

FEEDBACK on the Sample and Users STAP Report from October 2018

GENERAL

Sample Environment Labspace – As an outside comment to sample environment, there was an immediate feeling that the distance from the site-offices to the temporary Utgård labs is becoming an increasing problem. We could suggest to prioritize finishing the new labs on site ASAP.

The Utgård lab is in principle fully functional now. Travel between Utgård and site is indeed a problem, with typically 15-30 mins lost several days per week for some of the team. The fit out of the on-site sample environment labs have been integrated with the fit out of the chemistry labs and will start soon after hand-over of the E buildings.

Money - It is good to hear that SAD received additional funding to cover the unexpected costs for installations in the laboratory buildings.

The plans for the laboratory fit-out have been refined and the installation schedule integrated into the over-all ESS planning. We are preparing for the practical aspects - from worker cabins to overtime / shift work.

Management & Interactions - Group and section leaders will set you up for better communication.

The team increasingly works together on joint projects though there is always potential for improvement and creating synergies. This collaboration involves all of SAD e.g. interactions between the lab and sample environment teams.

ESH - The updates on ESH and Procurement/Logistics are quite troublesome. Both of these activities are crucial to the success of a user program. It needs to become a priority for ESH to support SAD activities. The STAP sees the lack of urgency as a critical oversight. User experiments cannot wait months for common activities such as glass blowing to be reviewed. At all times there will be new situations arise that need immediate safety attention. Beam time is not cheap. The entire mission of this facility is to provide instruments for experiments. Doing experiments safely is key to that mission. Press upon the ESS organization that practicing now for when users are present will result in a much higher rate of success. Make clear to ESH how instrumental the OSH engineer was in getting work done and ask them to ensure that there is an appropriate handover between the retiring ESH OSH contact and their replacement. The current state of things is not acceptable and unnecessarily slowing down work. Can SULF show LEL calculations with worst case H₂ amounts and sufficient air flow and best practices from fire engineers to MV for the go ahead of the compressor use? The typical rule of thumb is no chance of spark within 4.5 m. Can the compressor be this distance from the H₂ source? While waiting for ESS to step up is MV willing to discuss what needs to be done directly to SULF?

The SULF team shares the concerns of the STAP with regard to the environment, safety and health division, ESH. We are trying to resolve the situation of lacking support after retirement of our former safety officer by spending extra efforts in frequent meetings with the new ESH team member that started in February. So far this has not been entirely successful. SULF is spending an increasing amount of time to explain reasoning and logic behind laboratory work and safety procedures as well as responding to new safety requirements that often are not suitable for the type of work ongoing in chemistry laboratories. SULF is currently exploring possibilities to perform the hydrogen work and glass blowing activities in labs at the ESS site. This is not convenient but easier as the safety rules and responsibilities are fully in ESS hands and issues can be resolved promptly.

Procurement/Logistics - We will reiterate our comments in March regarding the procurement process. It is good that as well as identifying the problems you are having with the processes, you are working on eliminating them/or minimising their effects, but this is on a critical path for DEMAX. Users will expect their samples in a certain time frame to make beam time allocation, for use in research tied to funding with milestones, to support graduate thesis work, etc. Chemicals are needed to fulfill these proposals. As well, shipping seems to be in this same department. It is unacceptable that DEMAX has a package sit, waiting to be shipped. The expense of overnight shipping is trivial compared to time and money put into making samples. The viability of samples packed in dry ice is on a ticking clock. Speed and reliability

are key to the success of the DEMAX user program as well as the ESS neutron user program. For the neutron user program there is time to work out these kinks, for DEMAX, there is not. Impress upon the Procurement and Logistics department that the early reputation of ESS is dependent on being able to send and receive shipments. Not just receive shipments, but actually order chemicals and supplies in a timely manner. The extra approvals are still in place and slowing down the process. Employees should be able to order things under a certain amount (e.g., 10,000SEK) without extra oversight. More flexible administrative procedures could be helpful (e.g. non signature for small priced items). Furthermore, SULF should not be restricted to two suppliers, but free to choose its preferred supplier under considerations as pricing, availability, quality and delivery time. However, overnight deliveries are hardly possible if internal administration is involved. It is suggested that SULF establishes "rapid orders" with one or two suppliers, e.g. Merck (Sigma-Aldrich) or Fisher Scientific. Those companies have a broad range of chemicals and consumables available. Prices and estimated delivery dates can be checked directly online. A rapid order can be placed at the beginning of the year for a certain amount of money and subsequent online purchases will be withdrawn from it. Such a system is the fastest way to obtain chemicals or consumables. A general question to think about is, who is going to order chemicals requested by users? SULF or the instrument teams? Ask them to visit LU. There must be a way to make this process better. Other facilities have found a way. They must reach out for solutions and revamp their policies in order to accommodate a large staff with obvious needs to ensure facility success. The situation as is, is unacceptable. It would be a real shame to tell the scientific community that you would love to make contributions, but the Procurement and Logistics department just doesn't seem to be on board.

