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Concepts of Operations for the T-REX Instrument

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TABLE OF CONTENT	PAGE
1. INTRODUCTION.....	4
2. HIGH LEVEL SCIENTIFIC REQUIREMENTS.....	4
3. SYSTEM CHARACTERISTICS	8
3.1 System purpose.....	8
3.2 High Level System Requirements.....	8
3.3 System Life-Cycle.....	10
3.4 System overview.....	11
3.4.1 Functional building blocks.....	11
3.4.2 Neutron Optics Systems.....	12
3.4.3 Shielding.....	13
3.4.4 Choppers	14
3.4.4.1 Bandwidth chopper subsystem.....	14
3.4.4.2 Resolution defining chopper subsystem	14
3.4.4.3 T0 chopper	15
3.4.4.4 Fan chopper.....	15
3.4.5 Shutters.....	15
3.4.6 Experimental cave	15
3.4.7 Detectors	16
3.4.8 Beam Stop.....	17
3.4.9 Personnel Safety System, PSS	17
3.4.10 Control Hutch.....	17
3.4.11 Future upgrade possibilities.....	17
3.4.12 Key System Interfaces	18
4. SYSTEM STAKEHOLDERS.....	20
5. OPERATIONAL CONCEPTS.....	23
5.1 Operational environment.....	23
5.2 Operational scenarios.....	23
5.2.1 Samples.....	24
5.2.2 Sample geometry and exposure system.....	24
5.2.3 Sample preparation	24
5.2.4 Instrument configuration	25
5.2.5 Measurements.....	25
5.2.6 Data visualization and Data Analysis.....	25
5.3 Maintenance Concepts	26
5.3.1 Levels and categories of maintenance	26
5.3.3 Maintenance philosophy.....	27
6. CONSEQUENCES OF THE CONCEPTS	29
6.1 Upgrade options.....	29
6.2 Robust design.....	29

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

6.3 Training of personnel	29
GLOSSARY	30
REFERENCES	30
DOCUMENT REVISION HISTORY	31

LIST OF TABLES

Table 1 An overview of stakeholders interactions	22
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LIST OF FIGURES

Figure 1 Proposed life-cycle of T-REX	11
Figure 2 Sketch of T-REX showing the major functional building blocks.	12
Figure 3 Context diagram shows group of stakeholders and their high-level interactions.....	20

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

1. INTRODUCTION

The purpose of this Concepts of Operations, ConOps, is to provide a brief description of T-REX, Time of Flight Reciprocal Space Explorer, including both a high level introduction to its science case, as well as providing the framework and context within which the instrument will be designed, operated and maintained through its life-cycle.

The intended audience for this document includes everyone involved in the construction and operation of T-REX, i.e. all central stakeholders. It will also serve the function as a quick overview of the instrument's purpose, construction and operation for persons familiar with the field of neutron science, and spectroscopy in particular, and those who are not.

2. HIGH LEVEL SCIENTIFIC REQUIREMENTS

The high level scientific requirements for T-REX are derived from the science case presented in the instrument proposal and represent the expectation of the wide user community for spectroscopy at the ESS. Based on these requirements, a number of core capabilities shall be delivered to users in the early days of operation, as best as reasonably achievable within the time and budgetary boundaries. On the other hand, advanced features of T-REX should be considered as part of the instrument design from the earliest stage, to ensure that the instrument will implement these features successfully and to guarantee a continuous broadening of the instrument scope through the entire life-cycle.

Here we list the expected core and advanced features of T-REX.

I. Spectroscopy for a broad user community

T-REX will be the ESS spectrometer to measure wide energy transfer with good wave vector resolution and to provide Polarization Analysis (PA) over the energy transfer range from 20 μeV to 140 meV. The instrument will support different operational modes and configurations to match the expected flexibility and versatility requested by the wide user community. Measurements will be supported in two modes, using polarized and non-polarized neutrons. In particular, **polarized neutrons** will enable the separation of the magnetic spectra from nuclear scattering, the analysis of polarization and eigenvectors of magnetic excitations and permit the separation of coherent and nuclear spin incoherent scattering, which is of particular importance for hydrogen containing samples in energy research, soft matter and life sciences. Spectroscopy using non-polarized neutrons in the wide dynamical range offered by T-REX will enable the investigation of coherent excitations, spin correlations and fluctuations, relaxations and diffusion processes in a broad range of samples and applications.

The instrument can be configured in a versatile fashion. By choosing the choppers frequencies the users can match the requested energy resolution, thanks to the flexible pulse shaping of the long ESS pulse and the use of both the moderators. In particular, the illumination of the sample with a polychromatic beam allows the optimization of a narrow relative energy transfer range for an individual pulse, but still covering a wide energy transfer range with optimized conditions by all pulses from a band. This optimization is crucial for the study of large energy transfer to the sample. By choosing the beam collimation

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

at the sample the Q-resolution can be tailored to the needs, and the proper back-ground condition at the lowest detection angles can be achieved to perform clean measurements.

In view of various user communities, the sample area shall be spacious and capable to host various sample environment equipment, enabling high/low temperature, control of pressure, installation of magnetic/electric field. More complex studies, e.g. in-operando studies or levitation experiments request an easy access to the sample area, also from the side, and the application of auxiliary characterization tools in parallel to the scattering experiment.

II. Quantum phenomena

Studies of excitations in quantum condensed matter request to explore the energy range from several tenth of μeV , for the determination of small energy gaps, to several hundreds of meV, for studies of e.g. excitations in the parent compounds of high T_c superconductors or excitations into the Stoner continuum.

The most stringent information about the excitation spectrum comes from studies on single crystals, which usually have only limited size and mass in the order of a few hundred of mm^3 or mg. Typical samples are low dimensional, topological and frustrated materials, quantum magnets, high temperature superconductors, multi-functional oxides, molecular magnets. Most of the investigations not amenable today because of flux limitations will be within reach thanks to the tuneable time structure combined with the outstanding brightness of ESS that allows tailoring the resolution of time-of-flight spectroscopy. Often the line shape of a specific excitation provides the information about the microscopic interactions requesting a high resolution at the specific energy and wave vector transfer. To explore the reciprocal space continuously the sample will be rotated and the scattered neutrons will be detected position sensitively. The state of the sample will be controlled with various sample environment equipment. In particular, to study quantum phase transitions, it is requested to control the temperature reaching the mK range and beyond 1000K, it should be possible to apply magnetic fields up to 10 T, and pressure up to several 10 GPa.

The asset of PA is manifold: it distinguishes different cross sections in the typically rich spectra of complex compounds and provides as such the most solid test of theory. In particular, for heterogeneous systems like magnetic thin films one may suppress the sample inherent background from a non-magnetic substrate, which dominates the scattering. Another example comes from new multiferroics with a strong magneto-electric coupling: here either chiral magnetic structures or magnetostriction cause multiferroicity. Their fingerprints in the excitation spectra can be identified uniquely by PA.

III. Functional Materials

One of the strongest scientific missions of T-REX constitutes in the study of functional materials, including catalysis metals, ion-transport materials, fuel cell membranes, nanomaterials (such as nanoporous or metal-organic frameworks for hydrogen storage, nanomembranes for filtration), thermo-electric and magneto-caloric materials, which all promise potential societal applications in fields such as new and sustainable energies, energy harvesting, environmental pollution, water purification. Many of the above systems present a characteristic coupling mechanism between phonon dynamics and spin waves (e.g. magneto-calorics), or between phonon dynamics and ion diffusion (e.g. ion-transport materials), which determine and govern the promising functional capabilities of these materials. The study of

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

such coupling mechanisms requires, for instance, the measurement and separation of phonon and spin excitations, for which both PA and high incident energies are simultaneously necessary. Or again, it requires simultaneous access to the relatively high energies of phonons and the high energy resolution for the quasielastic signal of diffusion processes. In addition, the latter often take place in non-trivial spatial geometries, determined by the complex atomic structure of ion conductors, which therefore require also a wide Q -range. The example of hydrogen storage materials needs thermal incident energies to access the quantum rotational peak of the H_2 molecule at low temperatures, which is the best spectral signature to get information about number, strength and nature of the hydrogen binding sites. At the same time, most of the information lies in the detailed lineshape and Q -dependence of the rotational peak, which requires both very good energy resolution and wide Q -range. As a last example, *in-operando* studies of prototype membranes, for fuel cells or nanofiltration, are nowadays severely limited by the reduced volumes of the working devices that can be reasonably exposed to the neutron beam. Such studies will strongly benefit from the increased and concentrated beam fluxes expected on T-REX. As a whole, the science case for functional materials provides a typical example of scientific fields that strongly need the wide capabilities of T-REX simultaneously, combining its large dynamical range with very good energy Q - E resolution and polarization analysis.

