

Comments to STAP report & Q1 2021 update (Spring 2021)

We would like to thank the STAP for their thoughtful comments and good advice in the last report submitted (Autumn 2020). Below we respond to the main points in the STAP report that are not addressed in the Q1 2021 summary tables that follow later in the document.

1.1 SULF

As of January 2021, SULF is now operating the laboratories on-site. All equipment, chemicals and glassware have been moved from the rented lab space and our instrumentation has been recommissioned.

Installation of labs and Covid-19 impact

SULF is still battling with the travel restrictions and quarantine for the UK contractors fitting out the labs. The contractors managed to be back at ESS in October and progress with the installation. The electrical work in E03/E04 is 100% done, the inert gas lines are complete in 90% of the areas, and the plumbing is 90% finished. The lab installations have been on hold again since Christmas. Fortunately, the main contractor arranged to come over for 4 weeks in March to finalize the official testing of the ventilation in the fume hoods in E04, connecting all fume hoods, overhead extraction arms and solvent cabinets leaving the labs in E04 completely finished and the E03 labs only in need of testing. SULF can now officially use the fume hoods, extraction arms and all solvent cabinets.

SULF has worked with an electrical engineer (consultant) to verify and document the electrical installations for the past four months. The power distribution panels for the lab spaces in D and E-buildings have been brought up to standard with regard to safety and quality, and everything is documented according to ESS requirements. Furthermore, the E-plan drawings for the electrical installations as well as the necessary calculations for the finished E-buildings (E03/E04) and for the future D-buildings (D04/D08) have been completed. The consultant is now working for another project at ESS and could potentially be available again once installation in D-buildings starts in fall 2021 to support installation.

The commissioning of the glove boxes has not commenced as the quarantine conditions prevent the technician from coming to Sweden. The same is true for the UK workers expected to return for finishing the labs as well as other technicians for lab equipment. The possibility is currently being discussed at ESS to test the incoming workers for Covid-19 every morning for 5 consecutive days instead of forcing them into a 5-day quarantine. If this is possible, we will be able to finish the project on budget. Otherwise, we are facing further delays with the current fit-out as well as with the next installation in the D-buildings.

Resources and non-core business

SULF is now at a stage where a significant amount of time needs to be spent on developing routines for maintenance and use of equipment. This is especially true as we are only three full-time employees. However, with the utilities and the basic building support not (yet) fully in place, we are having to also deal with a lot of topics that facility management (FM) will long-term take care of, such as developing a procedure to test our waste water plus teaching FM to take water samples, getting the house vacuum and supply of N₂-gas going, writing cleaning requirements for our epoxy floor in the chemistry lab, request basic supplies for our offices that are taken care of automatically for the main building (white boards, lockers, copy paper, copy machine...) and so on. SULF is a bit in a conundrum, if we do not get involved in these topics, our work will be delayed, e.g. our 3m³ waste water tanks will not be emptied and we cannot use water in the labs anymore. If we do get involved, we are lacking time for other things.

Safety documentation for the labs will continue to be a part of the SULF work. However, the main risk assessment for the labs has been done and can be used across all labs. The discussions with the Quality Division are still ongoing (since Dec. 2019) and we are not sure what extra demands might arise as this seems to change over time. The latest example is the suggestion from February 2021 to test the quality of 2% of all brazing joints in the copper gas lines with X-rays. This will cause extra costs and it will be quite an effort as most of the joints are above the ceiling. SULF is now spending time to understand what the legal implications are in Sweden versus a “nice-to-have” quality check as testing is not standard in other labs such as the ISIS labs in the UK.

ESS project support and equipment

The equipment situation for SULF has improved greatly over the past few months. The single crystal machine made it from ISIS to ESS before BREXIT and is waiting to be installed. We were allowed to buy an X-ray powder diffraction machine that is expected to arrive in April (Thanks to the STAP for recommending it!). Both X-ray machines will be put into service together pending the technician being able to travel to Lund. The remaining in-kind money from the UK was spend on a fusion machine to prepare X-ray fluorescence (XRF) samples, a glove box and a scale for the labs. We also procured a microwave digestion furnace to prepare samples for the Ion-Coupled Plasma-Optical Emission Spectrometer (ICP-OES) that has been procured by Target Division and is expected in April. Both, the XRF and the ICP-OES will be used to support the ESS project with elemental analysis of various components, such as construction and shielding material. Target also procured an environmental Scanning Electron Microscope (SEM) that is setup in one of the SULF labs. While this machine is currently mainly used by Target, SULF supports the maintenance for it and has access to it. It is planned to be available to the neutron scattering users later on.

The close collaboration with Target Division on the instruments and on the material analysis for the ESS project as well as the joint effort with Accelerator Division to

understand and optimize the luminescence screen material for the proton beam window is continuing and benefitting all sides. SULF is also assisting in checking cooling water quality for several areas with simple pH and conductivity measurements that saves time and money for all involved.