SULF and DEMAX followed the STAP advice and managed to establish a blanket order system for three of the most common laboratory and chemical suppliers. Ordering items up to a fixed sum per year and supplier can now be done without authorization of every single procurement. We have extended the supplier to include Fisher Scientific and Sigma Aldrich. SULF is especially happy with Sigma-Aldrich as a lot of the chemicals are delivered fast and reliably. DEMAX is working with Procurement & Logistics to improve our workflow and make orders and goods pick-up smoother and faster. They are understanding and are sympathetic to our needs, but there remain obstacles both internally and externally to ESS. We will present these during the STAP. We have invited Luis Ortega from Procurement and Jörgen Larsson from Logistics to present the current working procedures and systems at ESS to the STAP in the April meeting. This also gives a chance to hear directly how our internal systems for support in these areas work.

VAT - The STAP has concern about the VAT issue. As it is an issue for the entirety of ESS and the accelerator will have the greatest need (and will have to have something worked out soon), this seems best left for the council to work out noting that it must indeed be worked out.

SCUO

User meeting - Joint ILL/ESS meeting is an excellent use of funds. ESS and users alike will profit from getting to know ESS with an early presence among European users and preparing for when they can make use of its capabilities. It will give a feeling of "reality" to the ESS as a future facility.

The user meeting was indeed a great success and we will soon need to plan for the event in 2020 taking place around Lund.

Funding - Brightness2 monies are great and will become an asset. Is there staff in place for this involvement? It does not seem time just yet for dedicated staff in the user office funded solely by ESS, just checking on the workload. Will DEMAX run the user office side of things for their upcoming activities until a time when dedicated user office staff is warranted? The foreseen addition to DEMAX from Brightness2 is a benefit to early success of its user program. Retaining Oliver is supported.

Brightness2 enabled us to recruit the SCUO officer (Carina Loble) starting in May. In this role she will also support the LENS initiative in addition to shaping SCUO internally at ESS

SULF

There are a lot of very positive things happening in SULF. There has been great progress and things appear to be moving in a good direction.

Communication - SULF clearly made efforts to inform the instrument teams on sample management procedures and established good cooperation, e.g. with DREAM. SULF is encouraged to continue those interactions with the different instrument teams. To clarify a point related to contacts from SAD to the instrument teams, the STAP pointed out the interaction between DEMAX and NMX as an example. Perhaps that point was not well articulated. More to the point it is not about platforms but about specific expertise. Instruments are different and supplying sufficient support requires different skill sets. SULF is well positioned with expertise as is DEMAX and they have complimentary experience. The comment from last time was more meant to point out that the SAD contacts and the instruments should be better aligned with the expertise that best suits. SAD members who are unfamiliar with certain instrument types will find themselves very frustrated in those interactions. This is not a best case scenario for either the SAD member or the instrument. SAD has since readjusted the contacts to the instrument teams. As well, the tollgate process is better known and these interactions are hopefully more understood. Creating a checklist is a sound step toward streamlining this interaction.

SULF established direct communication to almost all instrument teams following the last IKON meeting. While SULF is not deeply involved in the tollgate process for the instruments, we will still provide guidance and review plans for instrument specific laboratories and sample handling.