IV. Soft-matter and Life Sciences

The use of neutron spectroscopy for studying soft matter and life sciences has steadily increased in the last decades and is nowadays rather widespread. The number of such systems that are or can be studied with neutrons is huge, ranging from natural and artificial polymers to proteins, nucleic acids and lipid membranes; from gels of all kinds to complex biological molecules like chromatin in the cell nucleus or entire living cells. More recently new smart and functionalized artificial polymers have been engineered to mimic the functional behaviour of real proteins, such as haemoglobin, at similar physiological conditions, which has further approached the two fields of soft matter and life sciences, and has enriched the scenario of fancy samples on neutron beam lines. In all such “functional” systems, be them artificial or natural, it is clear nowadays that biological functionality is governed by ps and ns dynamics, where low-energy single-particle diffusional and relaxational motions and higher-energy collective modes play equally important roles and often are even entangled to each other. Consequently, such scientific fields obviously need the very wide dynamical range of T-REX, capable of measuring both quasielastic and inelastic scattering, independently of the specific kind of sample under investigation. In addition to these obvious needs, very recent frontier experimental results have shown more challenging requests. Newly emerging results are showing that functional vibrational motions have often an anisotropic character. To deeply understand the mechanism that connects thermal vibrations to function, it is necessary to study oriented single-crystal samples. Those are very rare in soft matter and very small. Measurements on such samples are already at hand for other laboratory techniques (such as anisotropic light spectroscopies), but intrinsically those techniques cannot provide the richness of details that neutrons can achieve with a full 4D-mapping of the $S(\mathbf{Q},\omega)$. This is nowadays limited by the small size of the available crystals and the relatively low neutron beam intensity. The significant flux-gain factors of T-REX,

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

combined with the full mapping capability of its PSD detector, will mark a remarkable step forward for this branch of science. Finally, the availability of PA will be of great advantage for studying soft matter and life science samples, where hydrogen atoms are ubiquitous and abundant, as it will provide a clean way to separate coherent and incoherent scattering.

Correspondingly the high level scientific requirements are:

1. The instrument shall allow data to be collected to minimum energy transfer of 20 μeV .
2. The instrument shall allow data to be collected to maximum energy transfer of 140 meV.
3. The instrument shall allow data to be collected to minimum wavevector transfer of 0.05 \AA^{-1} .
4. The instrument shall allow data to be collected to maximum wavevector transfer of 10 \AA^{-1} .
5. The instrument shall match the size of the neutron beam to the size of the sample, assuring the homogenous illumination of rotating samples.
6. The instrument shall allow data to be collected to minimum scattering angle of 1° .
7. The instrument shall allow the analysis of neutron spin polarization.
8. The instrument shall allow the energy resolution to be optimized for the experiment.
9. The instrument should allow the Q resolution to be optimized for the experiment.
10. The instrument should be capable of providing elastic energy resolution of 1% at incident energy of 2 meV.
11. The instrument should be capable of providing energy resolution of 3% for an energy transfer of 100 meV.
12. The instrument should be capable of providing a Q resolution in elastic scattering condition of 0.05 \AA^{-1} at incident energy 80 meV.
13. The instrument should allow data collection from samples $< 10^2 \text{ mm}^3$ volume.
14. The instrument should maximize the signal-to-background (S/B) ratio in the scattering pattern.
15. The instrument shall allow the control of the physical and thermodynamical condition of the sample.
16. The System's design shall provide the space and flexibility necessary to host and drive the staging process to achieve the full scientific scope.
17. T-REX should serve the user, science and instrumental development program without interruptions during source operation.

3. SYSTEM CHARACTERISTICS

3.1 System purpose

Neutron spectroscopy is based on the inelastic scattering of neutrons from condensed matter. The analysis of the scattering pattern can reveal properties, nature and characteristics of collective excitations, spin correlations and fluctuations and, eventually, help understanding their role in quantum phenomena, functionality of materials in energy research, soft-matter and life science. An asset in the inelastic neutron scattering experiments is the determination of the dependence of dynamical properties of materials on external experimental parameters, such as temperature, application of magnetic or electric field and pressure. Thanks to the high brilliance of the ESS and its time structure, these characterizations, nowadays limited by the intensity, will be routinely performed on T-REX. The full scope layout offers its users a variety of configurations and capabilities to study a wide range of scientific questions. Here only a few examples, related to the scientific scope that T-REX should cover, are provided:

- Magnetism research: weak magnetic moments, interplay between magnetic order and superconductivity, quantum criticality, orbital and charge ordering, appearance of novel phases in low dimensional, topological and frustrated materials, electronic correlations and competing degrees of freedom in multifunctional oxides,
- Energy research: catalysis, nanomaterials such as nanoporous or metal-organic frameworks for hydrogen storage, thermo-electrics and magneto-calorics, ion-transport materials, *in-operando* batteries, fuel cell membranes, nanofiltering membranes,
- Soft matter and Life Science: disordered materials and liquids, natural and artificial polymers, functionalized “smart” polymers and gels, proteins, nucleic acids and lipid membranes, large biological complexes (e.g. chromatin), entire living cells.

3.2 High Level System Requirements

Firstly, in order to operate the instrument at the ESS, the safety requirements have to be fulfilled.

In order to achieve the high level scientific requirements, the following high level system requirements have to be met:

1. Studies in magnetism and material science require incident neutron energy up to 160 meV and consequently a neutron optics and guide system that is optimized for wavelengths down to 0.7 Å.
2. Studies in all the fields outlined in the scientific scope request incident neutron energy down to 2 meV to achieve ultimate resolution to perform QENS or to identify small excitation gaps.
3. The instrument should achieve the maximum performance in the so-called thermal band, from 0.7 Å to 2.4 Å, where the brilliance of the thermal moderator is higher than the brilliance of the cold moderator. Therefore, the beam extraction from the thermal moderator shall be undisturbed, the instrument length shall restrict the

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

instrument bandwidth to 1.7 \AA , the sample to detector distance shall be chosen such that pulse suppression is not needed in this wavelength band.

4. To achieve the wide energy band an additional extraction system for polarized cold neutrons shall be installed outside the monolith block. It shall be removable for experiments in the thermal band and shall be fail-safe, so that the instrument can run in case of failure.
5. The design of T-REX aims at reaching a 100 % duty cycle at the detector. The frequency of the MC defines the wavelength step between subsequent illuminating pulses and also the wavelength range of scattered neutrons recorded at the detector and hence the maximum energy loss that can be detected without frame overlap. The reminder of the chopper system shall ensure that the wavelength definition of each illuminating neutron pulse is sufficiently narrow (requirement on the PSC) and that neutrons passing through these chopper subsystems can be uniquely assigned to a source pulse (requirements on the wavelength band choppers).
6. While a high flux on the sample enables faster measurements, an improved signal to noise ratio enables the observation of hitherto undiscovered features. The large distance from the target building should provide an ideal position to achieve the lowest noise levels. Multiple means shall be taken to lower the background level as much as possible: avoiding the direct line-of-sight, evacuating the primary flight path, reducing the number of windows in the guide, moving the last window upstream from the secondary spectrometer, evacuating the entire secondary flight path, achieving low gamma sensitivity and providing sufficient shielding around the detector. Additionally, the provision of one TOC is considered, in order to contribute to suppress the background from the prompt pulse, if operational experience should show that it is necessary.
7. A key feature of T-REX is the use of polarization analysis. The polarizer devices must be able to achieve flipping ratios > 20 for the entire initial wavelength range from 0.7 to 6.5 \AA . XYZ polarization analysis shall be feasible for a wide solid angle range of the detector $> \pi/3$. Materials shall be selected to allow high magnetic fields without magnetizing any component of the scattering characterization system, i.e. the secondary spectrometer.
8. The energy resolution requires that a time uncertainty of $\leq 10 \text{ \mu s}$ is achieved by the critical components, such as monochromating choppers and detectors. We also request that the flight path uncertainty due to the spatial resolution of the detector is $\leq 20 \text{ mm}$, which correspond to 5 \mu s time uncertainty at 1 \AA .
9. To achieve the requested wave vector resolution, the collimation of the neutron beam at the sample shall increase with the neutron wavelength and be $\leq 1^\circ$, therefore the neutron optics shall be capable to achieve these properties.
10. Studies in magnetic and disordered systems need measurements at detection angles down to 1° , which in turn requires to limit the background produced by the direct beam, so that, when requested, the collimation of the neutron beam at the sample shall be reduced to 0.5° through primary beam collimators
11. Direct geometry chopper spectrometers feature the simultaneous detection of all momentum transfers accessible for a certain energy transfer and hence allow the most efficient mapping of reciprocal space within the kinematic borders of the

