

Scientific Activities Division – Q1/2021 report for STAP – 220406

Achievements

1. Scientific Activities Division (SAD) – General Comments

New Baseline: The new ESS baseline planning until 2027 is now established. As a result the overall scope for the SAD team to provide sample environment, sample and user services remains unchanged but we adjusted schedule and budget accordingly considering the new dates for beam-on-target, first science and the start of the user programme. All our activities are captured in the P6 project plan related to the science directorate incl. the remaining in-kind scope (which previously remained with NSS construction budget). The new science directorate sub-project is led by Oliver Kirstein and we are starting to implement a new streamlined and data-based reporting structure to ensure we remain on a good delivery path.

In-Kind (IK): We have submitted final IK reports on the glove boxes and gas adsorption systems from our Estonian partners to the IK review committee (IKRC) in March. We also agreed with our French partners to exclude the 2.5T warm bore magnet from their current IK scope and requested the resources to be transferred back to the ESS cash budget (IK2cash transfer). The remaining IK projects continue: pump probe, humidity control, stop flow units, electrochemistry, high-pressure systems as well as the diffraction cryo-magnet. A new technical annex had been prepared for the stress rig to be provided by our Czech partners but finally not submitted to this IKRC. We are investigating several new IK possibilities with (new) partners not least related to the spectroscopy magnet.

Team: To be able to execute this new-baseline plan additional resources are required and the recruitment process to ensure resource provision according to plan is (slowly) starting. In Q1/2022 the SAD team experienced some impact related to sick leave.

2. Scientific Coordination and User Office (SCUO)

SFT Newsletter: The quarterly newsletter continues and we have agreed that four quarterly newsletters will be the equivalent of the former annual research report that was prepared for each Science Day. On Science Day printed copies of the three newsletters already prepared, and copies of the 2021 publication library will be available.

Policies and Guidelines: The *Guidelines for Scientific Publications from ESS Users and Staff and Associates of the ESS Science Directorate including a Commitment to Scientific Integrity and Research Ethics*, released after the approval of SMT have been redrafted. The driving force for this was to prepare something that would be applicable

throughout ESS. Guidelines for Scientific Integrity was taken in to one document and Guidelines for Scientific Publications in to a second document. These have been approved by SAC, but must go to Technical Management and then the Executive Board. Progress with policies is difficult to achieve.

Internal Communication: The SCUO intranet pages have been significantly refactored, giving space to all elements of the office; the User Programme, Key Performance Indicator and a Science Focus. Of particular relevance are that this is becoming a repository for user office software (UOS) documentation and that it provides a space to organise work aimed at increasing the feel of scientific vibrance at ESS. Using JIRA and Confluence is supporting and altered way of working. In part digitising task management and making SCUO open within ESS provides some coverage in case of further absences.

ESS-ILL user meeting 2022: Registration and Call for Abstracts opened on time in March and all the plenary speakers have been invited. Scientists have been selected at ESS and ILL to complete the science programme and this is underway. Focus now shifting to the practicalities of the visit to ESS site.

User Office Software (UOS): The proposal submission system was used to collect proposals from the recent DEMAX call for proposals. A brief retrospective of the call enabled identification of small issues and reinforced the fact that the questions must be precise and accurate. Feasibility reviews are being carried out now and it is anticipated the science evaluation will begin around Easter. The review meeting will be facilitated using the UOS. STFC used the software for their CLF lasers call and will use it later in the year for the ISIS call.

3. Sample Services – Chemistry & Life Science User Laboratories (SULF)

Lab fit-out and installation: Glove boxes have been moved from their temporary location in E04 to the Radioactive Materials Lab in D08. Common areas (meetings room, kitchen, ground floor office spaces) in D08 are currently furnished and soon be available for several teams working in the D buildings. Procurement of the installation work package for the D04 fit-out is on-going to restart the fit-out activities in summer using lab furniture available and installing utilities lines, electricity and gases room-by-room during the next three years.

Using the E04 laboratories to support the ESS project: The luminescence coatings with the Beam Diagnostics Group have now been sprayed on the ESS target wheel. The collaboration continues to analyze the sprayed coatings for quality assurance and to continue to develop and optimize new coating materials. The SULF laboratories are continuing to perform water analysis for the waste water tanks until an online system

will be procured by the ES&H group. A materials team with members from the ESS Spallation Physics and the SULF group has been established to support the ESS project. Currently the main support is given to questions of water quality in the ESS cooling water loops servicing the accelerator components.

In-Kind and collaboration projects: Both in-kind projects have now officially been completed and have been approved. How further collaborations between the in-kind partners in the UK, Estonia and at ESS with respect to user support can continue will be discussed in an upcoming workshop in May.

4. Sample Services – Deuteration (DEMAX)

Supporting user proposals: DEMAX and SCUO – with support from DMSC – successfully launched the pilot call for deuteration proposals 2'b'. The call closed on 5 March and 16 proposals were submitted. Technical & feasibility reviews are underway before the review panel meets in Q2. Lab preparations in view of proposal support has started, specifically procurements or production of starting materials, equipment calibration & upgrade, as well an agreed way of working to organize proposal related data.

Grants & collaborations: Existing externally funded postdocs continue with no new updates. Recruitment for new postdoc under the VR-funded MeDCAN grant (UU, LU, ESS, ISIS) is underway. New publications from collaboration and/or user support are out (<https://europeanspallationsource.se/article/2021/09/27/highlights-published-papers>) and another is in progress.

DEUNET: Activities continued with preparing for an updated deuteration needs survey of the user community, planning for the annual facility network meeting, as well as requirements for an updated & functional website.