Sample handling - It may be a dangerous assumption to make that instrument teams will empty sample cans. You'd be surprised how time-consuming this job can be, especially if the dedicated powder box has thick (glove box) style gloves. And the cleaning up of the cans afterwards, ready for re-use, is not necessarily a quick procedure. If samples have been heated, some form of powder sintering may have occurred meaning the powders don't just flow out of the can, but need to be broken out. Also adhesion of the sample to, or reaction of it with, the walls of the sample can all increase the time taken to clean it. Not all beamline scientists will have the enthusiasm to undertake this sort of task; and lab technicians will need sufficient training to understand and deal with any chemical hazards present. If the users no longer need their samples, is ESS considering providing a disposal service for them? Or are all samples to be returned to users (once any induced activity has decayed)? The shipping of samples can be quite time consuming (paperwork) and shipping of hazardous samples is complicated and expensive. Considering work and costs, disposal on site might be the better solution. Be cautious to consider sending sample containers to the users for emptying after an experiment. Apart from the general issues with shipping, the containers may not be returned in a timely manner if at all. Moreover, unless the users are 100% trustworthy it would almost certainly be prudent to clean the containers again in order to avoid the risk of providing the next users with contaminated ones. It will also require some effort from the instrument teams to keep track where the containers went. Nevertheless, some degree of unloading samples which remain active for long periods will probably need to be done at ESS, if only to get the sample cans back into circulation.

SULF will not take the responsibility to empty the cans to the instrument teams. However, we have started discussions on where and how the cans can be emptied as some of the teams (e.g. DREAM) are aware of the issue and planning for it.

Experiments - Working through some of the typical experiments is a good test whether the lab is functioning. However, care should be taken to adjust expectations - the service level to local users will surely decrease when the facility starts operating. As stated in the section on making samples for users, a lot is learned on what may be needed. For thought, such experiments may involve studying air sensitive samples at high (or low) temperatures along with gas flow. Make sure that there is appropriate coordination between Sample Environment and SULF teams to ensure that sample cells and holders are designed to be able to fit within the posting ports of the glove boxes (or that large enough posting ports are available to accommodate any existing designs). The scenarios for sample preparation for a powder diffraction, spectrometer and SANS experiment are not unlikely. It may be worth preparing similar scenarios for soft matter/biology experiments on a reflectometer, as those often require the most intensive sample preparation. Concerning the simple sample preparation for the nanopowder measurement, a standard glovebox is not necessarily the best equipment for handling nanopowders. If

the particles can be handled at ambient, a specific fume hood for handling nanopowders will facilitate sample handling and decontamination.

Also - a Sample Environment consideration - these experiments may have multiple samples, in which case provision of multiple sample holders/sticks needs to be considered to allow for efficient changeover (or a holder/stick being out of commission due to e.g. still containing an active sample, or chemical contamination).

Consider committing MESI efforts to allow LabView controlled sample environment to run at ESS since this is a major platform for user groups who build their own sample environment and would bring it to the facility.

SULF will continue the evaluation of what is needed for experiments at various instruments while we follow the teams through construction. The point to go through a reflectometer experiment is well taken. The laboratory in D04 is designed with extra free space for preparing and moving reflectometry equipment such as Langmuir troughs easily from instrument to lab.

Staff - SULF seems to be well staffed for now. The responsibilities seem to be well allocated to cover all of the current major tasks. Apparently planning for future staff has already progressed. The current SULF team's background covers a broad field, which is necessary to deal with future user requests that will come from quite different scientific areas. Just for clarification, is there or will there be a SULF member (or health and safety officer) with a profound knowledge in biology to judge handling of samples that pose a potential biological risk? SULF might consider sharing a technician with a more mechanical background on part-time (maybe 20% to 50%). Some of the standard equipment that will be bought may need modification to fit the needs, e.g. Langmuir troughs must be modified to carry silicon blocks used on the reflectometers. Such work can also be done with help of sample environment and/or technicians of the instruments that would profit of the work. However, their priorities may be different and work may take longer to be completed.

We have now started the recruitment of a laboratory technician for FLUCO but working also synergistically with the SULF team to cover exactly these aspects.

In-kind - The glovebox in-kind project seems to run smoothly and the future steps until the delivery and installation of the glovebox are well planned. This is an in-kind success in a system that has many challenges. The main issue seems to be the temporary placement of the boxes. Evidently, the laboratory outfit with the in-kind partners from the UK is more complex and we hope that SULF gets the administrative support it needs to resolve the VAT problem. It is a bit worrying that only 1/3 of the lab space can be fitted out with the UK in-kind package. From the document (SAD accomplishments/next steps), it is not really clear whether funding for the additional 2/3 of the lab space is secured and whether it will have an impact on the schedule. Fitting out the labs with the UK in-kind is progressing quite well. Great news on the UK visit and how well they reacted to the state of the buildings. The time line seems to be right on for having everything in place for when the buildings are turned over in December 2019. Hopefully the leftover from the high cost estimate can be put to good use. It seems that NSS could provide cabins that can be shared throughout and the "hot desk" model can be used, which requires much less office space as they are shared.