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

neutron scattering process. Therefore, the widest detector coverage is beneficial to these type of instruments. In particular, full scope of T-REX requires a wide range of scattering angles to access sufficient volume in reciprocal space, when using cold neutrons. The instrument shall therefore be equipped to cover an angle $-36^\circ < \vartheta_h < 144^\circ$ in the horizontal plane and $-25^\circ < \varphi_v < 15^\circ$ in the vertical plane. There shall be only a gap from -1° to 1° horizontally and vertically for the direct beam, to host the beam stop. The asymmetric coverage of the vertical scattering angle aims for a wider coverage of momentum transfer in the vertical direction in particular for single crystal work, while still providing the possibility to integrate large parts of powder rings. The detector in the first day, shall cover horizontal angular range from $1^\circ < \vartheta_h < 70^\circ$. The ratio of the active area of the detector to the total area shall exceed 90% and gaps should be avoided or, if not avoidable, shall not exceed the dimensions of a detector pixel.

12. Typical single crystal specimens have a surface of $5 \times 20 \text{ mm}^2$ or smaller. Exposing them to the beam in an oriented fashion requires a larger beam cross section to ensure a constant illumination also under rotation. Assemblies of co-aligned single crystals and powder samples can benefit from an increased scattering volume, if the flight path uncertainties remain small. The beam cross section at the sample position shall therefore be $10 \text{ mm} \times 30 \text{ mm}$.
Single crystal studies require homogeneous illumination of the sample with a smooth divergence distribution; therefore, we request a variation within 10 % of the beam intensity and a smooth divergence profile at the sample position. The sample shall be rotated whilst keeping it fully illuminated, which require slits and beam masking, for an appropriate beam tailoring. In addition, all means to lower background are important.
13. In situ and levitation experiments will require side access to the sample position.
14. The time and position resolution of the detector provide 3 degrees of freedom to parameterize 2 momentum transfer vector components and the energy transfer. The rotation of the sample enables continuous access to the full $S(\mathbf{Q}, \omega)$. The alignment of the coordinate system set by the detector and the rotation to the sample coordinate system can be achieved by software.

3.3 System Life-Cycle

The figure below shows the proposed life-cycle of T-REX, which consists of engineering design, construction, commissioning, users' operations and upgrades, and decommissioning. At the end of the relevant phases, Toll Gate (TG) reviews are foreseen to validate the progress to the next phase. The instrument life cycle need to be aligned to the overall ESS development phases.

The schematic process is a streamlined depiction of the real construction process, as we expect overlaps between the seemingly distinct separations of the phases. For example, long lead time components, like detectors and neutron guides, will presumably start tendering and production during phase 2, but the procurement of non-critical and off-the-shelf components could be made towards the end of phase 3. Close attention will be paid to those components, which can be procured by a limited number of suppliers, like choppers and neutron guides.

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

The installation phase needs to be aligned to the overall ESS operational phases, in close coordination with the ESS and in consideration of the status and needs of the neighbour beamlines, to ensure efficient use of resources and availability of space in the halls.

The hot commissioning will ramp down in parallel with ramping up of the Early User Access that will involve the instrument team and expert users in demonstration experiments to show the capabilities of T-REX and help trouble shooting of hardware and software. Once the hot commissioning activities have ramped down, the beam will be available for users according to the ESS overall operations.

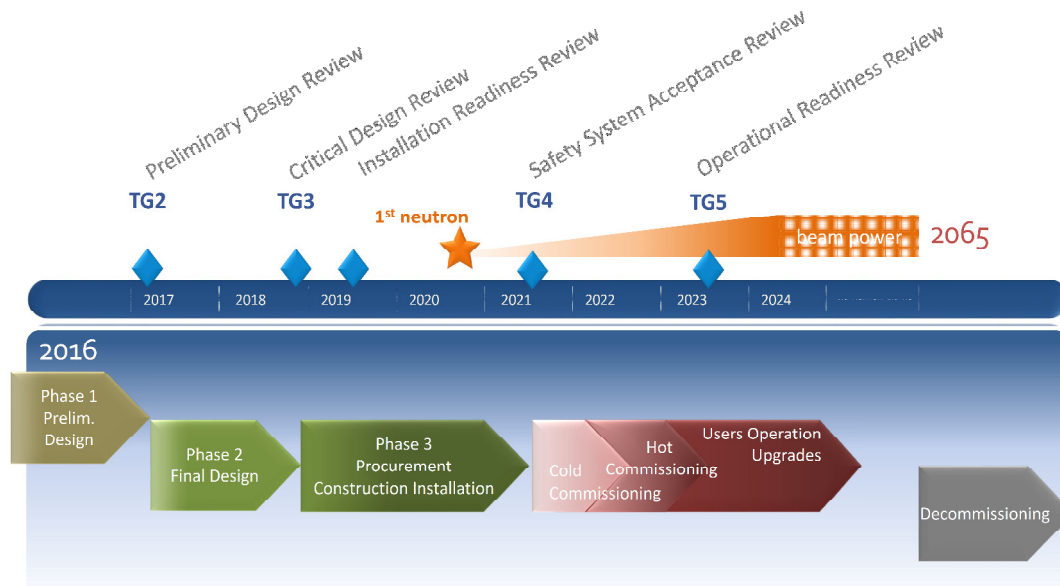


Figure 1 Proposed life-cycle of T-REX.

The development of an upgrade program should be staged during the life-cycle to adapt constantly to the evolving scientific demands and cutting-edge research.

The Instrument Development process provides the framework within which the instrument will be developed with timely milestones in order to measure progress, still allowing for the overlap to exist. The controlling document for the instrument development is: Process for Neutron Instrument Design and Construction: ESS-0051706.

3.4 System overview

The T-REX instrument is identified as the system number 13.6.15, within the NSS project of the ESS. It is composed of the subsystems identified in its Product Breakdown Structure (PBS) and described in the Preliminary System Design Description. Here we describe the main building blocks according to their function and relevance in achieving the scientific scope. We analyse some design and installation aspects, along with the key interfaces with the whole ESS, which are relevant to the fulfilment of the high level system requirements.

3.4.1 Functional building blocks

The here-described main building blocks of the T-REX instrument that are relevant to ensure its operation and functionalities, are: neutron optics systems, shielding, chopper systems,

shutters, experimental cave, detectors, Beam Stop, Personnel Safety System (PSS), control hut. We give also a brief overview of potential upgrade possibilities.

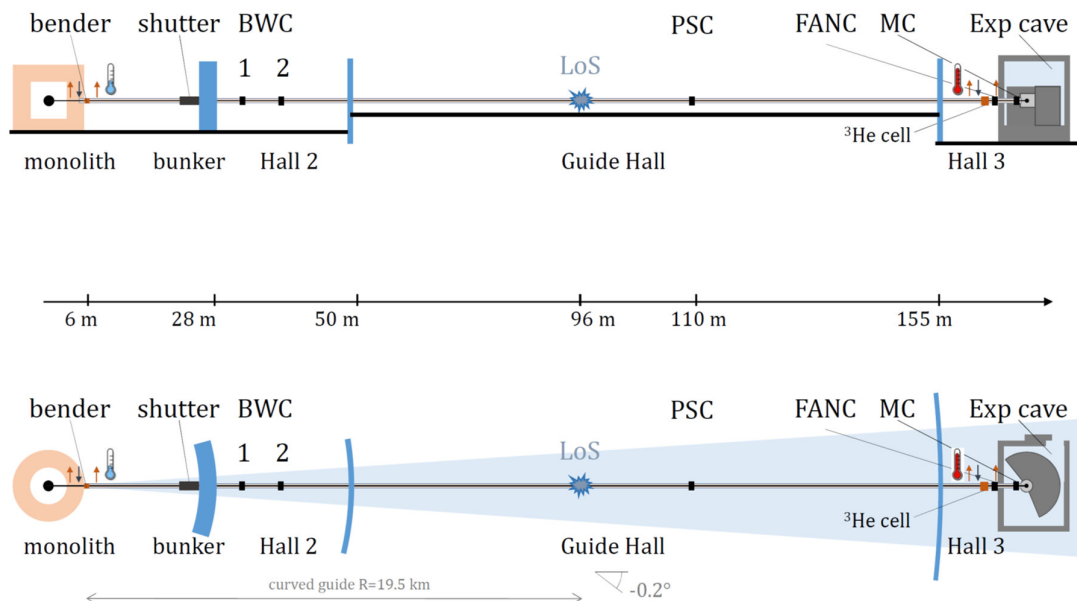


Figure 2 Sketch of T-REX showing the major functional building blocks.

