IKON19

SAMPLE ENVIRONMENT REPORT FOR IKON19

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1. INTRODUCTION

This brief IKON report provides an update on mechanical interfaces, helium management as well as on the prioritised sample environment systems for instruments #1-8. We shall be delighted to exchange on any further topics during IKON shall a need arise.

2. MECHANICAL INTERFACES FOR SAMPLE ENVIRONMENT SYSTEMS

Two mounting interfaces for standardised installation of sample environment equipment have been developed matching the requirements related to reference document ESS-0038078: one to allow installation where the mass of the equipment rests on the floor (floor-mounting or bottom-loading) and one to allow installation where the mass of the equipment hangs via a flange from above (flange-mounting or top-loading). Within each system, three different levels are defined (levels L1,L2 and L3). Each level consists of standardised mass, size and sample-to-beam distance specification. As level number increases, equipment size and mass decreases and precision of installation improves.

Floor-mounting system: Following CDR on Nov 2019, ESS formally selected the Kipp 50mm mounting component as the standard interface for installation of pool equipment on levels L0, L1, L2. Subsequently, ESS-1797666.2 was released on Q1/20 detailing the standard locations of the components within an ESS neutron instrument. Recently we defined magnetic requirements for a specially manufactured non-magnetic version of the Kipp 50mm interface (NMKIPP) as tracked on confluence to enable magnet use and polarisation analysis:

https://confluence.esss.lu.se/display/SA/Magnetic+considerations+for+mounting+hardware

The design work to incorporate the Kipp standard into the SAD prototype mounting system (the "torta") has been underway. As part of this work, a provisional Level 3 has been defined also using Kipp 50mm

components and the height and tilt adjustments have been moved below the x-y adjustments. The latter modification improves speed and efficiency of alignment operations.

Flange mounting system: Following a critical SAMS review the prototype for the flange interface L1 was redesigned and released Q3/20 after subsequently reviewing all drawings. Manufacturing process has started and current plan is to have the prototype installed in E03 and to complete a metrological study of its performance before the end of 2020. In parallel, design work for the L2 flange, started by the MIRACLES team was completed and included in the L1 system, along with an L1-to-L2 adapter. Still outstanding tasks are the development of a non-magnetic variant of the flange system and verification of vacuum capability.

Universal sample coordinate system: Since the earliest drafts of the mechanical interface documentation, SAD has consistently implemented a universal sample coordinate system (USCS). This was defined to follow the instrument engineering coordinate system:

(a) a right-handed Cartesian system defined by the three unit vectors ex,ey and ez, and an origin centred on the sample position,

(b) ez points vertically up,

(c) ex is the horizontal vector closest to parallel to the beam (which may not be horizontal).

However, on some instruments, it is conceptually preferred to have an alternative system where the "z-axis" is parallel to the beam. In addition, internationally agreed conventions in some analysis software (e.g. MANTID) also uses this convention. The possible risks of operating with multiple definitions of coordinate systems were raised during several TG3 reviews. Subsequently, this was discussed in the instrument scientists Meeting June 2020. And the following proposals made:

(a) stick with the current definition of the USCS because this also agrees with the engineering coordinate system used for installation. Introduce a set of standard transform routines

(b) Suggesting to refrain from using x,y,z convention when talking about movements, rather say parallel to beam, up and down, right and left, etc.

Instrument teams were asked to consider, and report back any conflicts with their current coordinate system proposal and how it fits with SEE, software, etc. IKON19 represents a good opportunity to revisit.

3. HELIUM MANAGEMENT

Helium recovery and management will be increasingly important for sustainable and cost efficient operation of ESS. Facilities such as ISIS typically use more that 50,000 liquid litres per year, with costs per litre rising year on year. The Test and Instruments Cryoplant (TICP) at ESS is currently operational, and being used for testing of accelerator cryomodules before installation. In addition, it will provide liquid helium for the instruments and sample environment workshops, as well as supplying MAX IV and LU on a collaborative basis.

Liquid helium will be distributed to the D and E buildings, and the Campus, in 100-250l mobile Dewars. Space has been allocated in or around each instrument hall for a parking station for these. Site transport from the cryoplant to the instrument halls will be handled by Logistics, for self-service by SAD, instrument teams, and eventually trained users. Storage Dewars will be a common resource, but most instruments will require dedicated transfer siphons adapted to the geometry of the instrument, to be procured in consultation with SAD.