5. Sample Environment (SE)

Workshops: The main sample environment workshop in the E03 building is now in routine operation. We have power, ethernet, wifi, compressed air, helium gas, and working cranes. The lathe and drill press are working, the milling machine has some electrical issues that are being investigated. Benches, storage and general workshop furniture have been purchased and assembled. Safety risk assessments have been carried out for a number of activities (Cryogenics, use of machine tools, ODH...), or are in process (use of strong magnetic fields). The YMIR test beamline installed in B02 SE space is now also used for first commissioning activities by the various stakeholders (SE, ECDL, MCA, ...).

Sample Environment systems:

Magnets:

- The 8T diffraction magnet tender process is now complete and the bidders have been notified. A kick-off meeting will be organized shortly. At that point the tender for the dilution insert can be finalized, in order to ensure compatibility with this magnet.
- Transfer of cash and scope for the warm bore magnet from LLB to ESS has been agreed, including discussion with ESS procurement division. The specifications have already been agreed and discussed with the most likely potential manufacturer. The procurement process for this will be launched at ESS shortly.
- The second hand HZB magnets are in the process of being refurbished. We have purchased fresh o-rings and will replace accessible superinsulation. Once reassembled and the original software is in place we will cool down and test the 15T magnet V1MB. In parallel we are working on integration of the new generation Mercury controllers. In order to avoid wasting a large amount of helium we have discussed with the rigging team the possibility to do the initial cooldown in the coldbox hall, where helium recovery is available. We will first do a warm trial run using accelerometers attached to the magnet to ensure that it can be transported safely.
- LLB have declined to be involved in the procurement of the planned high-field spectroscopy magnet. This opens the possibility of other (Swedish?) in-kind, or in-house procurement by ESS. In any case the next step will be a design study in order to get a realistic idea of possible and affordable configurations.

Cryostats:

- The BIFROST cryostat has been received but not yet tested for acceptance as the tail needed re-machining. Once this is received we are ready for acceptance testing. We have a lakeshore 336 controller connected and integrated into the EPICS network and ready for temperature control and logging, helium siphons, and pumps available for
- We are stripping down and refurbishing the old orange cryostat received from HZB. This will involve installing new thermometers, o-rings/indium seals, and fresh superinsulation, which is on order, to be used also for refurbishing magnets.
- We are building a prototype of the new standard pumping cart, following the STAPs advice for a modular design, with automation but also retaining the possibility of manual operation. Progress is ongoing with the needle valve motor control using the Beckhoff system, using its additional capabilities to provide automatic pumping and flushing of the sample space with a separate pump. Currently this is all integrated into one pumping cart, but we will evaluate if the pump/flush mechanism is better located as close as possible to the cryostat itself, while retaining the possibility of keeping control electronics out of the instrument caves. The control logic will use Octopy.

- We have a quote for the electrochemistry cryostat, though procurement has not yet started as other activities have been prioritised, and resources are limited.

High-Pressure:

- The in-kind project with LLB regarding the procurement of high-pressure equipment is progressing well. Discussions with ILL on specifications for the dedicated cryogenic equipment but also test protocols and documentation are converging.

Mechanical Processing:

- An in-kind technical annex between NPI and the SE team has been prepared but was not submitted for the IKRC in March 22) to transfer the 60 (100) kN stress rig developed by NPI to ESS. Though the equipment should still arrive on site before the end of year 2022 to be able to start the commissioning and finish the control integration in 2023.

Soft Matter, Surface and Interface, In-Situ techniques and Physical Chemistry:

- CDR of the SANS sample changer for Loki, driven by the instrument team, was successful and manufacturing is starting (soon).
- Control integration has started for the rheometer and the pumps for the stop flow system.
- The projects in this area will remain on hold until Alice is back from maternity leave and the recruitment of a soft matter expert is done.

Control Integration:

- Octopy: With a running version and after several demos to stakeholders, Octopy gets some traction at ESS as a tool relevant even beyond purely the SE team.
- SECoP: collaboration with the HZB meta data project continues.

Mechanical integration

- Parts for the non-magnetic force sensors for the magnetic force testing device have been delivered.
- The design of the top loading version of the device has also been finalized, having agreed on the common interface on the instruments that will use it. Mechanical simulation has been carried out to verify the structures with a successful result.
- The non-magnetic kinematic mounting devices are now integrated at the existing alignment stations at E03.

Helium management

- The helium recovery backbone network is being installed in the experimental halls and galleries.

- In consultation with the NSS infrastructure team the end connections (instrument/workshop and parking stations) are being specified and will go into detailed design.
- We plan to use the HZB helium management software and hardware solution, and are ordering compatible equipment. It is not yet clear who will take care of the integration side (i.e. hosting database, maintaining software up to date, configuration), but the relevant stakeholders are aware of this need, and some informal support has been offered by ECDC.

Challenges

The main challenge for the SAD team remains the lack of manpower and subject matter experts due to staff turnover, sickness and maternity leave. With only one FTE supporting each technical area, it is not possible to deliver reliable service or even engage in sufficient scientific and technical collaboration with our partners. It is sometime even a struggle to find adequate coverage for workshops / laboratories and scientific supervision (postdoc activities). This issue will only grow in the lead-up to First Science on ESS instruments when we can expect additional demands from instrument teams and the user community. We are hence emphasising the need to recruit resources according to the new baseline plan.

Due to the global situation in supply chain and increasing costs, we are also under financial pressure. We are already seeing impact on cost of aluminium but also (deuterated) chemicals. We will continuously monitor to deliver maximum value for money not least related to the deuteration support provided as part of the current pilot calls.