3.4.2 Neutron Optics Systems

Since the TG1 review, we have optimized the neutron optic systems of T-REX for the top butterfly moderator, paying close attention to ensure that they can be integrated in the overall ESS facility, e.g. the optical elements inside the monolith insert, the guide system within the piling corridor in the guide hall.

The extraction system has been conceived to enable the view of both cold and thermal moderators, therefore in the monolith insert there is a neutron mirror to enlarge horizontally the view on the cold moderator.

The vertical shape of the neutron guide has been changed since the proposal and is now ballistic with elliptical end sections, focusing on the moderator. The m-coating variation is optimized for a high brilliance transfer and is particularly tailored towards the transport of short wavelength neutrons down to 0.7 \AA . The horizontal shape has not been modified since the proposal, it consists of a curved section, 90 m long, to guarantee that the direct line-of-sight is broken, as a measure to reduce the background. The beam at the sample is $10 \times 30 \text{ mm}^2$, the beam profile is homogeneous within a 10% variation, the divergence increases with wavelength and shows a smooth profile, in agreement with the Q-resolution requirements. Collimators on the incident beam will be placed at the end section of the guide, close to the sample area, to enable measurements at the lowest detection angle of 1° , for which the width of the direct beam has to be reduced. The mechanics of such a device shall allow an easy removal from the beam, in order to increase flux at the expenses of divergence, for experiments where access to the lowest scattering angles is not necessary. Although the mechanics details are currently under investigation, they can be easily optimized for T-REX starting from the design of similar existing systems.

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

According to the new vertical shape of the guide, the solid state bender has been re-dimensioned in height, being now smaller: 60x48 mm². The other design parameters have not been changed. This component is an asset for some high level requirements, like the request for a wide energy range, and allows combining the thermal and cold neutron spectra in one instrument for the first time. Many facilities operate thermal and cold neutron beamlines, which are complementary, for many applications.

The combination with the polarizing function by a polarizing bender provides the ideal 50% transmission for cold neutrons. A guide field for cold polarized neutrons will be provided. The polarizer for thermal neutrons will be realized as a continuously spin optical exchange pumped (SEOP) ³He spin filter cell, yielding a neutron polarization constant in time and including a near ideal spin flipper by adiabatic fast passage (AFP). We have conceived a guide field configuration, which allows an adiabatic spin rotation for thermal and cold neutrons in XYZ, which is combined with a PASTIS coil setup to analyse the spin with a wide angle ³He spin filter cell.

The guide system requires a vacuum system and potentially a ventilation system for dry Nitrogen. The guide system is in principle a non-moving fixed installation, which in optimum case does not require maintenance. Settling of the ESS ground might however set a requirement for re-alignment at some point in time.

Beam Scrubbers/Slits are also part of the system, and are to be installed close to the sample position to limit the beam to the required size.

3.4.3 Shielding

The shielding shall avoid exceeding an actual dose rate of 3 µSv/h, outside it, as requested in Supervised Areas at the ESS. Moreover, shielding optimization is crucial to achieve the low level of background requested, but it can only be finalized during phase 2, although a conceptual design is part of the deliverables of phase 1, both with respect to cost and safety. The requirements are set by operational safety, optimization of the background level and cost.

Outside the bunker, the instrument shielding stretches from the bunker wall to the end of the instrument in the beamstop and hence includes in particular the experimental cave, for which the corresponding requirements apply not only with respect to safety but also with respect to achievement of low background level by reducing the skyshine and groundshine and by preventing the instrument to be source of skyshine for neighbour beamlines.

Since the instrument emphasizes the use of thermal neutrons and requests a fairly large divergence, avoiding the direct-line-of-sight is not straightforward. The neutron transport concept relies on extracting a wide, low divergent beam, which is then curved with a large radius of curvature to avoid too many reflections and large scattering angles. As a result, the direct line of sight is broken at 96 m from the origin. Within the line of sight the shielding shall absorb and reduce primarily the dose of fast neutrons and muons originated at the spallation source escaped from the bunker collimation. Around the choppers the shielding shall absorb backscattered neutrons as well. Materials requirements are under investigation and their finalization depends on detailed information about the energy spectra of particles produced at the spallation source, but some considerations can be applied already here. We expect that, within the LoS, a significant fraction of shielding will be of steel and/or lead and boron enriched concrete.

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

Outside the LoS, the beamline shielding shall absorb mainly the gamma radiation originating from the supermirror, therefore a fraction of it will be steel and/or lead. Outside the LoS the shielding has to stop fast neutrons escaped from the collimation and the less energetic particles generated in the secondary spallation events within the LoS, therefore a big fraction of concrete is foreseen, similar to typical shielding layouts as used on reactor based instruments. The shielding design parameters along the instrument are chosen according to the 'ESS process for shielding cost', as further described in Preliminary System Design document and the relative budget is calculated according to the ESS cost book values for materials.

3.4.4 Choppers

Choppers can be classified according to their function in bandwidth choppers (BWC, 2 single discs), pulse shaping choppers (PSC, 2 single discs) monochromating choppers (MC, 1 pair of discs in butterfly configuration), FAN chopper (FANC, 10 single blades) and T0 chopper (TOC, final design specs tbd). The chopper system is being optimized and specified with respect to the boundary conditions of the source time structure, the guide system, technical feasibility, failure modes and maintenance requirements. The chopper casings should share the vacuum atmosphere with the neutron guide system to avoid windows as much as possible. Following [ESS-0034513], metal bellows should connect the guide vacuum tubes to respective flanges on the chopper housing, to enable extraction of the chopper unit. In particular close to the secondary spectrometers, neutron windows should be placed as far upstream of the detector area as possible.

3.4.4.1 Bandwidth chopper subsystem

The 14 Hz BWC shall select a band of 1.67 \AA from each source pulse, whilst preventing higher orders transmission bands within the wavelength band transmitted by the PC. They are placed at a position outside the bunker to facilitate access. The discs have a large diameter similar to existing instruments such as LET. They should also scatter fast neutrons significantly to contribute additionally to the background suppression.

3.4.4.2 Resolution defining chopper subsystem

Due to the 55 m distance between PSC and MC, their required burst times differ considerably. As a consequence, the MC mainly controls the illumination time of the sample and accordingly the resolution of the final neutron velocity, while the PSC controls the width of the initial neutron velocity/wavelength distribution. The repetition rate of both chopper pairs is locked to the inverse ratio of their distances from the moderator. The repetition rate of these choppers defines the step in wavelength between subsequent pulses illuminating the sample. Furthermore, the repetition rate of the MC defines also the maximum final wavelength and hence the maximum neutron energy loss, which can be recorded before the sample is illuminated again. In order to achieve the highest requested energy resolution, the PSC shall define the width of the velocity/wavelength distributions for neutrons with a mean energy $E_i=160 \text{ meV}$ to 1%. Hence the minimum burst time of the PSC shall be 100 \mu s . For the highest repetition rate of the MC the band of final wavelength is limited to $0 \text{ \AA} < \lambda_f < 4.03 \text{ \AA}$. The minimum burst time prepared by the MC shall be 10 \mu s (FWHM of the distribution)

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

providing $\Delta\lambda/\lambda = 1\%$ for a final neutron wavelength $\lambda_f = 1.5 \text{ \AA}$, i.e. for elastic scattering at the center of the overall band. MC might operate in multiples of 14 Hz, up to 336 Hz, therefore varying the energy resolution. A higher frequency $\geq 350 \text{ Hz}$ might be possible thanks to new chopper developments, however, we still consider the 336 Hz as the baseline specification, as in the proposal.

3.4.4.3 T0 chopper

As resulting from the scope setting meeting, the project makes provision for a T0C which may be installed if operational experience should show that it is necessary. A preliminary design of the component has been investigated within the DREAM project, which can be also used for T-REX. The current design has a single hammer of 20 cm thickness along the beam direction, spinning at 14 Hz. The hammer material is a combination of the tungsten alloy and B_4C .