1.2 DEMAX

Second pilot call & Covid-19 projects

There are many challenges related to lab access, supply chain issues, and delayed/cancelled beamtimes for our users that have slowed us down during the pandemic. Work has continued for a number of projects, but at a reduced rate. Due to schedule delays and impact to BoT, FS, and SOUP, we decided to postpone the 3rd pilot call that was supposed to happen December 2020. A new date has not been decided. We face resource constraints that do not enable us to expand our team for at least 24 months. We need to balance this with continuing to deliver (some) support and materials to our users in order to build collaborations and keep the momentum and interest of the user community.

Grants, collaboration, outreach

We have several activities ongoing, including working on the deuteration pilot project in BrightnESS², participating in two VR grants, co-supervision of a PhD student at LU, and two new grant-funded postdocs that have joined us. Jenny Andersson is funded by a Nordforsk grant and is in a shared position between DEMAX and LU with her primary workplace being our chemistry labs. Her projects involved deuterated natural lipid preparations and neutron scattering. We also have Jia-Fei Poon, who is co-funded between DEMAX and LU by Tillväxtverket and his primary work place is also our chemistry labs. He is an organic synthetic chemist and is working on deuterated surfactant projects with our LU partner.

DEMAX continues as the coordinator for the Deuteration Network (DEUNET) and maintains the Twitter account and website. Hanna is leading the LENS Priority Action 3 in biomedical science (“Role of cell membranes in health and disease”) and ESS and external partners are committed to participating in this activity. The LENS webinar series under this topic has been very successful and popular. Hanna is also working with the “Grants and external relations” team on being part of various consortia to enable ESS participation in larger Horizon Europe grant applications. There are two relevant themes (Cancer and Infectious Disease) and we are very supportive of expanding our capabilities with these efforts.

Resources & timeline impact to staffing and planning

Our staffing of the labs in the different subject areas continues to be lean and we lack overlapping competence and redundancy/ability to help each other scientifically and technically. This means we can help a wider range of scientific users but we don't have depth if someone is sick or leaves. Due to current funding constraints and schedule delays this will not change for the next 24 months. Fatima was hired as maternity replacement and her contract will end in August 2021. We would very much like to extend her contract to be able to support our postdocs in lipid preparation as well as working on LENS PA3 deliverables.

1.3 SCUO

User office software

DEMAX, SCUO and DMSC continue to collaborate on expanding and improving the proposal submission portal. The focus in this period was to set-up the ability to have different types of calls, set up different expert/peer-review panels, and allows for calibration and discussion of awarded scores. There are a large number of components missing: sample declaration & tracking, sample shipping, data accessibility, visit management for users with regards to travel/hotel/training/site access etc that has to be developed or at least integrated into other existing systems at ESS.

Policies

The policy on Scientific Evaluation and User Access is still awaiting submission to Council. The policy for User Scientific Publication is approved by the Science Management Team but requires alignment with other ESS stakeholders. DMSC is currently revising the ESS policy on Scientific Data.

Grant activities

We continue to work under BrightnESS2 work package related to establishing best practices for KPI tracking for ESS. This is a very important activity as it will establish what we track and will form the basis for measuring our performance in terms of scientific output and effects on society. A comprehensive report has been generated and can be shared with the STAP if interested. For another work package in BrightnESS2, we have contracted Grethe to do the industry interviews to develop access and pricing guidelines that can be implemented at ESS for proprietary beamtime.

Staffing

Due to a staff member being out sick for a significant part of 2020, we have redistributed some tasks within ESS to keep momentum going and also to continue making progress. This is not sustainable in the long term and we may need more help going forward.

1) SULF Summary

Top achievements – and benefits/value they bring

Importance 1-5	Team	Achievement	Enables
1	Science SAD/SULF	Labs in E04 transitioned into operations: SULF team moved out of Medicon Village and into E04. All SULF capabilities have been recovered. The basic installation in all technical areas in E03/E04 is almost complete. Labs are fully functional and used daily for commissioning of equipment and supporting the ESS project.	Enables ESS project support. Enables developing routines to be able to support the user program such as: <ul style="list-style-type: none"> - Maintenance / operation of equipment - Chemical safety/training/first aid - Ordering/disposing of chemicals Setting up of glassware/consumables
2	Science SAD/SULF	D-buildings basic installation is being negotiated: D-building early access is coming closer. We are in process of ordering the fume hoods and the installation. If this happens within the next two weeks, we can install in April-June 2021 in D04 and D08. Installing now prevents additional costs later that are due to adjusting of components such as ducting, dampers, sensors and alarms (lessons learned from E-buildings).	Enables installation of fume hoods in D04 and D08 during early access. This saves money and time if done at this stage of the building construction.
3	Science SAD/SULF	Single crystal x-ray diffractometer ready for commissioning, powder x-ray system expected in April.	Enables structural characterisation of materials. Supports the ESS project now and user operations later.
3	Science SAD/SULF	Supervising two master students (collaboration with the Beam Diagnostics Group, ESS) and one postdoctoral research assistant (funded by Melissa Sharp's HFSP grant on cyano bacteria).	Enables testing the functionality of the laboratories for user operations with emphasis on physical characterization and chemistry (master students project) and life science (postdoc). Extends SULFs capability in the areas of life science and soft matter.

