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Concepts Of Operations for CSPEC, the cold chopper spectrometer of the ESS

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Table of Contents

1. INTRODUCTION

The purpose of this ConOps document is to provide a brief description of the cold chopper spectrometer instrument at the ESS, CSPEC. The description includes both a high level introduction to the science case of the instrument as well as providing the framework and context within which the instrument will be designed, operated and maintained through its life-cycle. The document does not represent a detailed design. A deailed design will be provided during the detailed engineering phase, phase 2.

The intended audience for this document includes all those involved in the construction and operation of CSPEC. It will also serve as a quick overview of the instrument's purpose, construction and operation for person/-s familiar in the field of neutron science. This document will be frequently updated.

2. HIGH LEVEL SCIENTIFIC REQUIREMENTS

The high level scientific capabilities of the cold chopper spectrometer CSPEC are based on the spatial and dynamic capabilities outlined in the CSPEC proposal May 2014. In the CSPEC proposal, the long pulse structure and enhanced brilliance of the ESS have been exploited to develop a high performing cold chopper spectrometer that will gain an order of magnitude in neutron counting rate with respect to existing cold chopper spectrometers. It will probe low-lying excitations and relaxation processes in materials ranging from hydrogenous materials, polymers to strong electronic correlations, to name a few. A main focus of CSPEC is to enable routine in-situ or time dependent experiments that will open new scientific frontiers. Further details can be found in the CSPEC proposal.

CSPEC high level scientific requirements:

1. Wavelength range = 2 – 20 Å.
2. CSPEC shall probe excitations from 0.005 up to 20 meV.
3. CSPEC shall measure in repetition rate multiplication configuration for all measurement modes.
4. The CSPEC guide shall extract flux with +/-1^{o} divergence at 3 Å and more, if possible for

higher wavelengths.

5. CSPEC shall be capable of energy resolutions down to and better than $\Delta E/E = 1.5\%$ for wavelengths greater than 4 Å.
6. CSPEC shall be capable of momentum transfer resolution $\Delta Q/Q = 2\%$.
7. CSPEC shall provide a signal to noise of 10^5 at 5 Å. Signal to noise is defined as the peak of the intensity at the elastic line of a vanadium sample versus background obtained far away at a time of flight when the background level has been reached.
8. The chopper cascade shall ensure that, for each impinging pulse on the sample with energy Ei, an energy transfer = $\hbar\omega = \infty < E_i < 0.8E_i$ will be measured.
9. The neutron beam at the sample position shall illuminate a sample area ranging from 4 x 2 cm^2 to 1 x 1 cm^2 (height x width)
10. CSPEC should follow kinetic processes with time steps of one minute.
11. The detectors provide a detectable angular range of $5^o < 2\theta < 140^o$ with a sample to detector distance of 3.5 m and a vertical detect-able range of +/- 26.5^o.
12. CSPEC shall probe magnetic excitations in magnetic fields up to 12 T.
13. CSPEC shall ensure the possibility to perform polarization analysis in the future.
14. The systems design shall provide the space and flexibility necessary to host and drive future developments, for instance further focusing optics for smaller sample sizes, possibly integrated into the sample environment, further in-situ sample environment such as secondary characterization (RAMAN or NMR), XYZ polarization analysis.
15. Sample environment within the CSPEC scope for the wide range of scientific cases studied on CSPEC should be consistent with the demands of signal to noise.

3. SUPPORTED SPECTROSCOPY MODALITIES:

3.1 Quasielastic scattering (non-crystalline condensed matter, powders, soft matter liquids)

Quasielastic scattering probes dynamics on the pico- to nanosecond scales and includes diffusion processes, tunneling, librational and rotational motions. The aforementioned motions are typically found in hydrogenous materials, soft-matter, biological systems and glassy compounds. Typically, these materials have very broad spatial correlations and as such the Q-resolution can be degraded to improve flux, or focus the neutron beam on a smaller sample with the resultant degradation of divergence and thus Q-profiles. In contrast, the energy resolution must be freely tunable, from 5 μeV upwards, to adjust the experimental time window to the time scales of the motions of interest. The data that one extracts in a quasielastic experiment lie very close to the strong elastic line and any deviation from a triangular or Gaussian energy resolution function makes it difficult to extract the information required. It is imperative that the signal to noise is optimised (10^5 at 5 Å) and the background is minimized and well understood. The demand for a signal to noise of 10^5 at 5 Å comes from the optimized signal to noise current day chopper spectrometers which CSPEC must be able to compete with. The neutron beam spot size for quasielastic scattering of non-crystalline materials must be able to vary from large, 4 x 2 cm^2, thereby optimizing the scattering intensities of dilute but abundant samples, to 1 x 1 cm^2 for compounds with small sample volumes. Repetition Rate Multiplication (RRM) may allow the cumulative use of adjacent incident pulses for incident energy wavelengths > 6 Å, with small variations in energy and momentum transfer, to increase flux.

3.2 Quasielastic scattering (Single crystal)

The comments made in the previous section remain true for quasielastic scattering from a single crystal except that the Q-resolution, which is closely matched to the energy transfer, must remain adequate to determine the lifetimes and spatial correlations across the entire S(**Q**, ω). The scientific interest in quasielastic scattering of single crystals is rooted firmly in hard condensed matter, typically magnetism or glassy behaviour of functional materials. Novel materials in these scientific domains are difficult to synthetize and result in small crystals as small as mm^3 size. It is therefore important to be able to focus the neutron beam to a small spot size while maintaining a clean divergence profile that can adequately probe S(**Q**, ω).

3.3 Inelastic neutron scattering (non-crystalline condensed matter, powders, liquids)

Inelastic scattering occurs due to processes with discrete energy steps. These include collective excitations such as vibrational modes, stretching modes, density of states and spin waves. A powdered sample will scatter broadly (in Q) due to the almost isotropic texturing of the sample. As such the scattering profiles are broadened and the instrumental background must be minimal, well understood and free from spurious scattering. To gain optimal information from the scattering profiles it will be imperative to have access to theoretical models convoluted with the instrumental resolution and powder averaged.

3.4 Inelastic neutron scattering (Single crystal)

Inelastic scattering profiles from single crystals on CSPEC will provide 4 dimensional S(**Q**,ω) profiles across 8-10 incident wavelengths via RRM. Single crystal excitations are of most interest in the field of hard condensed matter. The single crystal sample will be rotated to provide the extra **Q** dimensions and it will be possible to measure S(**Q,** ω) in event recording as the sample is continuously rotated. To gain optimal information from the scattering profiles it will be imperative to have access to theoretical models convoluted with the instrumental resolution.

3.5 Kinetic measurements for all modes

A combination of the high flux and the multi-energy mode via RRM makes CSPEC most suitable for experiments that investigate time resolved kinetic phenomena, including pump-probe experiments and out of equilibrium behaviour. The high flux (potentially further enhanced by combining several RRM pulses) will enable monitoring of transient phenomena with a time resolution of minutes. For cyclic processes, time-resolved stroboscopic measurements will benefit both from the high flux and the multi-energy mode to probe the dynamic response of a compound to an external trigger with a time resolution in the order of milliseconds.