3.4.4.4 Fan chopper

The FANC takes over the function of the frame overlap chopper used at monochromatic chopper spectrometers at continuous sources. It suppresses arbitrarily an illuminating pulse, if the time frame is too short to cover the requested range of λ_f . This chopper consists of 10 independently phased blades that spin on a common axle. The blade dimensions are small enough to sweep over the beam cross section in less than two periods of the M chopper and large enough to cover the beam cross section completely during the time, the M chopper transmits neutrons.

3.4.5 Shutters

The instrument requires a heavy shutter for access in conventional operation. However, a standard heavy shutter system is not specified yet. It is currently expected that a shutter would be placed either inside the bunker wall or as-close-as achievable to it and it will have a length of up to 1.5 meters, shall be fail-safe and accurate enough as to carry a corresponding length of guide, which also requires to be evacuated. A possible rotatory mechanism is foreseen. The system shall be fail-safe.

In order to guarantee safe access to the beamline during the source shutdown, a light shutter is foreseen just outside of the monolith insert. The design parameters will be finalized during phase 2, but the safety function will be made by a gamma attenuator.

3.4.6 Experimental cave

Looking at it from outside, the experimental cave is a massive shielding resembling the one of other neutron instruments. The access to the cave is from the side through a sliding door. The door will be wide enough to haul the basic sample environment components and some of the instrument components, which might be removed for maintenance, like MC, FANC, ^3He Polarizer and detector elements. However, as this depends on boundary conditions and interfaces with neighbours and the overall facility, the layout will be finalized during phase 2. Inside the experimental cave, the largest room will be occupied by the detector vessel, which will lean on a raised floor realized in wedges, so that a cavity is left in between wedges to

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

install vacuum pumps on the floor. Enough clearance will be left to allow bulky sample environment to be installed from the side, when requested by users. T-REX will be a top-down instrument, where the sample will typically hang inside SEE from a top flange, thus top access to the sample tank will be routinely used for conventional sample environment equipment, like cryostats, pressure cells and for the MAGIC PASTIS equipment. Due to the dimensions of the MAGIC PASTIS, which will be 1000 mm in diameter, the flange inner diameter will be larger than the 800 mm requested to install the XL SEE, according to the ESS standards defined by the SAD in ESS-0038078. According to the latter document, a cryomagnet can weigh up to 1000 kg with a height of 1.7 m and a diameter of 0.8 m, so we plan to have a dedicated crane inside the experimental cave, which will enable to move and install such equipment. This also requires that sufficient clearance is left between the instrument crane and the taller level inside the cave, which is the roof of the detector vessel. This still leaves enough clearance between the roof of the cave and the hall crane to enable dismantling of elements. Moreover, the roof of the detector vessel could be used for the auxiliary equipment to support the sample environment. The crane, gas cylinders and sample environment stick holders are going to be located at the experimental cave as well, and there is going to be a number of PSS components installed within it. Their purpose is to monitor and prevent radiation, fire, oxygen deficiency, cryogenics and electrical hazards during operation of the beamline. The instrument operation also requires various utilities for gas, exhaust, electricity and corresponding surveillance equipment installations.

3.4.7 Detectors

The 3D arrangement shall imitate a vertical cylinder and a foreseen coverage of about 2.2sr , corresponding to horizontal angles between -36° and $+144^\circ$, vertical angles between -25° and $+15^\circ$, i.e. 2.2m active vertical length. In the first day detectors shall cover the full height and the horizontal angles from -1° to 70° at least, to avoid compromising the core scientific scope, represented by investigations on single crystals in magnetism. The asymmetric detector layout provides access to a larger vertical component of the momentum transfer in particular for single crystal studies, while it still allows the integration of large parts of powder rings. The minimum detection angle is 1° , as requested by investigation in magnetic and disordered systems. The required energy resolution can be achieved with a contribution to the time resolution from detectors of $\sim 5 \mu\text{s}$. Currently this is state of the art using presently available electronics, e.g. commercial FPGA (Fast Programmable Gate Array) chips. In order to limit the contribution to the wave vector resolution the requested pixel dimension is 20×20 (W x H) mm^2 .

The detectors will be optimized to reach 70% efficiency at 1.8 \AA , which is the benchmark of 6 bars ^3He detector tubes assemblies, with construction blind areas taken into consideration. The latter wavelength has been chosen, because the detector needs to record all final neutron wavelengths from 0 to the maximum λ_f , so that the average final wavelength will be around this value. Moreover, when using neutrons with high initial energy, typically the focus is in the access to large neutron energy loss processes.

The detector shall be capable of handling the count rate generated by the experiments, which is at the edge of capabilities of today's detectors, and largely insensitive to gamma radiation

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

3.4.8 Beam Stop

A beam dump is foreseen at nearly 96 m, where the line of sight is broken, to prevent fast and epithermal neutrons from reaching the sample and detector areas. Dimensions and characteristics will be defined during phase 2, since MCNPX calculations are needed. Most likely it will consist of a block of tungsten integrated into the shielding. As the instrument leaves the line of sight at a large distance from the sample area, the beam stop at detector position has to catch only the thermal/cold neutron beam and will likely consist of B₄C or PE and concrete.

3.4.9 Personnel Safety System, PSS

PSS will manage the risks associated with running a user program at the instrument. The risk assessment and PSS requirements for operating T-REX will be provided by ESS along with the system and its integration.

3.4.10 Control Hutch

The instrument personnel will be able to change the instrument and sample environment parameters remotely from the control hutch. Additional computers for monitoring chopper and data acquisition systems will be also located in the hutch. At least two separate workstations inside the hutch will be dedicated to data reduction and analysis. Activities related to the sample handling will be carried inside the sample preparation lab and in the sample environment preparation area.

3.4.11 Future upgrade possibilities

We foresee several upgrade options for T-REX, which will further expand its scientific scope and secure the relevance of the instrument for the user community in future. The list of possible upgrades includes:

- I. Detector coverage. T-REX detectors have modular structure and their coverage can be increased to the full scope. The overall performance of the instrument is, generally speaking, proportional to the detector coverage.
- II. The state-of-the art SEE. Considering that magnetism is one of the main science drivers of the instrument, availability of various magnets in sample environment pool is important, either being instrument specific or in shared efforts with other instruments. Also important to develop the user program efficiently is the availability of pressure cells (like Paris Edinburgh and clamp), HT furnace, IR furnace, Sorption Stick, 6kV HV supply, pulsed magnet, pump and probe and gas processing.
- III. The project will make provision for an additional T0 chopper to improve the background level by means of attenuation of the prompt pulse. At the moment of writing two alternative positions are considered for the chopper: either inside the bunker or downstream 96 m, where the LoS is broken.

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

- IV. The resolution limits considered in the present proposal are determined by the maximum chopper speed available nowadays. Future developments can provide a higher resolution with very similar flux, as the reduction of intensity in an individual pulse is compensated by a higher pulse density. Additionally, the realization of an optically blind four chopper system, as introduced in the VOR proposal, would allow a continuous optimization of the energy transfer region of interest as compared to the discrete choice offered by the combination of different windows on the PSC and MC discs.
- V. A supermirror analyser array could be considered as an alternative analyser. While not working for high final neutron energies, it would be efficient for deep inelastic scattering with low final neutron energy. As it would cut out the high neutron energies it would avoid frame overlap from the subsequent pulse and therefore enable higher repetition rates with the respective flux gains. However, the cost of such a device is much higher and the flexibility is lower compared to a wide angle ^3He spin filter cell.

3.4.12 Key System Interfaces

For the entire instrument life-cycle several system interfaces will arise and need to be analysed already in phase 1, to ensure that the instrument will successfully be integrated and operated in the ESS facility and achieve the scope at which it is aimed.

- Target System, moderators and monolith: impact the design of the bispectral extraction system, neutron optics, neutron guides and shutters; might impact the instrument overall performance, if any change to the baseline will be applied.
- Bunker System: will host several components of the instrument: light shutter, cold neutrons extraction system including the polarizing bender and the guide field (≤ 10 G), heavy shutter and about 26 meters of the neutron guide. The current design of the instrument does not imply the modification of the bunker wall. Considerations of the expected background level might require that during the upgrade program a TOC might be located within the bunker, at a position where it will not interfere with bunker support pillars, bunker wall and any components of neighbour beamlines. A proper system for the extraction of the chopper assembly would be developed, with consideration of the bunker design.
- Conventional Facilities and neighbour beamlines: T-REX will be installed across three different buildings, Experimental Hall 1 (EH1), Guide Hall (GH) and Experimental Hall 3 (EH3). Every building is characterized by a different floor load and different cranes will be available, with various crane load and clearance. The beam centreline is at a different height with respect to the floor in the three buildings. Regarding EH1, where neighbour beamlines are closer to each other, we foresee to investigate the shielding design in collaboration with neighbour beamlines (W6 and W8), which will avoid any possible clash, but might also lead to the proposal of a communal shielding structure, to improve background conditions and/or lower the cost.