Helium will be recovered at the instruments and workshops, with flow meters and other instrumentation enabling detailed management of helium supplies and losses, and rapid identification

of leaks and contamination. ESS is part of a helium management collaboration involving HZB, ILL and STFC, sharing knowledge and technology including a sophisticated helium inventory system developed at HZB over many years, including wireless tracking of equipment. Test equipment from this system is currently being set up for testing and integration with our own systems at ESS. Design of the recovery backbone is well underway, covering the first phase of design up to the connections to individual instruments and workshops. The E buildings are being prioritised as this building is already handed over.

The helium recovery project is complex and has many stakeholders across the whole of ESS, and an offer of coordination support from NSS has been gratefully received.

4. UPDATE ON SAMPLE ENVIRONMENT PRIORITY SYSTEMS FOR FIRST 8 INSTRUMENTS #1-8

Here the various sample environment systems are presented grouped by different classes:

(a) sample environment systems for low temperature, high temperature, magnetic fields

(b) sample environment systems for high pressure and mechanical processing

(c) sample environment systems for fluids incl. gases, liquids and complex fluids.

We refer to the attached slides presenting the priorities as expressed by the different instrument teams.

Sample environment systems for low temperature, high temperature, magnetic fields

20 position cryofurnace (DREAM instrument specific): This cryofurnace is intended to allow long series of measurements on the DREAM instrument without significant interruption. The project is being managed at LLB, and has passed its CTV with the tender currently being finalised. The specifications are very ambitious, with a wide temperature range, and in-vacuum sample changing envisaged. In the event of delays, pool cryostat and furnace will be used.

8T Magnet (MAGIC DREAM): This wide aperture diffraction magnet is optimised for MAGiC but intended for general use on diffraction instruments, including DREAM and HEIMDAL. It is an in-kind contribution from LLB, who are managing the procurement. The TA was agreed in January and formally signed in August. The CTV has been passed and the procurement in progress for publication in September/October.

Ultra-low-temperature ULT systems (pool, compatible with 8T magnet): This is part of the French in-kind package for temperature and fields. Two 50mm diameter dilution inserts and a He3 sorption insert will be procured, ensuring compatibility with the 8T magnet and pool cryostats. Specifications have been collected for the dilution inserts, the 3He is in preparation. In order to be sure of compatibility with the 8T magnet, final specs will be determined once a preliminary design is approved. Two additional second hand dilution inserts will be procured from HZB in Q4/2020 and will be available for integration and training.

6.5T magnet (POOL/CSPEC): Second hand magnet to be procured from HZB. Contract is in preparation. Drawings have been obtained and mechanical integration with CSPEC vacuum tank via standard flange mount will be overseen by SAD mechanical engineer. Modern control electronics (compatible with legacy magnets) have been procured from Oxford instruments in order to start integration in a timely manner.

Cryofurnace 70mm with 6 pos sample changer (CSPEC instrument specific): SAD and CSPEC have agreed on scope and specifications for the instrument specific cryofurnace with temperature range

1.6-550 K. A draft tender document has been prepared by the CSPEC team and is being reviewed by SAD and the instrument team. An automated sample changer will be additionally procured as a modular insert for this cryostat.

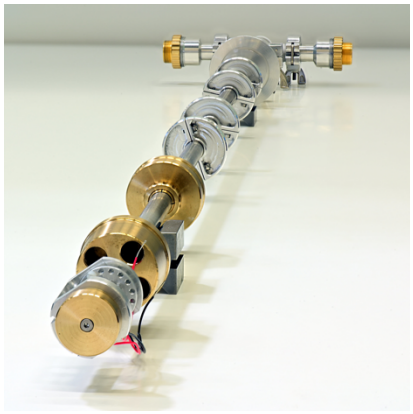
15 T magnet (BIFROST): This is a second-hand magnet procured from HZB. It was due to be shipped with ESS participation in dismantling and packing, just before covid-19 restrictions prohibited travel. This process is to be restarted ASAP as restrictions permit. Modern control electronics (compatible with legacy magnets) have been procured from Oxford instruments in order to start integration in a timely manner. Mechanical integration with the kinematic mounting system is being overseen by the BIFROST team.

Wet cryostat 70mm (BIFROST): This instrument specific cryostat tender has been prepared by the BIFROST team with SAD input, and procurement is ongoing via DTU. It is intended for use on Bifrost in the absence of a cryomagnet using a goniometer on the sample stack. Mechanical integration is being overseen by BIFROST, this equipment will not be installed using the L2 kinematic mount standard (though the goniometer will) due to geometrical constraints, though it will be possible via an adapter.