4. SYSTEM CHARACTERICS

4.1 System purpose

CSPEC is a cold chopper spectrometer that will extract cold neutrons ($2 < \lambda < 20$ Å) from the 3 cm butterfly moderator. The ~160 m, moderator to sample, distance enables measurements across a ~1.72 Å wavelength bandwidth using RRM within each ESS frame. By rephasing the choppers the energy transfer range measured by CSPEC will cover 3 to 4 orders of magnitude, from few µeV (quasielastic scattering) up to 20 meV (inelastic scattering). The chopper cascade, optimised for energy resolutions down to $\Delta E/E = 1.5$ %, for $\lambda \geq 4$ Å, must ensure that the distance in time between incident adjacent RRM pulses can be adjusted to ensure that the complete energy transfer region of interest, energy transfer = $\hbar\omega = \infty < E_i < 0.8E_i$, can be measured.

The technique is highly background sensitive. The instrument must be considered and designed with signal to noise in mind. Special care has been focused on the design to minimize the background generated by the source, the primary and secondary spectrometer components. This is especially pertinent in a scientific age where the well-defined scattering features have been probed and the exciting science lies in scattering functions that are typically weak and broad in both energy and reciprocal space. Sample environment for the wide range of scientific cases studied on CSPEC must be consistent with these demands of signal to noise, 10^5 at 5 Å. The signal to noise requirement is based on current state of the art cold chopper spectrometers: CNCS, IN5, TOFTOF, AMATERAS and LET with typical signal to noise levels of $10^4 – 10^5$. The signal is defined as the peak neutron intensity on detectors by an incoherent scatterer, such as Vanadium, and compared to the noise which is defined as the neutron intensity at a time when the signal has decayed to background levels. A high signal to noise makes it possible to probe the weakest of neutron scattering signatures for instance: signatures of spinon pairs, spin-liquids or the exact details of diffusion. Uniquely LET can offer a signal to noise of 10^5 and is therefore perfectly placed to probed the most interesting scientific phenomena. CSPEC, as the world leading cold chopper spectrometer, must be able to offer an equivalent or better signal to noise.

The neutron beam at the sample position will illuminate a sample area ranging from 4 x 2 cm^2 to 1 x 1 cm^2 (height x width). The detectors will ensure the E and Q requirements (including ΔE and ΔQ) as defined in the high level scientific requirements, 4-6.

The science case for CSPEC is very broad and will satisfy communities who study systems as diverse as strongly correlated physics to life sciences. A few examples include:

- Spin wave excitation spectra of novel materials, such as those with strong spin-orbit interactions that may lead to novel nanodevices.
- Magnon-phonon interactions in magnetothermal or multiferroic materials.
- Time dependence of the rotational or translational diffusive processes in enzyme catalysis.
- Dynamics of hydration processes and the structural relaxation of the glassy water.

- Time dependent phenomena of hydrogen storage in clathrates.
- Proton diffusion in metal organic frameworks.
- Diffusion dynamics and the relation to the ordering mechanism of solidification.
- Studies of in-operando proteins such as those involved in photosynthesis: light-induced dynamics of the antenna pigment/protein complexes.

4.2 System Life-Cycle

The figure below shows the high level life-cycle of the CSPEC instrument without the details of each development phase. Each phase of the instrument development is concluded with a TG review and with accompanying design review. 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.

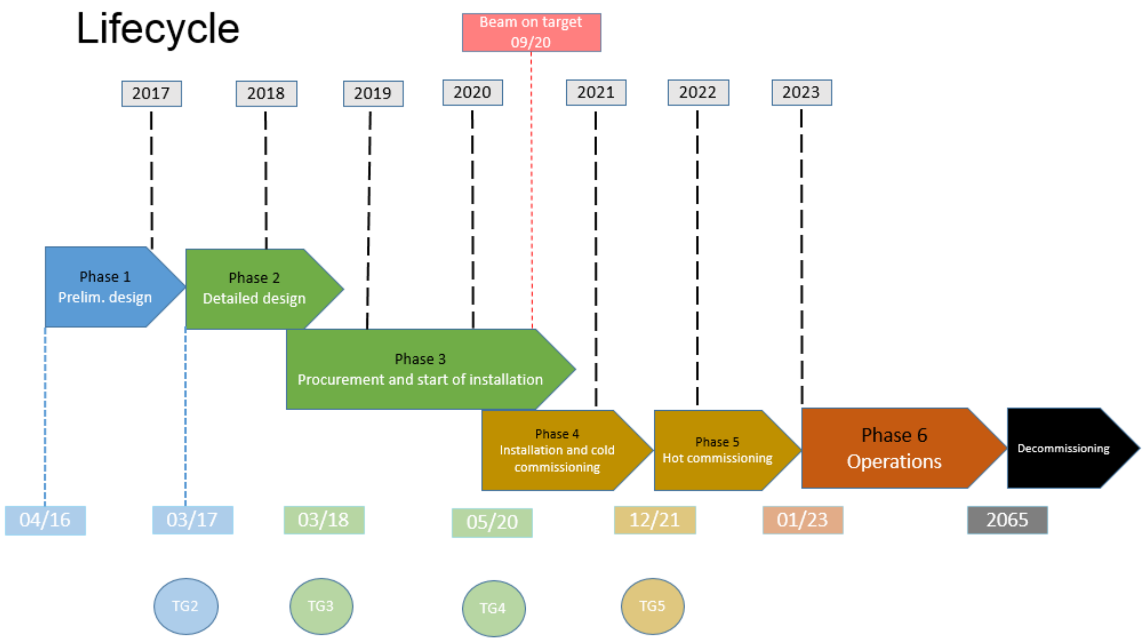

Figure 1:Schematic overview of the instrument development process for CSPEC with the related life-cycle.

4.3 System overview

The conceptual CSPEC instrument is subdivided into the following main functional blocks:

- Neutron optics
- Chopper system
- Shielding

- Shutters
- Detector tank
- Detectors
- Sample environment
- Beam monitoring
- Beam stop
- Control hutch
- Instrument control
- Personnel Safety System, PSS.

All components have to be defined and designed to fulfill the high-level requirements as the basis for the detailed functional and non-functional instrument and component requirements.

