Project Specification	
Document Number	
Date	2017-01-31
Revision	1 (1)
State	Preliminary

Initial Operations and Staging plan, CSPEC
the cold chopper spectrometer of the ESS

	Name	Role/Title
Owner	Pascale Deen Joseph Guyon Le Bouffy Wiebke Lohstroh Stephane Longeville	Instrument Lead Scientist Instrument Lead Engineer Scientific coordinator (TUM) Scientific coordinator (LLB)
Reviewer	Shane Kennedy, Ken Andersen, Oliver Kirstein, Arno Hiess, Gabor Laszlo, Peter Sångberg	Science Directorate
Approver	Shane Kennedy	Science Directorate

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

www.esss.se

SUMMARY

The initial operations and staging plan describes the preliminary plan for the validation of the instrument function and scientific performance using spallation neutrons. This 'hot commissioning' is beyond the scope of the instrument construction workpackage. This document also describes the potential upgrades beyond the allocated cost category.

1. HOT COMMISSIONING

The 'hot' commissioning of an instrument refers to the testing and validation of the instrument using spallation neutrons from the ESS target station. The main objective of the hot commissioning of CSPEC is to prepare the instrument for the user program in the operations phase of the ESS. In the spirit of the ESS Early Success Strategy the hot commissioning phase will also aim to show how the instrument can deliver its full scientific performance with challenging samples. These two objectives have very different requirements for the samples on the one hand and beam intensity and availability on the other. In this preliminary plan the two objectives will therefore be discussed separately, bearing in mind that the successful completion of the first is a necessary prerequisite for the second.

1.1 Validating instrument function

A neutron scattering instrument is a complex machine with many custom-built subsystems (e.g. optical system, detector system) that in turn consist of technical components (e.g. guides, choppers, detector units, electronic control units). The factory acceptance tests, installation and site acceptance tests of each individual component are included in the cold commissioning of the instrument, but their function together as system to perform scientific experiments can only be tested when neutrons are being produced by the target. The goal of the function validation of the individual systems is to establish the readiness of the instrument to produce reliable experimental data. The validation of the instrument function starts with the validation of the neutron beam characteristics, verifying that the functional requirements (see System Requirements document) have been met. The second part of instrument function validation is data collection from well known and characterised samples.

1.1.1 Beam validation

The Neutron Optics and Shielding group (NOSG) will provide guidelines and assistance in measuring the beam characteristics. The NOSG will provide a detailed plan and schedule for beam characterisation for the hot commissioning phase.

The beam monitoring system provides diagnostics for neutron beam presence in the various parts of the beam transport and conditioning system (BTS). A beam monitor will be positioned after each chopper set. This enables monitoring of the guide performance over time and the transmission through the choppers when aligning the instrument. A final beam monitor in the experimental cave provides a relative measure of the beam intensity as a function of the time-of-flight (TOF). The neutron flux at the sample position will be measured with the flux measurement assembly. The beam divergence and size at the sample position will be measured with the beam visualisation system. The pulse length at various wavelengths will be measured using a Vanadium rod. Measurements of the various types of unwanted radiation (gamma rays, fast neutrons, thermal neutrons outside the desired bandwidth) will be made if deemed necessary by the instrument team or the ESS technical groups concerned.

1.1.2 Spectroscopic data collection from a well-characterised samples

The objective of this part of the commissioning is to verify that the instrument is ready for data collection. Well-characterised samples will be positioned at the sample position, including:

- A Vanadium rod to quantify the elastic line.
- A crystal with well defined crystal field excitations in the required energy range such as PrAu2Si2 (~ 1meV) (Nature Physics, 4, 766, 2008).
- Soft matter with well defined quasielastic scattering (Water, Alkanes).
- A crystal with well defined excitations (phonons or FM spin waves), e.g. a Tb single crystal with excitations up to 13 meV.

Scattering from well-defined samples will not only enable the characterisation of primary/secondary spectrometer but also include data analysis in the characterisation.

1.1.3 Validating scientific performance

1.1.3.1 Time dependent phenomena

The scientific performance of the instrument will be validated using the aforementioned test samples. However the main scientific aim of CSPEC is to enable the study of time dependent phenomena. We have developed a collaboration with J. Pieper (Univ.Tartu) that will aim to study the time dependent behaviour of proteins excited by a laser pump probe. This project will partly validate the sample environment requirements of CSPEC.

Further time dependent experiments that display the capability of the CSPEC are under consideration and these include:

- Charging / discharging of batteries
- Hydrogen uptake in hydrogen storage materials such as metal-organic frameworks.
- Viscoelastic effects in polymeric materials.

1.1.3.2 Background evaluation and reduction

The background level on a time of flight chopper spectrometer will determine the success of the instrument. Although MCMPX simulations will be performed to determine the high-energy background at the sample positions and the shielding requirements will be followed, it is nevertheless clear that hot commissioning will entail a focus on further background reduction. This is clear from commissioning of instruments at ISIS, J-Parc, SNS etc.

The duration of this phase is extremely difficult to predict, but several months of beamtime should be dedicated to “friendly user” experiments. The 150 beamdays foreseen by the

Instruments Division is expected to be sufficient. This phase should also overlap with regular user operations and sufficient beamtime should be allocated at the discretion of the instrument team for resolving issues that have arisen as well as for experiments to demonstrate the scientific potential of the instrument.

