrons with 100% *brilliance transfer* within the selected wavelength and divergence range.
   8.2. **Rationale**: The more neutrons are incident on the sample the higher the signal (see 13.6.3 (8))
   8.3. **Verification**: Measurement of the flux at sample vs. flux at moderator surface
9. **Intensity profile**
   9.1. The BTS should transport from the moderator to the sample a beam of neutrons with a uniform, smooth intensity and the same spectrum over the sample area.
   9.2. **Rationale**: The sample needs to be evenly illuminated with the same spectrum of neutrons in order to ensure that the scattering can be correctly normalised.
   9.3. **Verification**: Measurement of the beam intensity profile at the sample.
10. **Divergence profile**
    10.1. The BTS should transport from the moderator to the sample a beam of neutrons with a smooth divergence profile.
    10.2. **Rationale**: The beam divergence profile is convoluted with the scattering pattern and a smooth profile is needed for correct normalisation of the scattering data.
    10.3. **Verification**: Measurement of the beam divergence profile at sample
11. **Wavelength rejection**
    11.1. The BTS shall transport from the moderator to the sample a beam of neutrons where the total *brilliance* outside the selected wavelength band is <1%
    11.2. **Rationale**: The neutrons outside the used wavelength band add to the background (see 13.6.3 (8))
    11.3. **Verification**: Measurement of the neutron spectrum at sample
12. **Accessibility**
    12.1. The BTS should be accessible for repairs while the *proton beam is on target*.
    12.2. **Rationale**: The instrument will be more fault tolerant hence increasing throughput of experiments (see ConOps)
    12.3. **Verification**: Measurement of the dose rate at the relevant technical component

4.1.2 Sample exposure system (SES) (13.6.3.2)

Initial function statement

The sample exposure system positions one of a number of samples in a beam of neutrons and controls the physical and chemical environment of the sample as dictated by the needs of the experiment.

Functional requirements

1. **Horizontal and Vertical Positioning**
   1.1. The SES shall position the sample in the beam of neutrons with an accuracy of +/- 0.1mm and a precision of +/- 0.05 mm
   1.2. **Rationale**: The sample needs to be in the beam of neutrons and correctly illuminated (see ConOps).

- 1.3. **Verification**: Test.

2. **Rotational Positioning**
   - 2.1. The SES shall position the sample in the beam of neutrons with an accuracy of +/- 0.1 degrees and a precision of +/- 0.05 degrees
   - 2.2. **Rationale**: The sample orientation must be controlled and known (ConOps).
   - 2.3. **Verification**: Test
3. **Sample Environment Equipment**
   - 3.1. The SES shall permit the installation and positioning of sample environment equipment <= 1m diameter and <= 2000kg mass
   - 3.2. **Rationale**: The experiment may require equipment to control the physical and chemical environment of samples (see ConOps).
   - 3.3. **Verification**: Test.
4. **Automatic sample changing**
   - 4.1. The SES should be able to change the sample automatically without physical user intervention.
   - 4.2. **Rationale**: Automated sample changing is required in order to optimise the use of the available beamtime. (see ConOps).
   - 4.3. **Verification**: Test

4.1.3 Scattering characterisation system (SCS) (13.6.3.3)

Initial function statement

The scattering characterisation system detects the neutrons scattered by the sample to produce meaningful experimental data.