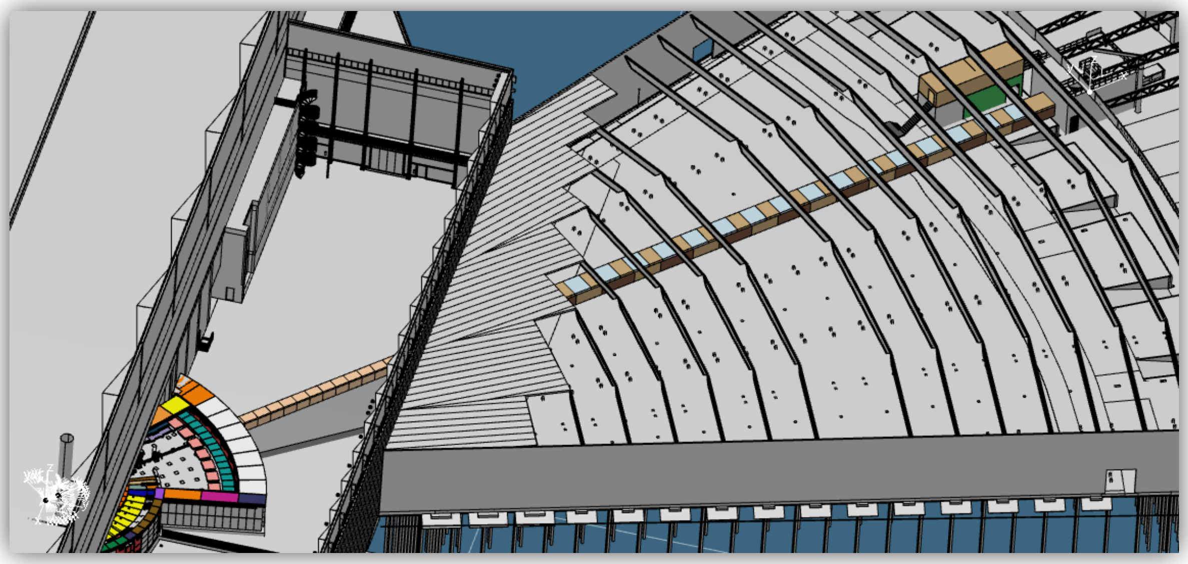

Figure 2: Engineering drawing of the CSPEC layout from moderator to sample cave.

CSPEC is positioned in the west sector on beamport W3. The spectrometer will extend over three different buildings – experimental hall 2 with building designation D03, the guide hall with building designation E02 and finally the experimental hall 3 with building designation E01.

4.4 Neutron Optics:

4.4.1 Beam extraction

The guide begins at 2 m and will view the cold moderator of the top butterfly moderator. CSPEC requires extraction of a broad divergent (+/- 1^{o} @ 3Å) cold neutron beam ranging from 2 to 20 Å. It should be noted that time of flight spectroscopy is a very flux intensive technique that is rarely Q limited. As such it is important to extract and transport a wide divergence. For example, scattering from soft matter compounds, typically with λ > 5 Å, can accept a divergence of ± 2^{o} due to the broad features in the Q-dependence of the scattering profiles.

4.4.2 Beam transport system (BTS).

The instrument length, moderator to sample ~160 m, provides a 1.72 Å wavelength bandwidth. The beam transportation system is optimized using the following parameters:

- Guide must transport 2 < λ < 20 Å.
- Beam dimensions vary from 4 x 2 cm^2 (height x width) at the sample position to 1 x 1 cm^2 .
- < 10 % intensity variation across the sample position, necessary to extract the correct neutron scattering cross sections.
- The guide will transport at least ±1^{o} divergence at 3 Å but can transport more if possible, especially at higher wavelengths.
- The divergence profile must be smooth to facilitate scattering from single crystals.
- The guide dimensions at the pulse and monochromating chopper positions must be consistent with the requirement for $\Delta E/E_i$ = 1.5 % for λ ≥ 4 Å .
- The guide must be optimised for signal to noise.

Guide overview

An overview of the guide is provided in Figures 3. The guide starts with a vertical s-curve that curves the guide 2 times out of line of slight with once out of line of sight just before the bunker wall. Horizontally, the guide is constrained by the piling corridor and the engineering constraints of the ramp between E01 and E02. A curved guide to accommodate these requirements is the result. Beyond the curved guide, a single ballistic component describes the width of the guide up to the monochromatic chopper, while vertically two ballistic components, separated at the pulse-shaping chopper, are required up to the monochromatic chopper. A final tapered nose delivers neutrons up to 20 cm from the sample.

The guide parameters have been optimized with respect to neutron transport and cost. The absolute values of the guide reflectivities, m-values, have been chosen to limit cost and ease of production. A substantial portion of the CSPEC guide will be developed at the TUM optics facility under the direction of P. Link.

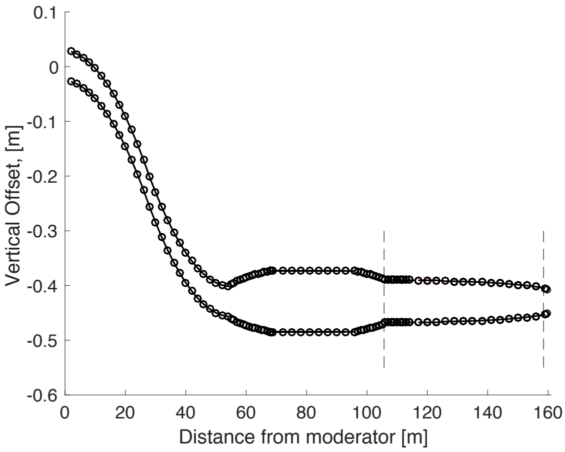

Figure 3(left): Vertical guide overview, distances are McStas coordinate system. The dashed lines show the position of the pulse shaping and monochromating chopper.

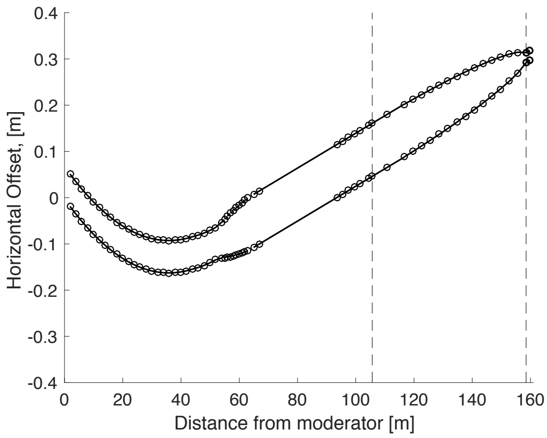

Figure 3(right): Lateral guide overview, distances are given in McStas coordinate system. The dashed lines show the position of the pulse shaping and monochromating chopper.

4.4.3 Further optics components:

Slits: a set of movable slits will be placed at the end of the guide that will make it possible to finely tune the beam size and shape.
Collimation: an oscillating radial collimator will be used to reduce background from sample environment and is positioned outside the sample environment pot.

An upgrade path to enable polarisation analysis is foreseen. To enable incident beam polarisation an exchangeable approximate 2 m guide section before the monochromating chopper is incorporated into the guide design.

An upgrade path to enable the placement of a T0 chopper before the end of the bunker wall by incorporating a 0.5m exchangeable guide piece.