2. STAGING

The Scope Setting meeting allocated a 16.5 M€ budget, including 10 % contingency, to deliver CSPEC, a cold time of flight chopper spectrometer with world-leading performance.

The scope setting report stated: *It was agreed that the instrument presented as configuration 2 in the scope-setting report will form the basis of the scope and budget for CSPEC. It will be world-leading already at 2MW beam power and has a clear upgrade path to the full scope. The following conditions were agreed on:*

- *A cost book value of 16.5 M€ was agreed, including a 10% contingency of 1.65 M€.*
- *The agreed cost book value is based on the configuration 2 instrument in the scope-setting report, which had a budget of 17.38 M€, adjusted as follows:*
- *VAT is not included. ESS and TUM will continue to work together to ensure that no VAT is charged to the project. TUM can highlight the VAT on procurements as a risk to the project until the issue is resolved.*
- *The personnel cost book values of the lead scientist and engineer were adjusted down from 77 € /hour to 60 € /hour, resulting in a cost saving of 419 k€ .*
- *The travel budget was reduced from 235 k€ to 190k€.*
- *The bandwidth choppers should remain in the bunker but use magnetic bearings to reduce maintenance requirements, resulting in a cost increase of 160 k€.*
- *The detector height is reduced from 4m to 3.5m, resulting in a cost saving of 330 k€ .*
- *The detector vessel is reduced in height, range of scattering angles and sample detector distance, compared to the detector vessel used for the costing. This is conservatively estimated to result in a cost saving of 150 k€ .*
- *The agreed cost book value is based on the costing of the boron multigrid detectors. ESS feels that the risks are comparable for multigrid and 3 He detectors and advocates to continue planning for boron technology. The CSPEC team will pursue evaluation of 10 B and 3 He detector options. The decision on detector technology will be taken at TG2.*
- *In case 10 B detectors are used, detector modules covering the full range of scattering angles are included in the scope. However, only about 50% of the detector electronics are included in the scope. This should be used to provide an active detection area covering the full range of scattering angles in the horizontal direction and +/- 8° in the vertical direction.*
- *In case 3 He detectors are used, ESS will work with the CSPEC team to provide an alternative solution within the instrument budget, likely resulting in a smaller detection area.*
- *It was felt that some cost savings could still be made to the guide system, which should be studied in collaboration with the Neutron Optics and Shielding Group. Any savings will stay within the CSPEC project.*

- *This detector configuration provides a straightforward upgrade path to full detector coverage.*
- *Any cost savings elsewhere in the CSPEC budget could be used to increase the active detection area.*
- *ESS will propose to Council that CSPEC is one of the first 8 instruments.*
- *It is envisaged that procurement of critical items (detector vessel, choppers and optics) could start shortly after TG2. The CSPEC team needs to work closely with ESS to include this in the early procurement plans before procurement otherwise starts after TG3.*

It is therefore clear that in comparison to day 1 performance, the upgraded performance of the instrument could be significantly increased by detector upgrades to 100% coverage.

2.1 Optimise signal to noise.

Although every effort will be made to minimise the background levels on CSPEC, there will invariable be unforeseen background issues as demonstrated by instruments that have recently been commissioned on high power spallation sources, J-Parc and SNS. It is essential that both manpower, time and money is foreseen in the hot commissioning stage to deal with background reduction. This will ensure that the instrument will produce high profile science as soon as possible and the community remains enthusiastic.

2.2 Full detector coverage.

It has been estimated that 1 M€ will upgrade the detector coverage to 100% via fully connecting the electronics. This must be performed as soon as possible after hot commissioning to ensure that the scientific community is not disappointed.

2.3 Complete sample environment

The local sample environment suite on CSPEC must be expanded to include:

- Cryofurnace
- Cryostat
- High temperature furnace,
- Multiple sample changer,
- Dilution and access to a 12 T magnet,
- Optimised hydrostatic and uniaxial pressure cells (T_{min} ~ 0.3 K & P_{max} up to 5 GPa),
- Huber goniometer: Rotating 2 axis table +/- 10 degrees,
- Internal goniometer for single crystals (attocube style),
- Levitation furnace,
- Gas handling panels for catalysis,
- Humidity chamber for life science research,

Secondary sample characterization: NMR sample cells, coupled impedance spectrometer.

2.4 Polarisation analysis

CSPEC team envisage using a polarising supermirror guide and a neutron polarisation Mezei flipper before the monochromating chopper with ^{3}He analysis of the scattering beam using a ^3He cell in the sample environment pot. The length of the polarising guide must be adequate to provide a uniform magnetic field across the guide. A 50 cm exchangeable guide piece is foreseen. In addition the Mezei flipper must also be long enough to enable flipping of the incident neutrons. A 2 m exchangeable guide piece is foreseen before the monochromating chopper to enable this upgrade, in addition to the use of materials with very low relative magnetic permeability in this region, < 1.02.

2.5 T0 chopper

The implementation of the T0 chopper is considered but will not be acted upon unless the background is not suitable.