We have established a clear plan for fitting the labs and workshops using both in-kind contributions but also ESS procurements. Details will be presented during the STAP meeting.

Chemicals - The STAP supports the movement toward obtaining a chemical inventory. Having a functioning chemical inventory from the start is important and should receive more priority than it currently (apart from SULF) does. As a temporary solution for SULF "Quartz", a free web-based inventory system, might be an option. Apart from inventory, one can also use it to manage orders and purchases; an option that can be very useful to track orders during busy times with many purchases. Bar code scanning is possible. The STAP endorses the use of bar code scanning for chemical inventory – SAD should also consider linking this to user chemicals/samples arriving onsite, and (at end of experiment) being checked by Health Physics if they are to leave site/for disposal, so that there is one process for chemical handling and a one-stop shop for accessing safety information about any sample/chemical onsite. Also tracking when a container is thrown out could indicate the need to restock. (the ANSTO system for user samples works well and includes such bar-coding).

The chemical inventory that includes all Swedish legal requirements has been procured and will be implemented in the coming months.

Training - The safety training classes are a good start. Can ESS gain the ability to train within ESS? Meaning, does everyone who wants to flame seal a vial have to attend this class? What are the thoughts on users being able to do activities such as “hot works”? The incorporation of a user lab training into the official database seems to be right on track. For the future SULF, SCUO and the instrument teams should think about the way lab access will be managed. What are the requirements to obtain access? Who will provide the physical access? An option for requesting lab access should be integrated into the SCUO software. Access should be requested by users well in advance so that SULF (or the instrument team) has sufficient time to check the availability of chemicals and equipment, etc. Well done on exploring opportunities for getting equipment funded.

DEMAX

DEMAX continues to make excellent progress and is well placed to strengthen apparent delivery of value to the ESS through its upcoming friendly user call for proposals which, it should be noted, will cover a range of fields of application and neutron instrument type. The approach that will be taken for the call is appropriate.

The call for proposals went out at the end of February. Our internal and external review committees are ready to review proposals and give feedback and we look forward to reporting back to the STAP on how it all went (receiving proposals, reviewing them, user communications, project execution etc) later in the year.

SMT endorsed this event as news story to promote ESS moving towards first science. We also had a chance to tell instrument teams about DEMAX, proposal call, and offered services at IKON16 and the message was very well received. DEMAX going through this process required a lot of effort and shows that ESS is not quite ready for users. For e.g. we are still lacking an access policy, nobody thought about where and how to register users. In the face of these challenges, many people worked very hard to push the various issues forward and helped us navigate “being first” with users & proposals. All details will be presented during the STAP meeting 2-3 April 2019.

Previous concerns about the security of lab and office availability for the DEMAX team (particularly Chemical Deuteration) have been allayed by progress – renewal of the MV lab lease for 5 years and continuation of arrangements with Lund University’s LP3/LU platform. Access to external key infrastructure such as NMR, ESI-MS and MS is in place and makes financial sense.

We are happy to report that MV lab space has been secured for 5 years (2018 – 2023) for an annual cost of 600 000 SEK. This is higher than what we anticipated or planned for and we will work to reduce our footprint in an effort to bring this to a more reasonable level. When SULF moves on site in 2020, DEMAX will take over the payment from Admin. The service agreement with LU is entering its 4th year and we will soon start negotiating for the next five year contract.

Concerns expressed by the SAC about value delivery by DEMAX appears to be based on the misconception that it will only deliver in the area of neutron crystallography of deuterated proteins. As stated in SAD’s reply, the deuteration platform at the ESS is highly relevant to a broad range of instruments and spans many different types of neutron science application through its developed and planned capabilities in production of a broad range of deuterated small molecules such as lipids, phospholipids and surfactants which are highly relevant to neutron reflectometry (ESTIA) and SANS experiments (LOKI) and through the ability to produce partially deuterated proteins for SANS of protein complexes and interactions. The ability to produce perdeuterated proteins is relevant not only to the determination of the position of individual hydrogens in crystal structures (NMX) but also to the measurement of the dynamics of proteins using neutron spectroscopy (C-SPEC). The recently developed capability to produce deuterated lactic acid which enables production of poly-lactic acid (PLA) also opens up SANS and spectroscopy polymer applications requiring deuterated PLA. These observations are based on the experience of other deuteration facilities in Australia and Europe where chemical deuteration capabilities predominantly serve reflectometry, SANS and diffraction and biodeuteration SANS, neutron crystallography, spectroscopy and reflectometry depending on the capability of the instruments. DEMAX has demonstrated considerable progress and success in a