4.5 Chopper System

The chopper cascade, in conjunction with the guide and detectors, must access the energy resolutions stated in the high-level requirements. The technical choice for choppers considers, as a high priority, reliability. It is for this reason that:

- High speed choppers are all positioned outside the bunker with easy access to the chopper pits.
- The high speed chopper disks are symmetric.

- The chopper blade diameter does not exceed 700 mm.
- Frequencies do not exceed 350 Hz (most experiments will run at frequencies of 250 Hz or less.

Table 1 gives an overview over the chopper system and the characteristics of the various axes. The absolute positions of the bandwidth choppers may change slightly when engineering realities are considered.

Chopper Name	Position (m) McStas ISCS coordinate system	Single Blade (SB) or Counter rotating (CR)	Diameter (mm)	Number of openings & slit width (angle)	Max Frequency (Hz)	Blade material (Absorber)	Bearing
BandWidth 1	(-0.077, -0.07, 15.5)	SB	700	1 & 34.30°	14	Aluminium (^{10}B coated)	Magnetic
BandWidth 2	(-0.1, -0.12, 20.03)	SB	700	1 & 44.32°	14	Aluminium (^{10}B coated)	Magnetic
Pulse Shaping	(-0.319, -0.423, 105.666)	CR	700	3 & 23.45°	175	Carbon fibre (^{10}B coated)	Magnetic
Mono_RRM	(-0.318, -0.423,,158.450)	SB	700	1 & 4.15°	350	Carbon fibre (^{10}B coated)	Magnetic
Monochromating	(-0.318,-0.423,158.50)	CR	700	1 & 4.15°	350	Carbon fibre (^{10}B coated)	Magnetic

Table 1: Overview of the chopper cascade with relevant parameters.

The system is comprised of two bandwidth choppers (BW) that define the useful wavelength band at the detector position, a pulsing chopper pair at 2x/3 m and a monochromating chopper pair at x m (x = distance from the moderator to the monochromating chopper). A pulse removal chopper, denoted as mono_RRM, just in front of the monochromating chopper pair will ensure the clean separation of pulses in repetition rate configuration. The monochromating chopper and the mono_RRM chopper will be in a single housing.

It is currently unclear what the signal to noise at the sample will be. In particular, there is substantial concern about the high energy prompt pulse resulting from the protons on the target. These high energy particles are observed on all chopper spectrometers at spallation facilities with varying degrees of intensity. Curving the guide twice out of line of sight in conjunction with the long instrument length should limit the prompt pulse. However, due to the substantial uncertainty there should be a mitigation strategy. A T0 chopper at 18 m rotating at 14 Hz will allow the transmission of 2 Å neutrons while reducing the prompt pulse feature by an order of magnitude. The guide and vacuum housing will be designed to enable to placement of a T0 chopper, if required, however the cost of a T0 chopper is not within the day 1 scope of the instrument.

4.6 Shielding

4.6.1 Guide and chopper shielding

The shielding will satisfy the biological safety requirements in and around the length of the instrument for those operating in the vicinity with beam on sample.

Shielding within the bunker will be required to limit the activation of components and minimize cross talk between CSPEC and the guides of the adjacent instrument, BEER and BIFROST.

The shielding beyond line of sight is designed to shield against gamma flux only. These flux estimates are obtained by considering that all the neutrons escaping from the guide or absorbed are converted to 4.4 MeV photons, the photon energy of the gamma released after the interaction between the neutron and Ni/Ti of the supermirror coating.

In addition, extra care will be taken to limit any fast neutrons that have been able to stream through the guide housing by using steel shielding closely placed around the guides at relevant positions.

The chopper pits will be used to enable maintenance work but also to create large volumes in which the fast neutron stream can diffuse, and thereby reduce the intensity and energy of high-energy particles in the forward direction along the guide.

The shielding calculations that have been performed to date consider all choppers in the open position at 3 Å (highest flux). These calculations estimate the biological shielding requirements and not the stringent signal to noise requirements on the time of flight spectrometer. MCMPX calculations will be performed in the next phase to determine shielding requirements to optimise the signal to noise on the instrument.

4.6.2 Detector tank shielding

The shielding estimates for the detector tank are obtained by considering that all the neutrons absorbed by a hydrogen sample that will release 2.31 MeV gamma photons. Secondary scattering effects that will increase the background levels of the experiment are however of great concern. The floor beneath the detector tank will consist of boronated concrete to limit floor shine. Skyshine will be limited by a polyethelene/B4C laminate cover that will cover the detector tank.

The shielding will also ensure that the signal to noise (signal = elastic line) on the sample is at least 10^5 at 5 Å for a typical vanadium sample, with signal determined by the elastic intensity and the noise measured at a time of flight position where the signal has decayed to background levels. The calculations performed to achieve this signal to noise should include all components on CSPEC and scattering background contributions from nearby instruments.

It should be noted that although we are now costing HD concrete for shielding purposes, it is more likely that a laminate of other materials (boronated PE, steel cans containing Fe_3O_4 nanoparticles and a hydrogen rich fluid or wax) will be employed to optimise shielding and cost.

4.6.3 Beam stop

CSPEC will require to access low Q regions to deliver its scientific case and this requires careful consideration of the materials that the transmitted beam comes into contact with. After experience from LET and AMATERAS, the first material the transmitted beam will encounter is a layer of $^{10}B_4C$ equidistant to the sample to detector distance. This will limit any inelastic spurious contributions since most of the scattering, inclusive of the gamma background, will occur simultaneously as the elastic line of the scattering. Beyond the $^{10}B_4C$ layer a further beam tube will extend behind the detector tank ending in an opening surrounded by concrete.

4.7 Sample environment:

The science case for CSPEC covers a broad user community. The ESS science case strongly focuses on the ability to probe time dependent phenomena. Equally, the science case for CSPEC has a strong component that focuses on time dependent phenomena and in-operando experiments. The sample environment, which includes the sample environment pot, must provide for such experiments.

The area for sample environment is integral in the design of the detector tank and is designed with a broad range of apparatus in mind. Sample environments will be optimized for the instrument with stringent signal to noise requirements and, where possible, the tails of cryostats and furnaces will be removed to limit background contributions.

To address the scientific questions as outlined in the CSPEC proposal the following sample environments will be available from day one, as outlined in the minutes of the Scope Setting Meeting.

- Cryofurnace (3-600 K, ΔT= 0.1 K) (CSPEC - in scope),
- multiple sample changer (up to 8 samples), possible collaboration between ESS and TUM (CSPEC – in scope),
- sample rotation stage and goniometer (CSPEC – in scope),
- Dilution insert (in-scope)
- Access to a 12 T magnet (ESS Pool – not in scope).
- In-situ capabilities (in-kind – not in scope).

In-situ environments will be provided by in-kind contributions and collaborations. A current collaboration with J. Pieper (University of Tartu) will develop the technical requirements for a pump probe experiment on biological systems.

