

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

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Summary	3
1. Hot Commissioning	3
1.1 Validating instrument function	3
1.1.1 <i>Beam validation</i>	3
1.1.2 <i>Spectroscopic data collection from a well-characterised samples</i>	4
1.1.3 <i>Validating scientific performance</i>	4
2. Staging	5
2.1 Optimise signal to noise.	5
2.2 Full detector coverage.	5
2.3 Complete sample environment.....	5
2.4 Polarisation analysis.....	6
2.5 T0 chopper	6

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 book value.

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 the start of hot commissioning will entail a focus on further background reduction. This is clear from commissioning of instruments at ISIS, J-Parc, SNS etc. 1-2 months should be allocated to minimise background issues. The signal to noise will be validated.

The duration of the hot commissioning phase is extremely difficult to predict both due to technical uncertainties on the instrument but also due to the current uncertainty surrounding the operation of the target. 150 beamdays, as currently foreseen by the Instruments Division for hot commissioning, 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 precise details of the conditions are outlined in the CSPEC scope setting meeting summary.

2.1 Optimise signal to noise.

Although every effort will be made to minimise the background levels on CSPEC, there will invariably 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.

50 % of the detector electronics is available in the day 1 scope of the instrument. The grid modules will have all of their connections into the electronics part of the detector vessel. Here, only some of the channels will have ASIC boards connected to them.

Between the feed throughs and the ASIC boards, an intermediate adapter boards will map the channels that are connected to the ASICS. When upgrading, these boards would need to be replaced, so that the detector channels can be mapped more naturally to the electronics channels. For a full grid stack of 140 grids high, 40 – 48 grids will be connected to cover +/- 8°.

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 ($T_{\min} \sim 0.3 \text{ K}$ & 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 RF flipper before the monochromating chopper with ^3He 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. In addition the 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 and an exchangeable guide piece is implemented in the design.