2.5T Warm bore magnet (LOKI/ESTIA): This dry cryomagnet is based on an existing design from HTS110 with minor modifications. It forms part of the first LLB in-kind packaged for temperature and fields. Specifications and detailed installation on LOKI and ESTIA have been considered in consultation with the instrument teams, and the CTV is in preparation, though slightly behind schedule as the 8T magnet and instrument component procurements have had priority.

Flow cryostat (ESTIA): This instrument specific equipment will be procured by PSI in accordance with the instrument schedule.

Pool cryostat and cryofurnaces: A number of pool cryostats, cryofurnaces and furnaces are envisaged as part of the LLB in-kind package for temperature and field sample environment. These will be defined in detail in a forthcoming meeting with the instrument teams, and a large part may be available as second hand equipment from other facilities. Highest priority is provision for DREAM. Integration for wet cryostats is already under way, however, with work on pumping carts, level meters and needle valve control which is broadly applicable across many systems including cryomagnets. Also sample sticks enabling fast temperature changed have been built (photo courtesy P Bentley)



Sample environment systems for high pressure and mechanical processing

Specific product requirements for all systems (apart from dilatometer) are available here: confluence.esss.lu.se/display/SA/Sample+Environment+Systems+Requirement+Documents

Clamp cells with medium sample volumes operating up to 2.5 GPa: Clamp cells with low-temperature capability are easily identified as the highest priority HP systems and shall be fully commissioned / available for instruments from Q4/22. The initial suite of devices will use well-established technologies and shall be available with a range of volumes and cell-body materials. They shall be provided through

an IK agreement with CEA (NIK 3.7) who will also provide training to ESS staff to build, maintain and operate these devices.

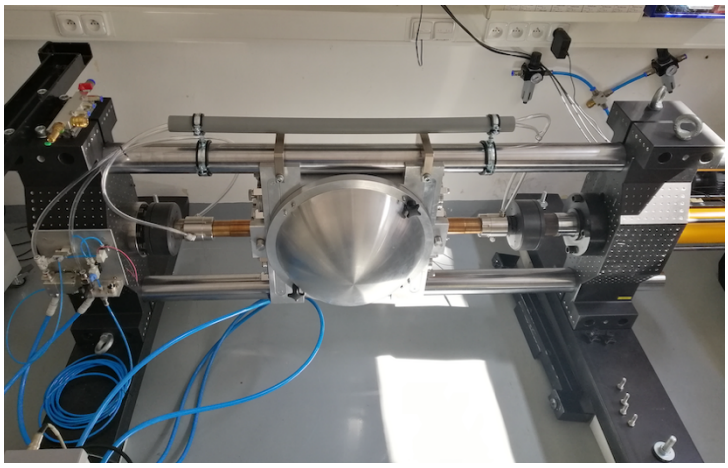
Gas and liquid cells with large sample volume operating up to 1 GPa: Gas and liquid cells are identified as the second highest priority and shall be provided as part of the same IK project as the clamp cells. As with the clamp cells, these devices are well established and the IK partner CEA has world-leading expertise. If the TA is successfully agreed, this project shall be low risk. These devices shall be fully commissioned and available for ESS instruments in Q4/22

Paris-Edinburgh (PE) cells with small sample volume devices operating up to 25 GPa: Although Paris-Edinburgh (PE) cells are identified as the 3rd priority after the clamp and liquid and gas cells, they are still vital technology as they increase the accessible pressure range by a factor of 10. As such they are particularly important for First Science on the Diffraction Class instruments MAGIC and DREAM and also BIFROST. PE cells shall be delivered through NIK 3.7, which also includes a custom CCR-based device to enable low T operation and a hydrogen-compatible gas-loading system. For the past 2 years, ESS has borrowed two PE devices which have been used to develop the necessary mechanical and controls integration. Of equal importance, these have provided a testbed to ensure compliance with ESS Quality requirements.

Diamond Anvil cells (DAC's) with microscopic sample volumes, operating up to 60 GPa: DAC cells complete the suite of available high-pressure equipment, extending the available pressure range up to ~ 60 GPa. PREMP is currently pursuing a licensing agreement with ORNL to allow ESS to manufacture our own cells. Once this is obtained, 12 months will be sufficient time to integrate these cells into ESS mounting systems and other systems (for example, cryostats). This leads to a target date of Q1/23 to initial procurement.