The current guide layout is such that the piling corridor in GH can be used to support the guide system for the overall length. During the user program most of the

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

operational activities will be conducted in EH3, where special attention is needed to project the spaces for the preparation of the sample environment outside the experimental cave and the sample preparation lab at the instrument. Therefore, a close interaction with the project of neighbour beamlines will be necessary in the design phase, to realize the minimum impact and avoid any clash. A potential issue is represented by the use of extreme sample environment, like cryomagnets, which might alter the performance of the adjacent instruments.

- **Integrated Control System (ICS):** ICS will provide a framework for the integration of hardware, software, network infrastructure and timing system for the instrument, which is essential to the instrument operations.
- **Data Management and Software Centre (DMSC):** the instrument design enables data rates that can exceed 1 Tbyte/day in event mode recording, at full source power. A powerful and efficient data management system is required to transfer the large datasets, as well as tools for manipulation of the raw data, both online and offline. Moreover, reliable and user friendly data reduction and data analysis software solutions are crucial for the mission of T-REX. Computational resources for advanced data analysis must be available for the users at the control hutch.
- **Scientific Activities Division (SAD):** The support of the user office and sample environment teams is essential to run a successful user program, SAD will be providing solutions for processing beamtime requests and for receiving/disposing user samples. Apart from that, SAD is going to be responsible for the installation, operation and maintenance of the sample environment, including the instrument specific ones. Those activities will affect the scientific productivity of the instrument. In order to receive efficient support from SAD, new instrument specific sample environments should be specified and procured with information exchange and advice from SAD.

Maintenance and Service Groups: Both technical groups will provide the maintenance requirements and access strategies for the instrument. It is important to consider these requirements as early as possible in the design phase in order to ensure an easy and safe access to the instrument components for the maintenance and service work, in compliance with ESS standards.

4. SYSTEM STAKEHOLDERS

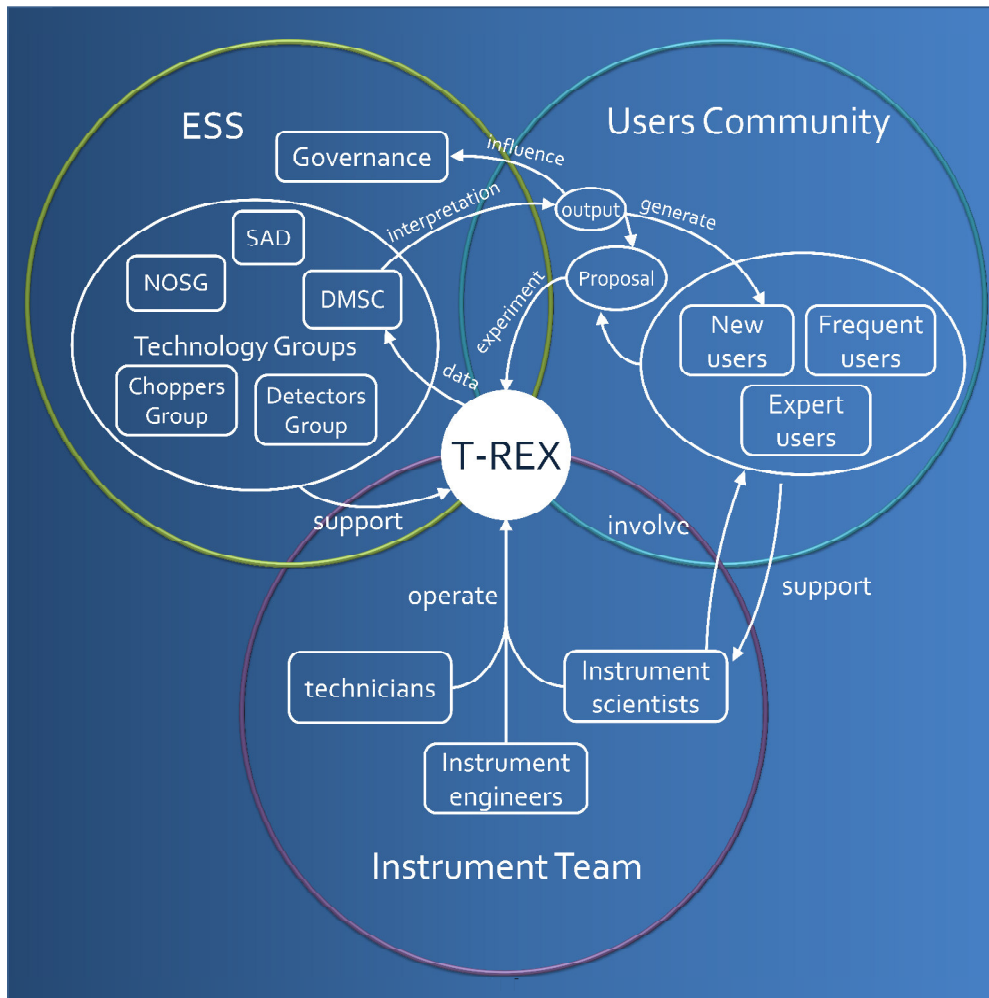


Figure 3 Context diagram shows group of stakeholders and their high-level interactions

- **Stakeholders Group 1: Users Community**

Members: Visiting scientific users, ESS scientific staff, commercial users. Within these categories users are grouped in expert, frequent and new users.

Their principal expectations are:

- Use the instrument to perform INS experiments
- Change experimental conditions during the experiment
- Obtain the scientific information and output from the experimental data
- Especially new users expect to handle the experiment and data analysis in easy fashion and may need support during the data evaluation and treatment after the experiment is finished

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

Interaction:

The level of interaction of expert users is high during the commissioning phase, when they are expected to run experiments first than others, and remains strong in production mode. Regular users with a limited experience should be more involved during production mode to minimize risk of unsuccessful experiments during commission. New users interact less as they may be less used to neutron science and the success of an experiment will be less affecting their work.

Any user will write a proposal of experiment, which will then be evaluated and, if accepted, eventually perform the experiment at the ESS. The data obtained from the experiment and their interpretation will enable to reach relevant scientific output, which is expected to be used as a parameter for evaluating the instrument performance and therefore will influence decisions and actions taken by the governance to ensure the operability of the facility.

- **Stakeholder Group 2: ESS organization**

Members: ESS governance: CEO, Council, Science Directorate, NSS Management, Instrument Division Head, ESS Technology Groups: Choppers Group, Detectors Group, NOSG, SAD, DMSC.

Their principal expectations are:

- Construction cost of the instrument to be maintained as low as achievable, whilst delivering the level of performance required by the agreed scientific scope,
- Operational cost to be maintained as low as possible whilst maintaining the agreed level of equipment performance and availability for the users community,
- Specifically for technical groups: development of new and optimized solutions to upcoming technical issues, to keep ESS at the cutting edge of neutron technology.

Interaction:

Members of the Governance are responsible for ensuring the operability of the facility for scientific use. They are not expected to interact directly with the instrument, but they lead the construction process through key decisions on the budget, the scope and the schedule. The high level of interaction is foreseen during the construction and commission phases. They are also responsible for most of the decommission activities.

Members of the Technology Groups, with the exception of the SAD, will not be involved in the normal operation, but they will interact directly with the instrument and its subsystems during installation, commissioning, maintenance. They are expected to lead breakdown situations and troubleshoot the issues affecting the subsystems of their competence.

Members of the SAD are expected to support the users during normal operation, through installation and handling of the sample environment equipment requested for the experiments. They lead the breakdown situations and troubleshoot the issues affecting the subsystems of their competence.

- **Stakeholder Group 3: Instrument Team**

Members: Instrument Scientists, Instrument Engineers, Technicians.

Their principal expectations are:

- Deliver the level of performance required by the agreed scientific scope, whilst maintaining the construction cost of the instrument as low as achievable and the construction process in line with the agreed schedule.
- Operate the instrument with the expected level of reliability, serviceability and availability, whilst keeping failures and breakdown level as low as achievable.
- Operate the instrument with the requested level of human and environmental safety.