The sample environment from the sample environment pool will be available for use on CSPEC, principally a high field magnet (12T). We are providing input to the design and manufacturing details of the high field magnet, with particular focus on the opening window and sample pot dimensions.

4.8 Sample and Detector vessel:

The secondary spectrometer is a 3.5 m flight path and the detector tank will accommodate the detector range with an angular range of 5 ➔ 140° horizontally, within scope of the instrument, and ± 26.5° in the vertical direction (total detector height: 3.5 m). Provisions will be made to extend the detector angular range to negative angles (max -30 °). To minimize secondary scattering, the internal walls of the detector tank will be covered in a neutron absorbing material, such as Cd or B_4C, that does not strongly degas. Vertical vanes between detectors columns will eliminate secondary scattering effects from the detectors and their housing. An oscillating radial collimator will further reduce background from bulky sample environments.

The sample environment pot, 1000 mm in diameter, will permit sample environments to be mounted and operated from the top as well as from the side. The side opening will also enable the user to view the sample environment. Non-standard equipment can also be aligned using a 6 axes goniometer positioned on the floor of the sample environment pot.

The sample and detector vessel will be evacuated to cryogenic pressures (10^{-6} mbar). This allows one to minimize the thickness of any tails on cryogenic equipment and thus any scattering from it. The cryogenic evacuation will extend to the monochromating chopper at which position there is an Al window.

The sample pot can be separated by the rest of the detector tank to facilitate the exchange of sample environments. The sample pot will be separated from the main detector vessel by an Al window that can also be used for experiments requiring ambient pressure conditions. Separating the sample pot from the rest of the detector vessel also makes it possible to reduce the thickness of the Al windows required before a ^{10}B-multigrid detector, the technology we are pursuing at this stage. Since the sample pot can be evacuated and brought up to ambient pressure independently from the detector tank, the detector tank vacuum can be considered as static. A technical solution to separate the sample environment pot from the rest of the detector tank is under consideration and is presented in the Preliminary System Design Description.

Special care is taken to ensure a non-magnetic vessel that enables high magnetic field measurements (up to 12 T) and polarization analysis as planned for the upgrade stage of the instrument.

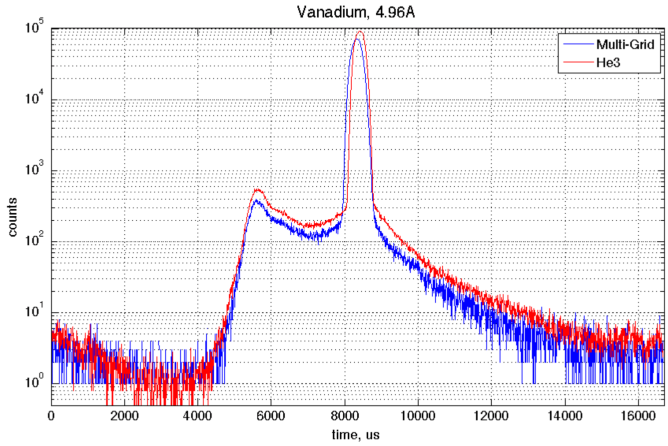

Figure 4: Comparison of the scattering from an isotropic scatterer (Vanadium) onto the ^{10}B multigrid detector demonstrator and He^3 detectors. Counts normalised to peak.

4.9 Detectors

The detectors will cover an angular range of 5° → 140° horizontally and ± 26.5° in the vertical direction. Assuming a minimum flight path uncertainty of ΔL = 15 mm, the time resolution of the detector is matched to the primary spectrometer. In the scope setting meeting the CSPEC team agreed to provide a path forward with respect to detector technology. The CSPEC team decide to use ^{10}B multigrid detector technology, however, since development is under way, we would like to clarify that if the technology does not meet the high level scientific requirements then an alternative will be pursued. Results from the position sensitive multigrid ^{10}B demonstrator, installed in the detector tank of the cold chopper spectrometer of the SNS, CNCS, adjacent to ^{3}He detectors, remain very convincing.

Comparisons between ^{3}He and ^{10}B detector technologies show very similar signal to noise and energy resolution over the entire time frame measured, Figure 13. Evaluations of a range of samples are underway. The latest results are shown on the ESS Wiki Detector group page and will be available in the Arc-xiv paper provided by the ESS detector group.

Within the CSPEC scope 100% of the detector modules will be implemented but only 50% of the detector electronics will be operational on day 1.

4.10 Shutters

A light shutter is provided by the ESS at the end of the monolith (5.5 m) and used only during beam shutdown to stop the photons after the beam has been switched off. An additional instrument shutter will be placed shortly before the bunker wall within the bunker. Closing the instrument shutter will enable access to the sample position and also access to the beamline, beyond the bunker, for maintenance purposes.

4.11 Beam monitoring

Beam monitoring will be essential both for commissioning and calibration purposes. Whether the monitors remain in place for the duration of the experiment or can be remotely removed is not yet clear. Provisions for neutron flux beam monitors after each chopper and at the beamstop will be made. The monitors that determine the transmission profile of the sample, after the monochromating chopper and at the beamstop, will resolve the incident wavelengths in rate repetition configuration.

4.12 Vacuum monitoring

The ESS vacuum team are responsible for monitoring of the instrument vacuum. This includes the guide vacuum (10^{-3} mbar) and the detector tank vacuum (10^{-6} mbar). It does not however include the vacuum of the chopper systems which is included in the chopper design and implementation.

4.13 Technical laboratories.

Within the CSPEC scope, CSPEC will maintain a laboratory for maintenance work and basic sample preparation. This laboratory is positioned close to the control hutch. Some preparation space is also available on top of the detector tank. Preparation space, within the laboratory, at least 20 m^2, is required and contains basic equipment. A range of crystal mounts and standardized Al and Cu sample cells should be available at the instrument to meet the needs of the experimental teams. The instrument will rely on the availability of a sample alignment station to ensure that single crystal experiments do not waste a substantial amount of time in the case of misaligned crystals. Storage space for samples before and after the experiment will be provided close to the instrument for samples with low radiation levels, and in the ESS sample storage area for high doses.

4.14 Personnel Safety System, PSS

Personal safety systems will be put in place as defined by ESS in line with Sweden's radiation safety regulation.

4.15 Control hutch

The control hutch must provide a good working environment that optimises the users ability to perform the experiment, from scientific discussion to data analysis. The work environment must provide natural light, thermal comfort, sufficient space to enable a team of 6 to work, reduced noise and limited vibrations.

4.18 Instrument control and data collection and processing

The instrument control, data storage and processing is provided by DMSC and is not part of the CSPEC instrument workpackage. It is therefore not costed. The instrument control shall enable to remotely control all necessary technical parts, i.e. the chopper parameters, motors, such as the slit systems, collimator, focussing guide and sample environment parameters. For commissioning and instrument control, monitor counts after each chopper set should be available and the count rate as a function of time-of-flight and voxel position of the detectors. These data must be available in minimal time to limit delays in the commissioning process.