Safety and Quality for High Pressure Cells: The decision that sample-environment equipment used at the ESS shall be CE-marked has come with particular challenges for high-pressure equipment. PREMP has had to develop approaches from scratch that allow compliance with internal ESS policies and also broader European and local Swedish regulations. These procedures and documentation approaches have been reviewed by ESS Quality consultant with final documentation expected by Q3/20.

Stress Rig #1 is a large 100kN stress rig optimised for BEER and shall be used on the majority of experiments on that instrument. It is critical that the device is available by the requested date of Q4/22 and it is the highest priority mechanical-processing system within PREMP. The device has been manufactured and tested by partners at the NPI, Prague. We are currently engaged in a period of controls and mechanical integration of the device. In parallel, we are developing the necessary safety and Quality integration of all stress rig-type devices. Figure shows the BEER stress rig undergoing testing at Nuclear Physics Institute, Czech Republic.



Stress Rig #2 is a modular portable rig 50kN rig optimised for rotation to allow torsional measurements and tomography. It is currently in the conceptual design phase which shall be completed during Q3/20, in this we are also exploring commercial solutions. Robin Woracek is supporting this project as a subject matter expert and class coordinator for imaging and engineering.

Stress Rig #3 a small portable 10kN rig specialised for soft matter applications. It is also in the conceptual design stage to be completed during Q3/20. As with Rig #2 we hope to find commercial solutions. Robin Woracek is supporting this project as a subject matter expert and class coordinator for imaging and engineering.

Dilatometer: The Dilatometer project has not yet started. However, as this device is a commercial product and not needed until Q1/23, we expect adequate time to complete the project if we start by Q2/21.

Pool equipment for mechanical processing: We are also in the process of integrating a second-hand, portable rig provided by Robin Woracek. This rig is physically present in Lund (Utgård) and provides an invaluable test bed to develop full controls integration into EPICs. In addition, it allows up to gain experience in the necessary safety and Quality integration (the device is not CE-marked). Lastly, we are designing a mechanical integration to the standard mounting system, allowing this rig to be installed on any 'Floor-mount' ESS instrument.

Sample environment systems for fluids incl. gases, liquids and complex fluids.

Gas handling systems: A first manual gas handling manifold usable for inert gases as well as flammable gases like hydrogen, methane is available. It allows gas adsorption experiments between 1 mbar and 10 bar in calibrated volumes of 50 ml, 150 ml and 500 ml. As part of the Estonian in-kind contribution a fully automated gas handling system has been built. It is on the way to ESS for integration which shall allow remote access to the gas handling system via instrument control (EPICS).

Pump probe laser system: A system is available from our Estonian in-kind partner and fist demonstration experiments had been performed at various facilities, the system is currently revised improving its mechanical integration prior to control integration.

Humidity chamber: based on a recent design developed between various collaboration partners an ESS humidity chamber is currently manufactured by our Estonian in-kind partenrs ready to perform first tests before the end of 2020.

Stopped flow units are again part of the Estonian in-kind contribution such units are currently manufactured and shall be tested at the end of the year.

Flow cells especially important for LOKI are intended to be provided as part of a collaborative (third-party) funded project. The partners have already made such system available to STFC and tested with neutrons.

In-situ techniques: Several systems including DLS, foam and humidity systems have been built as part a third-party funded collaboration project by several German university partners. Such systems shall be available to ESS as needed.

Electro chemistry cells: Gaining traction by the community for diffraction studies an additional in-kind contribution from our Estonian partners has recently been activated. Design is on-going for cells suitable for both, SANS instruments and direct geometry spectrometers.

SANS magazine: an instrument-specific thermalised SANS magazine for LOKI has to be delivered by ESS as part of the LOKI scope. Providing the capability to measure multiple samples under the right conditions (temperature, rotation) this system is key for first science on LOKI. A preliminary design study has been performed which enabled the revision of a (detailed) project plan. Following review with stakeholders, detailed design could start in Oct 2020 pending availability of engineering resources.

Solid Liquid cells are essential for first science on ESTIA. ESS is responsible for delivery as part of the ESTIA construction scope. Requirements were gathered but execution requires additional resources e.g. recruitment scientific engineer started. Also potential new expert partners were identified which might enable us to deliver not only the scope for ESTIA but also an initial set for FREIA provided additional third-party funding applications are successful.