Functional requirements

1. **Detection efficiency**
   - 1.1. The SCS shall detect the scattered neutrons with an *efficiency* >30% across the wavelength band
   - 1.2. **Rationale**: Neutron detection efficiency must be equivalent to current state-of-the-art technology (see ConOps).
   - 1.3. **Verification**: Measurement of detection efficiency.
2. **Angular resolution**
   - 2.1. The SCS shall detect the scattered neutrons with a *polar angular resolution* $d\theta/\theta < 10\%$ and an *azimuthal angular resolution* of < 5 degrees
   - 2.2. **Rationale**: The angular resolution contributes to the Q resolution and hence the precision with which the sample structure can be measured. (see 13.6.3. (6) and ConOps).
   - 2.3. **Verification**: Measurement (TBD).
3. **TOF resolution**
   - 3.1. The SCS shall detect the scattered neutrons with a *time-of-flight resolution* < 0.1 ms
   - 3.2. **Rationale**: The time-of-flight resolution should be less than 10% of the intrinsic pulse length (see 13.6.3.1 (5,6) and ConOps).
   - 3.3. **Verification**: Measurement (TBD).
4. **Neutron selectivity**
   - 4.1. The SCS should detect radiation incident to the detector system other than cold or thermal neutrons with a 0% efficiency
   - 4.2. **Rationale**: Non-neutron originated detector signals (*e.g.* gamma-rays) contribute to background and should be minimised (see 13.6.3 (8))
   - 4.3. **Verification**: Measurement of detection efficiency for gamma-rays.
5. **Accessible solid angle**
   - 5.1. The SCS shall be able to detect neutrons scattered by the sample within a polar angular range of ± 45 degrees and an azimuthal angular range of ± 180 degrees.

5.2. **Rationale**: Reach high Q and measure full scattering circle (see 13.6.3 (2) and ConOps).
5.3. **Verification**: Test.

6. **Detector positioning**
   6.1. The SCS shall position the detectors with an accuracy and precision of 1mm.
   6.2. **Rationale**: The position of the detectors needs to me known to accurately calculate Q (see 13.6.3.3(1-3) and ConOps)
   6.3. **Verification**: Survey and measurement.
7. **Detector noise**
   7.1. The SCS should record < 0.001 counts/s/cm^2 in the absence of incoming radiation.
   7.2. **Rationale**: The lower the background the higher the achievable S/B ratio, but the detector noise level must be lower than the background, otherwise the detector noise becomes limiting (see 13.6.3. (8)).
   7.3. **Verification**: Measurement with shutter closed

4.1.4 Experimental cave (13.6.3.5)

Initial function statement

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 system from external radiation.

Functional requirements

1. **Mounting components**
   1.1. The experimental cave 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.
   1.3. **Verification**: Metrology and acceleration measurement
2. **Utilities**
   2.1. The experimental cave shall provide the required utilities to the elements of the BTS, SES and SCS that are within it
   2.2. **Rationale**: The technical components need utilities (power, cooling vacuum, etc.).
   2.3. **Verification**: Test
3. **Access**
   3.1. The experimental cave shall allow personnel access when the proton beam is on target
   3.2. **Rationale**: Access for sample changes, maintenance, repairs or adjustments is necessary.
   1.1. **Verification**: Test
2. **Biological shielding**
   2.1. The experimental cave shall shield its surroundings against the radiation produced by the neutron beam to safe levels according to ESS radiation safety regulations.
   2.2. **Rationale**: The surroundings of the instrument must be safe for personnel
   2.3. **Verification**: Dose rate measurement
3. **Sample environment footprint**
   3.1. The experimental cave should allow the mounting of sample environment devices <= 1 m in diameter and <= 2000 kg in weight.
   3.2. **Rationale**: The experiments may require bulky sample environments (see ConOps)
   3.3. **Verification**: Test
4. **Detector shielding**
   4.1. The experimental cave should shield the detectors from radiation to <0.001 counts/s/cm^2.

4.2. **Rationale**: The lower the background the higher the achievable S/B ratio (see 13.6.3. (8))
4.3. **Verification**: Measurement with shutter closed

4.1.5 Control hutch (13.6.3.6)

Initial function statement

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.