Count rates:
To determine the count rates we consider quasielastic scattering as the most appropriate scattering profile for CSPEC. On CSPEC the highest flux obtained is at 3 Å, ~ 4e10 n/s/ Å onto the sample. A monochromatic pulse of approximately 100 µs extracted out of the 71 ms time period of the ESS, will provide a broad energy resolution at 3 Å, results in 5.63e+07 n/s on the sample, this is a time averaged count rate.

A 10% isotropic scatterer will scatter 5.6e6n/s into the complete detector tank, 2.1 steradian, out of a complete 4pi steradian. The count rate on the CSPEC detector range is therefore 9.36e+05 n/s which results in a daily rate of 8.09e+10 n/day. A neutronic event requires 12 bytes of storage space and thus the daily requirement is 9.7e11 bytes which translates into $9.7027e11/(1024)^4$ Tb = 0.8825Tb/day for a single incident pulse. However CSPEC will run in RRM mode with approximately 10 pulses per period and therefore the data rates will be approximately 8.8 Tb/day. This is typically an order of magnitude greater than data rates on current day chopper spectrometers.

Current day experiments on cold chopper spectrometers already struggle to extract and process data, with processing times up to 10 minutes. It will be essential for the ESS to process data on minute timescale, such that a data set can be viewed in minimal time, thereby enabling timely intervention during commissioning and experiments, in particular for in-situ and time dependent experiments, a main scientific goal, on CSPEC.

All instrument parameters are recorded in event mode for the data collection and processing. It is essential to provide software at the instrument that enables time-of-flight and absolute detector positions to be transformed to S(**Q**,ω) for each incident wavelength. The primary data analysis must considers instrumental resolution and background corrections. For user operation it will be essential to provide theoretical software to analyse the data extracted.

5. OPERATIONAL CONCEPTS CSPEC

5.1 Operational environment

CSPEC is positioned in the west sector on beamport W3, see Figure 14. CSPEC will extend over three different buildings – experimental hall 2 with building designation D03, the

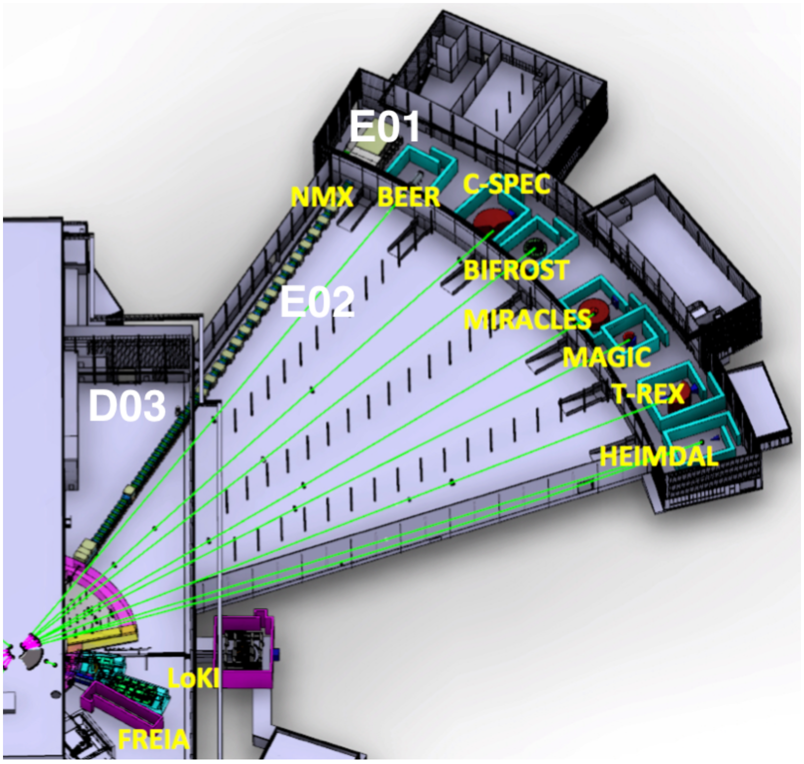

Figure 5: Beamport allocation in the west hall

guide hall with building designation E02 and finally the experimental hall 3 with building designation E01. The instrument will be operated in a controlled environment with a temperature of 22±2 °C all year round.

The floor height in D03 is 2 meters below target centerline. The floor in the E02 is 1 m below target centerline and in E01 it is 3 m below target centerline. Floor loading in the D03 is 14 tonne/m^2 and 20 tonne/m^2 in E02 and E01. Floor stability in the halls is specified to be maximum 3 mm w.r.t elastic movement and another maximum 3 mm due to creep/deformation.

In D03 there are three different cranes with weight limits 5 tonne and 30 tonne. The lifting height, from the floor, associated with the two cranes are 9.5 m for the 5 tonne crane, and 12 m for the 30 tonne. In E02 a gantry crane extends along the hall. In E01 there is only one 10 tonne crane and the hook height is at 10m from the floor.

Utilities and media are brought to the instrument via utility connection points situated close to the instrument. Media include: DIH_2O, N_2, instrument grade compressed air, cooling water. Utilities include: office IT, office communications, power, PSS, DMSC and ICS (provides the master clock). For detailed and updated listing of requirements and/or specifications related to operational environment see the System Requirements Document.

The ESS facility has 5 different operating modes, ref [ESS-0003640 Conops]: Shutdown, Studies, Studies on Target, Startup and Production. These modes have various impacts on instrument operations. Pure experimental work can only be conducted during ESS-mode Production. Access to instrument equipment for maintenance, calibration, cold commissioning is mainly done during Shutdown, Studies and Studies on Target – naturally after safety assessments are performed and maybe with some restrictions. During Startup instrument operations is limited to alignment, commissioning and calibration runs. When ESS has entered into a steady-state operations phase the following principal schedule may apply:

- 200 days/year of neutron production in steady state operation, of which 160 days will be delivered to the user programme.,
- 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 periods for studies on target,
- A series of study days to allow for fine-tuning of accelerator and target systems.

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

The CSPEC instrument is foreseen to be managed and operated by a team of 2 (Instrument scientists)+1 (SA) scientists or 1 technician in steady state operations. The technicians might split their time with other instruments. ESS will be manned 24 hours/day and such a model will provide flexibility for users before and during experiments in addition to time required to analyse results. Data collection, storage and analysis are provided by DMSC, physically located in Copenhagen. Currently it is foreseen that a DMSC member of staff will be an instrument team member, local contact for the users and focus on data analysis. This person must be fully integrated into the CSPEC team and frequently be on-site.

5.2 Operational scenarios

The beamtime for user experiments is allocated in a peer-review process based on scientific merit and feasibility. Proprietary access for industry is also envisaged. In order to partake in spectroscopy experiments the users will have employed bulk measurement techniques to characterize their samples.