Interaction:

Members of this group are expected to interact directly with the instrument and the subsystems during the installation and commissioning, they operate the instrument and the subsystems in production. The instrument scientists are expected to interact directly with the users during an experiment, are expected to keep the user community involved in the user program. Instrument engineers and technicians will interact with subsystems in breakdown and maintenance situations and troubleshoot minor issues.

		Installation	Commission	Production	Restart	Fault Detection	Maintenance	Repair	Decommission	Disposal
User Community										
SH-1	1.1 expert users	4	4	1	1	1	1	1	1	1
	1.2 regular users	2	3	1	1	1	1	1	1	1
	1.3 new users	1	2	1	1	1	1	1	1	1
ESS organization										
SH-2	2.1 ESS Governance	1	2	1	1	1	1	1	1	5
	2.2 NSS Management	5	5	2	1	1	1	1	5	4
	2.3 Optics&Shielding Group	4	4	1	1	5	5	5	1	1
	2.4 Detector Group	4	4	1	1	5	5	5	1	1
	2.5 Chopper Group	4	4	1	1	5	5	5	1	1
	2.6 Scientific Activities Division	3	4	4	1	5	1	4	1	1
	2.7 Automation Control Group	4	4	1	1	5	5	5	1	1
	2.8 DMSC	2	4	2	1	5	1	5	1	1
Instrument Team										
SH-3	3.1 Instrument Scientists	4	4	5	3	3	2	2	1	1
	3.2 Instrument Engineers	4	4	3	3	4	4	4	1	1
	3.3 Technicians	4	4	2	2	4	4	4	1	1

1	slight
2	limited
3	moderate
4	strong
5	leading

Table 1 An overview of stakeholders interactions

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

5. OPERATIONAL CONCEPTS

5.1 Operational environment

The instrument will be operated in a controlled environment with a temperature of 22 ± 2 °C all year round. It is envisaged that T-REX is located at the beamport W7, across three different buildings, D03 - Experimental Hall 1 (EH1), E02 - Guide Hall (GH), E01 - Experimental Hall 3 (EH3). The height of the target centreline with respect to the floor is 2.14 m, 1.14 m and 3.14 m in EH1, GH and EH3, respectively. Floor loading must not exceed 30 t/m², 20 t/m² and 20 t/m² in EH1, GH and EH3, respectively. Floor stability in the halls has been defined such that the elastic (initial) and creep (long term) deformation shall not exceed $3+3 = 6$ mm during the lifetime of the facility.

Utilities and media are brought to the instrument from the gallery. Media include: DIH₂O, N₂, instrument grade compressed air, cooling water. Utilities include: office IT, office comms, power, MPS, PSS, DMSC and ICS.

The ESS facility has 5 different operating modes [ref ESS-0011768]: Shutdown, Studies, Studies on Target, Startup and Production. Any of these modes has a different impact on instrument operations and operation modes, as experiments can only be conducted during ESS-mode Production. Access to instrument equipment for maintenance, calibration, cold commissioning is mainly done during shutdown, but possible with some restrictions during studies and studies on Target, after safety assessment. During Startup, instrument operations are limited to alignment, commissioning and calibration runs.

When ESS has entered into a steady-state operation phase, the following principal schedule is currently expected to apply:

- 200 days/year of neutron Production for the ESS users after 2026,
- Proton beam 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,
- 3 Optional Studies Days every second week to avoid long down time of instruments due to failures of activated components, followed by 2 days for Studies and Studies on Target,
- A series of Studies days to allow for fine-tuning of accelerator and target systems.

In accordance to the availability and reliability assessments made in ref [ESS-0017709] and [ESS-0008886], ESS aims to ensure that at least 90% of the users with accepted proposals receive a neutron beam allowing them to execute the full scope of their experiments.

ESS will be manned 24 hours/day, 7 days a week and the manning will allow for flexibility for users when conducting experiments and making preparations or analysing results.

The T-REX instrument is foreseen to be managed and operated by a team of at least 2 scientists and 1 engineer.

5.2 Operational scenarios

T-REX can be operated in various possible modes that result from the combination of the adopted neutron wavelength band and resolution and optional use of the polarization analysis. Before the measurements, the users and the instrument operators agree on how to

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

configure the instrument, according to program and aim of the experiment. It is foreseen that most of the experiments will request the use of sample environment equipment. The measurements consist of exposing a sample, under controlled environmental conditions, to the neutron beam to measure the pattern of scattered neutrons. To acquire sufficient statistics, the measurements typically will run for a few hundred to thousands of seconds. The scattering pattern so collected should then be transformed into scattering intensity as a function of energy and momentum transfer. The analysis of this data should reveal information about the dynamical features and characteristics of the sample, like fluctuations, excitations and vibrations.

5.2.1 Samples

Basically anything that is expected to show dynamical features in the time and length scale covered by the instrument is a potential sample. Examples are macroscopic solids, being either single crystals, powder or disordered; liquids or gels; liquids and gases infiltrated in nanoporous solid materials; proteins, other biological molecules and polymers, dried or in solutions. The high flux enables measurements on smaller amounts of sample as compared to today and to widen the scope of inelastic neutron scattering towards thin films and nano particles.

5.2.2 Sample geometry and exposure system

The sample should have known dimensions and a shape as symmetric as possible. This is achieved by shaping the sample in the case of solids, whereas in other cases the sample can be placed in a container, which should have a good neutron transmission. The shape of the sample holder should either be flat or a vertical cylinder to weakly affect the resolution function and the scattering pattern. The sample or the sample container can be placed within the sample environment equipment as part of the exposure system. If the sample is an oriented single crystal, it can be mounted on the sample stick directly. It should be kept stationary during an exposure long enough to acquire reasonable statistics, then the crystal orientation is varied and a new acquisition is started.

5.2.3 Sample preparation

Normally, users prepare the samples needed to run their experimental program. Depending on the kind of sample and the aim of the experiment different situations are foreseen for the sample preparation. Samples can be prepared in advance in the home-lab or facility and carried or shipped to the ESS. In the direct vicinity of the spectrometer area a working place equipped with the relevant tools is needed to mount the sample for installation at the spectrometer. This might include glove bags to install the sample under an inert gas atmosphere. As a spectrometer even on the ESS requires typical data acquisition times of the order of thousands of seconds also the samples should be stable on that time scale. Hence for more sophisticated sample preparation, access to the SULF preparation labs in building E04 is anticipated.

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

5.2.4 Instrument configuration

The instrument can be configured by remote control acting on various components. In order to fulfil the requirements of their experiment, the users will choose the instrument configuration within the available options for the band of incident energies and the energy resolution. This action is performed by changing the configuration of choppers. We envision two means of controlling the instrumental resolution: (i) via the change of the chopper speed of the PC and MC; (ii) via different disc windows on the chopper discs which can be selected by the relative phases of the discs of the PC and MC pairs, respectively. The second option enables the optimization for a specific energy transfer region of interest relative to the initial neutron energy, while the first one affects the resolution for all energy transfers similarly. Optionally the instrument can be configured to use polarization analysis. For cold neutrons the initial polarization is prepared by a using polarizing bender at the position of the cold beam extraction. Thermal neutrons will be polarized by a continuously pumped and hence autonomous ^3He spin filter cell, which can be exchanged with a neutron guide segment. Polarization analysis is foreseen using a wide angle ^3He spin filter cell in combination with a PASTIS like magnetic field arrangement, which enables the analysis of the spin in X, Y or Z direction. To achieve large solid angle coverage of the PA, the entire analysis device will be integrated with the sample environment.

5.2.5 Measurements

The measurements consist of exposing the sample to the neutron beam and collecting the pattern of scattered neutrons as a function of the position and time of flight. To work out the scattering signal from the sample a set of measurements should be performed: scattering from the empty container, scattering from sample + container, scattering with the sample replaced by a neutron absorber and a map of detectors efficiency, which can be obtained from the scattering of an incoherent scatterer, such as Vanadium. The experiment can foresee a series of scattering measurements under variable conditions. The user will visualize the scattering data and take decisions based on the observed results. Event mode recording enables a continuous variation of any SE parameter, as long as the change is slow compared to secondary time of flight.