relatively short period and the prospects are excellent for ESS to reap the value of this capability development through use of deuterated molecules at the first tranche of instruments.

We got very positive feedback from the last SAC meeting and buy-in from both SAC and management is now ensured.

However, the long-term value that DEMAX is likely to deliver as a platform with both biological and chemical deuteration capabilities, also needs to be considered. In the Australian context, the National Deuteration Facility which has operated both types of capabilities over the last 10 years (primarily for SANS, reflectometry and diffraction) has been able to demonstrate enabling of highly complex science relevant to: (a) New materials for Solar cells, Batteries, Electronic components such as Organic Light Emitting Diodes, and transistors. Drug delivery (lipid based liquid crystals), Tissue engineering, Hydrogen storage (energy) or CO₂ sequestration (climate change), Biosensors (biomedical and industrial applications), Catalysis and separation, Green solvents (e.g. ionic liquids). (b) Molecular structural basis for Disease causation (e.g. protein misfolding diseases like Alzheimers Disease, cancer, prion diseases, apoptosis, action of toxins), Drug design including antimicrobials for drug-resistant bacteria, Cell membrane integrity and membrane protein function, Nutrition and cell health – including understanding human digestion of lipids and triglycerides, and the role of antioxidants in maintaining cell health, Mineral processing including froth flotation and coal pyrolysis, Forensic detection, diomineralised structures in nature. DEMAX is a wise and judicious investment for the long-term success of the ESS and the best neutron facilities in the world have such capability platforms to leverage their neutron instrument investments.

The long term sustainability is a topic for the SIN2020 final deliverable but also part of Brightness2 (deuteration pilots). A sub-working group on deuteration has been established within the LENS partnership.

DMSC resources to work on User Office software (initially for DEMAX proposals process in early 2019 - is the aim still to have the call open for 6 weeks prior to a March deadline?) will commence in Oct 2018. "We are reasonably confident that some sort of system will be available for proposal submission next year," gives the STAP some anxiety. Ensure that the information collected by web form, and the (Survey Monkey/Google Form) customer feedback is stored in a database which is accessible, searchable, and can be expected to be easily exported to other systems in the future. How "short-term" is the short-term consultant? Continuity in developing/maintaining the system once s/he leaves is essential - the collaboration with MAX-IV should provide a good template to start work from, and also the longer-term commitment for the 2 facilities to work together should aid in providing continuity. The "Accomplishments in Q1/2018 & Next Steps in Q2/2018" (April 2018) document states you aim to have a web interface ready to accept DEMAX proposals by the end of 2018. Is just over 3 months long enough to create and test such a system?

The DEMAX user portal looks excellent and hard work from several individuals at DMSC made this possible. Jon Taylor, Tobias Richter, Gareth Murphy and Jeremias Hillerberg all worked hard to make this possible. All the functionality we asked for is there – users can register, download a proposal template, create a proposal, fill out info for us regarding their sample needs, attach a deuteration/crystallization proposal, beamtime proposal, chemical drawings etc and create an integrated PDF for review. On the back-end we need to be able to handle proposals, reviews, and reviewer comments and this is today still a rough prototype, lacking full functionality. As such we will handle reviews for the first round mainly "by hand". We created a restricted Confluence page where we put the proposals and a score sheet for internal reviewers to fill out. Proposals that pass the feasibility/safety review get sent out via e-mail for external review. We have prepared a review sheet that external reviewers will fill out and we will copy/paste the scores and comments back into a master Excel sheet. So - there is a bit of manual reviewing and scoring going on and we hope to have proper electronic tools for this last part in the future. Gareth and/or Jeremias will be able to support us once the call opens. We also expect quite some refinements to the portal in the future as we learn and grow. Continued support and expert help from DMSC is crucial in making this work.