The typical users of the CSPEC instrument are scientists, specialized in hard or soft condensed matter physics, material or biological science. The user team would typically consist of 1-4 scientists (PhD level, doctoral students and principal investigator) who perform the experiment within the allocated beamtime. Most users should be able to operate the instrument independently after a 2 hour introduction by the ESS instrument team. The less experienced users, who would require more support, would be expected to establish a collaboration with ESS scientists. Users will either bring their samples with them, ship them beforehand, or prepare them using ESS support facilities. After the experiment, the samples should be returned to the users, after clearance through radiation protection. The users will process the data at the ESS at least to the point where it can be input to third party software.

Outline of an experiment on a cold chopper spectrometer at the ESS.

A typical experiment at the direct geometry time-of-flight spectrometer CSPEC consists of the following steps:

Beam shaping and choice of energy resolution:

The energy resolution of the primary spectrometer is determined by the choice of the chopper rotation speed and phasing of the pulsing and the monochromating chopper pair. These parameters will be adjusted for each energy and energy resolution required. Similarly, the rotation speed and phases of the pulse removal chopper (mono_RRM) chopper will have to be set to select the time interval of the subpulses during the ESS time frame, according to the requirements of the experiment. The exchange guide (last piece of the beam transportation system) has to be chosen and moved into position to either measure with a standard extended beam, or a focussed beam. A slit system in front of the sample should adjust the beam dimensions to fit to the sample dimensions. The oscillating radial collimator will be in operation.

All of the above steps shall be executed remotely via the instrument control software that is common to all time-of-flight instruments. The settings shall be available as metadata for each data collection run in addition to the timing pulse of the accelerator to enable true time determination.

Preparation and mounting of samples:

Typical samples may consist of powders, liquids, layers on a substrate, and single crystals. For most standard experiments, they are packed into a container (mostly Aluminium, but other materials might be used according to pressure / magnetic field and temperature requirements). Laboratory space close the instrument will be used for the filling and preparation of the sample containers, including access to a glovebox for moisture and air sensitive materials, a balance and a furnace (not within CSPEC scope).

Powder samples can be attached to the end of the sample stick and positioned inside the sample environment, at the sample position, via the sample chamber top opening. An automatic thermalized sample changer will enable up to 5 sample changes without opening the sample chamber. Single crystals samples, held by a goniometer mount, or positioned on an alignment device attached to a goniometer head, can be attached to an in-situ 6-axes remote controlled goniometer. A range of crystal mounts should be available at the instrument to meet the needs of the user.

CSPEC will accommodate standard sample environments including cryostats, dilution stages, furnaces, and magnets that can be installed from the top of the sample area tank. A variety of non-standard sample environments will be available at CSPEC to accommodate *in-situ* and *in-operando* experiments. These non-generic sample environment can employ a 6 axis goniometer stage positioned below the sample position.

It is crucial for the long-term scientific productivity of the instrument that the spectroscopy experiments are as streamlined as possible. There must be flexibility to install a wide range of standard sample environments available in the ESS sample environment pool to cover temperature, magnetic and electric fields, pressure or humidity. It will be possible to study samples in more specialised sample environments, such as gas pressurisation equipment, levitation equipment, or perform complementary measurements such as optical spectroscopy (Raman or infrared spectroscopy) or specific heat measurements on the sample during the experiment. The use of such equipment will have to be agreed well in advance with the ESS instrument team. As a general principle, the user team is expected to be responsible for bringing in such special equipment and the ESS instrument team will provide support with mounting and integrating it at the instrument. For equipment developed by the ESS as part of an in-house research program, the users are expected to establish a collaboration with ESS scientists.

The sample environment area can be operated under cryogenic vacuum, under ambient conditions or under gas pressure. An Aluminium window will separate the detector vessel, at 10^{-6} mbar, from the higher pressures, up to 1 bar, in the sample environment area, and will be remotely controlled.

For the installation of sample environment and sample changes, safe access to the sample stage is required when the accelerator is on and the instrument shutter is in the closed position.

Multiple scattering shall be kept to a minimum, this implies that the transmission of the scattering must be greater than 90% for non-absorbing samples. In-situ checks of the sample transmission will be possible via incident and transmitted beam monitors. If the beam is collimated then a monitor at the entrance of the beam stop tube will be able to provide information on the sample transmission. A test beamline will be highly beneficial to determine sample transmissions as a function of sample rotation prior to the experiment, thereby improving the resultant data analysis.

Once the sample is mounted, the control of the sample environment should be remote. The control parameters (e.g temperatures, magnetic fields) shall be monitored continuously and available as time stamped meta-data for each measurement. Event recording will be the normal mode of operation.

Depending of the type of sample and the experimental questions, the frequency of sample changes might be as often as one sample change every 15 minutes and this will require an automatic sample changer.

Data collection runs

A single measurement consists of the registration of the scattered neutrons as function of (uniquely identified) detector voxel and arrival time at that position, for the duration of a preset time or a preset number of ESS source pulses. Data recording in event mode shall be standard. Typically, one sample is measured at different settings of the control parameter, e.g. at different temperatures, magnetic fields, sample orientations or at different energy resolutions. The instrument control software shall allow the change of these parameters to be included in an automated measurement script that should be easily modified during the experiment. The samples will be rotated to provide a fully consistent $S(\mathbf{Q},\omega)$ map in the case of highly textured samples and in the case of single crystals. The length of time that the samples are illuminated depends on the scattering strength of the sample constituents and the chosen instrument settings, the central wavelength and the energy resolution.

Besides the sample (+ container) run, each data collection run shall be complemented by (a) an empty container run and cadmium samples for background subtraction (at correct temperatures) and transmission purposes and (b) a vanadium calibration run at identical instrument settings to determine detector efficiencies and absolute scattering cross sections.

Data processing

Four dimensional energy/reciprocal space maps, $S(\mathbf{Q},\omega)$, will be generated in the case of single crystal measurements while 2 dimensional energy/reciprocal space maps $S(Q, \omega)$ will be provided for the case of non-crystalline or powdered materials. For each detector voxel and registered neutron, the energy transfer to the sample is calculated from the neutron velocity after scattering, i.e. via the time-of-flight needed to cover the known sample-to-detector distance. The neutron energy of the incoming pulses is known from the chopper parameters, and the time-of-flight of the elastically scattered neutrons can be either taken from geometry or determined from the vanadium calibration runs. During the data collection runs, data processing should allow the on-line display in the appropriate form. Intensity as a function of time and more processed S(**Q**,ω) will be required to check and monitor the experiment as it is running.