5.2.6 Data visualization and Data Analysis

In order to enable visualization and data analysis, raw data must be processed using dedicated software, which is expected to get the following functions ready in line with project phases:

- When entering hot commission, it will be possible to apply basic instrumental corrections, such as subtraction of the sample holder scattering and background signal and normalization to vanadium scattering. It will be possible to transform scattering intensity into the components of wavevector transfer and energy transfer. It will be possible to visualize tof spectra, $S(Q)$, inelastic spectra selecting single or multiple incident energy, at given Q vs energy transfer or at same energy transfer vs Q nearly in real time. It will be possible to quickly fit the data (e.g. vanadium) with basic functions (e.g. Gaussians) to monitor for instance the energy resolution in real time.

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

- When entering the Early User Access, "expert users" test the instrument, help trouble shooting software issues, and are expected to start a high-impact scientific program making combined use of RRM and Polarization Analysis, thus it will be possible to visualize contemporary spin-up and spin-down inelastic spectra and apply basic operations like adding up different spectra with a proper 'convolution' treatment.
- In production mode, when the regular user program starts, it will be possible to apply non-standard corrections, e.g. multi-phonon estimation from spectrum taken with the highest incident energy and subtraction from $S(Q, \omega)$ other energies, multiple scattering estimation, calculation of v-DOS and comparison in RRM, coherent-incoherent cross sections (weights) calculations and comparison to data, RRM modes available e.g. 'best data' visualization. A number of flexible data fitting functions and routines will be available for quick real-time considerations on data. QENS for instance requires calculation of mean square displacements and determination of the broadening of the elastic line vs Q by fitting the spectra with model functions.

5.3 Maintenance Concepts

5.3.1 Levels and categories of maintenance

Three levels of maintenance are considered in ref ESS-0003640:

- Organizational maintenance: maintenance conducted on site where the component is normally being operated,
- Intermediate maintenance: maintenance conducted on site at dedicated workshops,
- Supplier maintenance: maintenance conducted off site at the supplier premises, including In-Kind partners.

Besides this distinction in levels, the maintenance can be classified as corrective and preventative.

The preventative maintenance relies on the condition monitoring and as a general rule will not be carried out during periods of neutron production, but during periods of source shutdown, considering the ESS overall operational schedule, unless it is immediately required to support a safe and reliable operation of the instrument. Monitoring requirements of critical components will be considered during phase 2 and phase 3 of the project, as result of the instrument reliability analysis based on Reliability, Availability, Maintainability and Inspectability (RAMI).

The corrective maintenance will mainly apply when an unforeseen event happens forcing the maintenance to be done unscheduled. This occurs following either a component failure or detection of an issue that requires immediate action during the user operation. The instrument will likely have to stop the user operations for the duration of repairs or maintenance.

Access requirements and limitations define three categories: easy maintenance access, limited maintenance access and difficult maintenance access devices. In the first category all devices and components can be placed in areas located outside the radiation shield of the instrument, including devices located at the sample stations. These devices can be serviced

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

anytime when required, though downtimes are used for preventative maintenance in order to reduce the impact on the instrument operation. In the second category are the limited number of hardware components installed in the instrument shielding between the bunker shield and the sample station. They are downstream the heavy shutter system of the instrument. These components shall be accessible during the source operation in case corrective maintenance is required. The third category consists of components installed in the bunker area where access currently appears to be possible only during source downtimes and through remote handling. The access to components within the last two categories requires removal of the shielding with the corresponding implications of crane use, space requirement, radiation protection and probably can involve a necessary cool down time for the activated components. All of that will prolong the time needed for maintenance.

5.3.3 Maintenance philosophy

The maintenance philosophy of T-REX is in line with the approach of the ESS to utilize condition-control based preventative maintenance as much as possible, as a measure to minimize the resource requirements and potential downtimes. The critical components prone to regular maintenance consist of moving parts and can be easily identified. For the T-REX instrument they include the cold neutrons extraction bender, choppers and heavy and light shutters. We intend to implement the following maintenance approach:

- The bender is located within the bunker at ~6 m from the origin, inside or near to the Light Shutter System. The orientation for reflecting the cold beam requires accuracy and precision < 0.1 degrees. A change or loss of alignment will be seen in the spectra taken by the instrument beam monitors. The switch should have a motorized rotation, (if possible) with resolver, for realignment. The Si-wafers and the supermirror coating is sufficiently radiation hard, since no deterioration is expected before the radiation dose exceeds $>10^{19}$ n. A major issue could be to lose control on the motors and motion control, so that it should be a fail-safe device. Heat load and temperature still needs to be considered.
- Access to the choppers shall be possible when the heavy shutter blocks the beam. Choppers are removable without impact on the guide system; this will require a split housing approach for the choppers which are connected to the guide vacuum system. Choppers can be removed from the guide using a rail system. Chopper solutions using the magnetic bearings are preferred due to the minimum maintenance requirements. For mechanical bearings (as foreseen for BWC and, in case, for TOC) the maintenance interval is five years to replace grease and bearings.
- The heavy shutter shall be fail-safe, therefore its design has to be robust and reliable, since the failure of the component disables any instrument function. Removal of the shutter disables any instrument function; hence the components have to be designed as maintenance-free as possible. Removal is vertical, with remote handling as required.

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

- The neutron guide system is prone to failure, degradation of performance and misalignment of segments over the years. In case of failure, the guide outside the bunker should be accessible when the shutter is down, even with the source on, so partial removal of guide sections should be possible, while access to the guide inside the bunker or the monolith will only be possible during source shutdown and after safety assessment. Degradation will be limited thanks to a proper choice of the substrates, especially in the hard radiation environment, where the metallic substrate offers longer lifetime. Anyhow the performance can be monitored measuring the neutron flux. The realignment requirements of the guide have to be considered in the general design of the system. The guide design shall be robust enough to prevent misalignment as best as reasonably achievable within the budget and without compromising the overall performance of the instrument.
- All other components should be easily accessible and should allow for the failure mode operation and quick replacement. Spare components shall be available. The regular maintenance and check shall prevent their failure.

Document Type	Concepts of Operations Description
Date	01/02/2017
Revision	1 (2)
State	Preliminary
Confidentiality Level	TG2 Review

6. CONSEQUENCES OF THE CONCEPTS

The general design considerations related to all functional and non-functional requirements are/will be documented in detail in the System Requirements document.

6.1 Upgrade options

The upgrade options shall be considered and be catered for as much as possible in the design solutions, see section 2.

6.2 Robust design

The current preliminary design can be considered robust enough to address the scientific and technical requirements. However, there are several decisions to be made during the final design to finalize the design of the shielding, detectors, chopper system and neutron optics. The robust criterion has to be also applied to the interfaces of T-REX with the various supporting systems. It is expected that T-REX would be able to operate in the stand-alone mode in case of ICS and data streaming systems failures. The chopper system should be controlled via local hardware. In case the remote control has failed the manual access to the chopper system controls should be available. This applies to all motorized axis of the instrument, although less complex than chopper ones, e.g. bender, collimators, slits, etc. At least two workstations at the beamline will be used to store the data locally in order to prevent any interruption of the user experiment due to the failure in the data streaming system. After reduced data is saved in the appropriated format, the locally stored data may be deleted.

6.3 Training of personnel

The training of personnel will be further developed in future releases of this document when the design has matured enough for it to be included in a meaningful and contributing manner. Anyhow the training will include the walkthrough of the instrument, identification of all potential hazard situations and appropriate response. All training materials will be available on the instrument website. The hard copies of those documents will be available at the control hutch.

Glossary

Term	Definition
BWC	Bandwidth Chopper
PSC	Pulse Shaping Chopper
TOC	T0 Chopper
MC	Monochromating Chopper
FANC	FAN Chopper
T-REX	Time-of-Flight Reciprocal Space Explorer
PA	Polarization Analysis
PBS	Product Breakdown Structure
SAD	Scientific Activities Division
DMSC	Data Management and Software Centre
ICS	Integrated Control System
NOSG	Neutron Optics and Shielding Group
ConOps	Concepts of Operations
PSS	Personnel Safety System
EH1	Experimental Hall 1
GH	Guide Hall
EH3	Experimental Hall 3
TG	Toll gate

8. REFERENCES

- [1] Process for Neutron Instrument Design and Construction: ESS-0051706
- [2] Concepts of Operations for the ESS system: ESS-0003640
- [3] Concepts of Operations for the NSS system: ESS-0005817

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DOCUMENT REVISION HISTORY

Revision	Reason for and description of change	Author	Date
1	First issue – for STAP review	Nicolò Violini	2016-08-30
2	Second issue – for TG2 review	Nicolò Violini	2016-12-06