Functional requirements

1. **Instrument control terminal**
   1.1. The control hutch shall allow the user to remote control the technical components from a single dedicated computer terminal
   1.2. **Rationale**: The instrument control should be possible from one terminal
   1.3. **Verification**: Test
2. **Data reduction terminal**
   2.1. The control hutch shall allow the user to process the neutron data to an indexed list of scaled reflections at a single dedicated computer terminal (see ConOps)
   2.2. **Rationale**: Data reduction must be possible from one terminal during the experiment in order to verify data quality.
   2.3. **Verification**: Test
3. **Working space**
   3.1. The control hutch shall have sufficient working space for a four person user team
   3.2. **Rationale**: A user team typically consists of 1-4 people (see ConOps).
   3.3. **Verification**: User feedback
4. **Comfort**
   4.1. The control hutch should be a comfortable working environment for the users
   4.2. **Rationale**: Users work long hours and a comfortable environment reduces fatigue and increases productivity.
   4.3. **Verification**: User feedback
5. **Access to instrument**
   5.1. The control hutch should be located <15 m from the experimental cave door
   5.2. **Rationale**: Users need to mount and change samples during their experiment and hence need easy access. (see ConOps)
   5.3. **Verification**: Test

4.1.6 Hall Two Infrastructure (13.6.3.8)

Initial function statement

Hall two infrastructure includes all the shielding, infrastructure and support systems for the BTS elements within hall two.

Functional requirements

1. **Mounting components**
   1.1. The hall two shall allow the mounting of technical components of the BTS with the required *precision* and stability
   1.2. **Rationale**: The technical components have to be physically mounted on a suitable support.
   1.3. **Verification**: Metrology and acceleration measurement
2. **Utilities**
   2.1. The hall two shall provide the required utilities to the elements of the BTS that are within it

2.2. **Rationale**: The technical components need utilities (power, cooling vacuum, etc.).
2.3. **Verification**: Test

3. **Access**
   3.1. The hall two should allow access to personnel when the proton beam is on target
   3.2. **Rationale**: Access for maintenance, repairs or adjustments is necessary.
   3.3. **Verification**: Test
4. **Biological shielding**
   4.1. The hall two shall shield its surroundings against the radiation produced by the neutron beam to safe levels according to ESS radiation safety regulations.
   4.2. **Rationale**: The surroundings of the instrument must be safe for personnel
   4.3. **Verification**: Dose rate measurement

4.1.7 Integrated control and monitoring system (13.6.3.12)

Initial function statement

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.

Functional requirements

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 graphical user interface makes instrument control fast and easy (see ConOps).
   1.3. **Verification**: Test
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 (CLI)
   2.2. **Rationale**: A good a scriptable command line interface allows for flexibility for more experienced users and ESS staff (see ConOps).
   2.3. **Verification**: Test
3. **Scattering pattern visualisation**
   3.1. The integrated control and monitoring system shall allow the user to visualise the scattered neutron intensity as a function of detector coordinates and time-of-flight with user selectable binning.
   3.2. **Rationale**: Assessing the data for anomalies as it is collected allows the user to more efficiently perform experiments. (see ConOps).
   3.3. **Verification**: Test
4. **Data processing GUI**
   4.1. The Integrated control and monitoring system shall allow the user to process the recorded data through a graphical user interface to corrected intensities as a function of momentum transfer.
   4.2. **Rationale**: A good graphical user interface makes data processing fast and easy (see ConOps).
   4.3. **Verification**: Test
5. **Data processing CLI**
   5.1. The Integrated control and monitoring system shall allow the user to process the recorded data through a scriptable command line interface to corrected intensities as a function of momentum transfer.
   5.2. **Rationale**: A good a scriptable command line interface allows for flexibility for more experienced users and ESS staff (see ConOps).
   5.3. **Verification**: Test
6. **Hazard detection**

6.1. The Integrated control and monitoring system shall detect hazards that may compromise safety for personnel or equipment
6.2. **Rationale**: Detection of hazards such as fire, radiation, flooding or asphyxiating gasses can prevent injury to personnel or damage to equipment.
6.3. **Verification**: Test

DOCUMENT REVISION HISTORY

Version	Reason for revision	Date
1.0	New Document	2014-09-08