As previously stated, the amount of data gathered on a chopper spectrometer at the ESS will exceed the data on todays instruments by one to two orders of magnitude. It is thus essential that data visualization and analysis tools must be fast enough to make decisions while running the experiment. The tools must be ready to handle large complex data sets both during the experiment (on-line) and for the final data analysis.
It is imperative that there is a close collaboration between the instrument team, users, DMSC and theory groups. Theoretical expectation of the scattering must be available to compare data with expectation. Data processing requires software tools to perform profile fitting, scaling and comparison to basic models (e.g.SpinW, DFT, molecular dynamics). ESS scientists will support specific data processing and non-standard software (available at DMSC and with the DMSC instrument scientist) necessary to visualize and analyze data. The success or failure of the chopper spectrometers will depend on the ability of the user to extract data in a timely manner and to understand the results.

Sample handling.

After the experiment the sample will be stored according to the safety and radiation requirements. There will be some space provided on the instrument for sample storage.

5.3 Maintenance philosophy

CSPEC's maintenance philosophy aims to utilize condition based preventive maintenance as much as possible. In order to minimize time spent and increase efficiency when performing maintenance, accessibility is a requirement that requires a good deal of attention in the design work.

In general, access to instrument equipment along the beam guide shall be from the top, especially in the bunker region. In this area the aim is to utilize remotely operated vehicles to do the maintenance work, to the greatest possible extent. Further downstream, as the allocated beam line sector widens, more space will be available facilitating access from the sides for inspection and maintenance.

In the following a brief outline of the CSPEC components and the foreseen monitoring is given:

Guide and beam conditioning system:

(i) Operational parameters recorded
   a. Pressure in vacuum guide housing
   b. Regular checks of transported beam intensity using an incident beam monitor regularly and annually via gold foil measurements.
   c. Focussing guide configuration
   d. Beam aperture configuration

(ii) Regular maintenance required for
    a. Vacuum pumps and gauges
    b. Guide alignment: beam monitor at dedicated locations along the guide

Regular maintenance will be done during shut down periods. Realignment of guide sections requires removal of shielding blocks and (optical) access to the laser-tracking reference points. Maintenance and repairs of the focussing guide lift system requires access to the sample area as part of the detector tank.

Chopper system

(i) Operational parameters recorded for each chopper axis include:
    a. Cooling water temperature
    b. Cooling water flux
    c. Vacuum (Pressure, Vaccum pump on/off)
    d. Status of the magnetic bearing
    e. Vibration
    f. Rotation speed
    g. Temperature of the disks
(ii) Regular maintenance required for
    a. Vacuum pumps and gauges
    b. Cooling water circuit (filters etc.)

Preventive maintenance of each chopper axis can be done during regular shut-down periods. Chopper maintenance and repairs that require access to the chopper axis/disk will be possible since all choppers will be housed in large shielding housing with direct access (door) This provides a two fold advantage. First, visual and direct access to the choppers will limit down time and help in the commissioning phase. Second, large shielding housing around the choppers will provide secondary scattering opportunities for high-energy neutrons that will thereafter not continue their trajectories down the guide. CSPEC has no fast rotating disk choppers up to 100 m from the moderator.

Sample Environment:

Sample environment can always be removed from the beamline and all maintenance and repair is performed in dedicated workshops.

Detector tank:

(i) Monitoring includes:
    a. Vacuum (Pressure)
    b. Positioning and movement of radial collimator
    c. Partial water pressure
(ii) Regular Maintenance:
    a. Pumps and pressure gauges

Detectors:

The regular vanadium calibration runs allow for a continuous monitoring of the performance. Maintenance will need access to the detector tank inside the experimental cave and will be done by ESS detector group.

6. CONSEQUENCES OF THE CONCEPTS

6.1 General design considerations

6.1.1 Upgrade options

The scope setting meeting for CSPEC allocated 16.5 M€ from preliminary design, phase 1, to installation and cold commissioning, phase 4. The preliminary design phase, phase 1, has focussed on budget realities within the constraints of the science case presented in the STAP and SAC report of 2014.

Costing of the components has been in close collaboration with companies providing optics, shielding, chopper, detector tank and detector components. A chopper spectrometer does not have a great number of features that can be discarded. All components in the primary spectrometer are required for a functioning instrument. Some secondary spectrometer components may be considered for staging plans. The upgrade path for CSPEC include

Completion of detector electronics on the positive side of the detector bank.

Installation of further detector modules (+ electronics) on the negative side of the detector bank.

Sample environment.

Incident beam polariser

Polarisation analysis.

Further focussing optics.

T0 chopper (if required).

6.1.2 Robust design

Due to the hostile environment along the entire beamline, in particular inside the target monolith insert and the common shielding bunker area, design solutions should be made as robust as possible and minimise sensitivity to imperfections. Robust should be regarded in terms of e.g. minimizing number of components, moving parts (reducing maintenance efforts) and maximizing structural strength. Robust design solutions should also support the ability, where possible, to enable a degraded performance mode in case a failure or an unintentional misalignment occurs. Robust design applicability could include:

- Optics in the extraction system
- Optics in light shutter
- Monolith light shutter - position repeatability (not within the CSPEC scope)
- Neutron guide – mounting arrangement, components misalignment
- Chopper design solutions

Mitigating measures elsewhere along the beamline should be investigated should some of the issues/problems above occur.

6.1.3 Coordination with other systems

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

- CSPEC and TREX are being designed to scatter to the same side for ease of sharing sample environment equipment.
- CSPEC, BIFROST and TREX all have a great interest in the procurement of a high field magnet. Significant collaboration is envisaged.
- TREX and CSPEC may have the same detector technology. This has implications for the detector electronics and the detector vessel.
- Sample environments. Although slightly different in concept both TREX and CSPEC would like to be able to bring the sample space up to ambient pressure without evacuating the entire detector vessel. Significant collaboration is expected in the development of the sample environment pot.
- Neighbouring beamlines, BIFROST and BEER – especially the first 30 m from target center. Compromises cannot be ruled out possibly affecting design and performance of the CSPEC instrument. This should be kept in mind and possible scenarios of how to mitigate such compromises should be considered. Outside the bunker space monitoring of allocated space is mainly required for upstream chopper locations and various expected maintenance activities.
- Target monolith insert – optics alignment, cooling solution. The insert is provided by the Target System to NSS design specification.
- Light shutter – optics alignment, position repeatability and beam guide gap. The light shutter is provided by Target System to NSS design specification
- Bunker system – alignment components in the bunker, optics insert in bunker wall.

7. GLOSSARY

Term	Definition
BW	Bandwidth Chopper
RRM	Repetition Rate Multiplication
ConOps	Concepts of Operations
FOC	Frame Overlap Chopper
IRR	Installation Readiness Review
ORR	Operational Readiness Review
PDR	Preliminary Design Review
PPSC	Prompt Pulse Suppression Chopper
PSC	Pulse Shaping Chopper
PSS	Personnel Safety System
SAR	Safety System Acceptance Review
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

DOCUMENT REVISION HISTORY

Revision	Reason for and description of change	Author	Date
1	First issue	Pascale Deen	2017-03-03
2	Second issue	Pascale Deen	2017-06-19