Summary of SE priorities for the first instruments #1-8

SE Priorities for Imaging & Engineering

Systems as required for hot commissioning and first science of different instruments

BEER

System	Details	partners	comment	status
Stress strain rig 1	100kN 'workhorse'	NPI	system available and integration started	
Stress strain rig 2	40kN with rotation for imaging, torsion	NPI / MLZ / commercial	PDR completed; ready to start detailed design	
Dilatometer		commercial	not yet started pending final BEER requirements	

ODIN

System	Details	partners	comment	status
Stress strain rig 2	40kN with rotation for imaging, torsion	NPI / MLZ / commercial	PDR completed; ready to start detailed design	
Gas / liquid cells	5 kbar gas liquid cell	LLB	TA ready to be activated; based on existing design	

Some (pool) SE systems shown more than once – Details on delivery schedule provided on request

GREEN: according to plan; LIGHT GREEN: requires attention; YELLOW: mitigation to be implemented

SE Priorities for Diffraction

DREAM

System	Details	partners	comment	status
Cryofurnace	Instr. specific; 20-position changer	LLB	CTV completed; challenging specs.	
Wet Cryostat	Standard Orange Cryostat	LLB	2nd hand, OC sample sticks available, mechanical & control integration started	
Magnet	Asymmetric 8T + Dilution / ^{3}He	LLB	8T: CTV completed, LT: prepare CTV	
hi-p: clamp, PE	2, 20 GPa + low T	LLB	TA ready to be activated	
hi-p: PE, DAC	20, 50 GPa (RT and low T)	ESS/SNS	PE available with specific inserts (RT)	
Gas Processing	Automated	EE	commissioning started with partner	
Electrochemistry	Multi-parameter cell	EE	TA recently activated; some C-19 impact	

MAGIC

System	Details	partners	comment	status
Vertical Magnet	Asymmetric 8T + Dilution / ^{3}He	LLB	8T: CTV completed; LT: prepare CTV	
Wet Cryostat	Instrument specific	LLB	according to schedule not yet started	
hi-p: clamp, PE	2, 20 GPa + low T	LLB	TA ready to be activated	
hi-p: PE, DAC	20, 50 GPa (RT)	ESS/SNS	PE available with specific cells (RT)	

SE Priorities for Spectroscopy

CSPEC

System	Details	partners		status
6.5 T Magnet	Ex-HZB VM-2 +Dil. insert	ESS/HZB	2nd hand; integration to start Q1/2021	
Cryofurnace	Inst. specific 6 pos. changer	LLB	requirements agreed; similarities w. BIFROST	
Wet cryostat	Standard Orange Cryostat	LLB	to be started based on 2nd hand system	
DAC uniaxial	2 GPa + low T	LLB, KU	collaborative project completed	
hi-p: clamp, PE	2, 20, 50 Gpa + low T	LLB	TA ready to be activated; PE available	
Humidity cell	Wide angular access	ESS/EE	part of EE in-kind, based on existing design	
Pump-probe	In-situ laser trigger	EE	already used by partner; integration to be started	

BIFROST

System	Details	partners		status
15T Magnet	Ex HZB VM1B +Dil.	ESS/HZB	2nd hand; ready to be shipped; 2nd system avail.	
Wet Cryostat	Specific Orange Cryo 70mm	BIFROST	requirements agreed, procurement in progress	
hi-p: clamp, PE	2, 20, 50 Gpa + low T	LLB	TA ready to be activated; PE available	
hi-p: DAC cells	50GPa + low T	ESS/SNS	Generic DAC system already available	

SE Priorities for Large Scale Structures

LOKI

System	Details	partners	comment	status
SANS changer	Inst. spec.; (indiv.) thermalized, tumbler	ESS	Requirements agreed, conceptual design available; requires additional resources: design engineer 9/20; recruitment scientific engineer	
(Stopped) Flow cells	Inst. spec.; incl. pumps	ESS, EE	flow: collaborative, needs update integration stop flow: EE IK slightly late, CDR prepared	
In-situ techniques	Supplied via external grants	External	DLS, foam, humidity systems completed and used by partners; integration started	
Low field magnet	HTSC warm bore or electro.	LLB	CTV in preparation as part of FR TA	
stress-strain rig 3	5-10 kN versatile rig	LLB	Requirements gathered, kick-off pending	

ESTIA

System	Details	partners	comment	status
Low field magnet	2T HTSC warm bore magnet	LLB	CTV in preparation as part of FR TA	
Flow cryostat	Instrument specific	PSI	according to ESTIA schedule not yet started	
Solid Liquid Cells	Instrument specific	ESS	requirements gathered, requires additional resources: recruitment scientific engineer started; potential new partners identified	