Top challenges – and proposed mitigation

Importance 1-5	Team	Challenge	Mitigation
1	Science SAD/SULF	Planning of installation is complicated by the fact that costs for travel are unknown due to C19 and the varying requirements between countries. Finalization of E03 technical	Follow C19 regulations closely. Stay in close communication with Lab outfitter (weekly meetings) and follow up with Science Director for decision on C19 testing.

		installation and start of D04 / D08 fit-out pending return of UK IK partners. Decision to perform C19 testing on 5 consecutive days instead of 5 days of quarantine would save costs and make it easier to plan.	
2	Science SAD/SULF	Continuing requirements to be involved in topics not being core business of SULF leads to frustration and lack of time in other areas, such as participating in proposals for grants that might fund further equipment for the labs. Limited staffing does not help.	Try to prioritize the most important “additional” topics, i.e. the ones that will otherwise stop SULF from progressing.

2) DEMAX Summary

Top achievements – and benefits/value they bring

Importance 1-5	Directorate	Achievement	Enables
1	Science SAD/DEMAX	Second call for proposals concluded and work is being carried out. A special call for prioritized Covid-19 support has brought a strong project in.	Support the neutron user community with access to deuterated materials & crystals for neutron experiments. Covid-19 support enables collaboration and the chance to address the global health challenge. Success has led to several grant applications and a publication (one in print, another is being prepared). This is good visibility for the value that DEMAX adds to ESS to address global health challenges.
2	Science SAD/DEMAX	Successfully recruited two joint ESS-LU postdocs funded through external grants (Nordforsk, Tillväxtverket)	Drive deuteration methods and types of materials forward. Enhances our capabilities to develop methods and establish routines for preparing different types of deuterated molecules required by future ESS neutron users.
2	Science SAD/DEMAX	Coordinating LENS Global health challenges PA3 (“Role of cell membranes in health and disease”). Coordinating DEUNET. Coordinate ESS participation in Horizon Europe call related to Cancer & Infectious Disease.	Benefits are significant: engaging in these activities enables collaboration, attracts scientists to ESS, expands the scientific scope of what DEMAX can deliver, expansion of our capabilities and capacity to support users and life science research.

Top challenges – and proposed mitigation

Importance 1-5	Directorate	Challenge	Mitigation
1	Science SAD/DEMAX	Delivery schedule of deuterated materials affected by delayed/cancelled beamtime of users, negatively impacted by limited access to our labs at Lund University. Occupancy and work restrictions in our MV labs affect throughput. Supply chain issues for consumables & lab equipment.	Be flexible and adjust schedule and plans according to constraints. Transparency and communication with users on delays and possible impact are an ongoing process.
2	Science SAD/DEMAX	Staffing limited by recruitment freeze threatens capacity to develop and support user proposals and participate in grant collaborations that provide external funding	Adjust level of participation in grant collaborations, number of user proposals and manage expectations.

3) SCUO Summary

Top achievements – and benefits/value they bring

Importance 1-5	Directorate	Achievement	Enables
1	Science SAD/SCUO	Supports user office software development by DMSC, in collaboration with DEMAX. Identify other ESS stakeholder, expand capabilities	Implement and test portal for current and future proposal calls. Enables collaboration and coordination of stakeholders interests and aligns with policies regarding evaluation, access, and publication.
2	Science SAD/SCUO	Develop tools for reporting KPI	Help ESS to establish suitable KPIs, generate reports to demonstrate impact of ESS to funders & stakeholders
3	Science SAD/SCUO	Develop industry access modes, costs	Deliver on BrightnESS2 work package related to Industry access and costing. Will be useful for ESS during operations as well.

Top challenges – and proposed mitigation

Importance 1-5	Directorate	Challenge	Mitigation
1	Science SAD/SCUO	Coordinating across ESS to identify and engage all stakeholders related to user proposals, samples, and visits. Many key functions are not integrated (e.g. sample tracking, shipping) or even developed and are not part of UO software today.	This requires a lot of heavy work as there are so many stakeholders and system that have to be integrated to deliver the required information to UO software. Continue to work with DEMAX & DMSC to identify missing functionalities.
2	Science SAD/SCUO	User policies on evaluation / access and publication drafted, approved by SMT, but need to be presented to SAC and Council.	Work on implementation of procedures and guidelines for future user programme already now during initial ops.