Scientific Activities Division (SAD) – Recent Accomplishments and Next Steps
Q4/2018 Report – 14. Jan. 2019 – New Format

MANAGEMENT AND INTERACTIONS

Achievements

- Implementing line organisation
- Updating STAP reports following off-line meeting.

Enables smooth operation of the Scientific Activities Division

Mitigates line management issues.

Continuing to implement the line organization for the Scientific Activities Division we have established groups for deuteration and macromolecular crystalisation (DEMAX, Group leader Z Fisher) and sample and user lab facilities (SULF, group leader M. Hartl). To strengthen the team in its new line organization we went on a SAD retreat supported by HR.

An (off-line) STAP meeting was held and the STAP reports updated and presented to the SAC.

SAFETY AND LICENSING

Achievements

- NSS licensing core team complete with members from all relevant Science divisions
- Senior consultant Per-Olov Larsson is assuring our approach agrees with the ESS-wide approach and correct templates are used.
- Documentation for accident identification and classification are in informal review
- Detailed accident analysis has started with two out of six identified main accident scenarios involving subject matter experts.
- Planning for the sustainability of safety effort towards the SSM application (and beyond) needs to be started in Q1/2019

Enables timely delivery of documentation for SSM license application

Mitigates against delays due to licensing process.

The NSS licensing core coordination team has been extended to cover all parts of the NSS project. With Andrew Jackson joining we are putting an adequate emphasis on the safety and licensing aspects of the neutron instruments. We delivered (only) the required NSS documentation for the current license application e.g. documents related to the radioactive materials laboratory. Thought draft version of all NSS documents exist for the forthcoming license application. They are tracked in Jira by ESH and we have an agreed timeline with ESH on the documentation for the next license application.

In Q4/2018 our consultant Per-Olov continues to update the NSS top-level hazard analysis using the similar approach as other parts of ESS (accelerator / target) and to

link with the system specific hazard analysis performed by the various teams especially the bunker hazard analysis. The various subject matter experts continue to keep their documentation up-to-date but ensuring the adequate resourcing poses a challenge for several teams. This will require that during Q1/2019 we will be able to establish a more precise planning and the respective roles throughout construction and going forward to initial operation. We will need continuous support from ESH to provide us the expert knowledge especially related to our emissions resulting from certain accident scenarios.

Helena finalised the documentation on the work flow on performing the instrument hazard analysis. This serves as an important element to accompany the instrument teams in their detailed design work towards the instrument TG3.

Scientific Coordination and User Office (SCUO):

Achievements

- Successful ILL-ESS user meeting in Grenoble
- New SFT coordinators for 2019/2020 started
- Recruitment process started for scientific coordination and user office.
- Discussions with MAX IV on common seminar series started.

Enable better external and internal scientific collaboration
Mitigate against decrease of future user engagement and staff demotivation.

A main activity this quarter was the successful joint ILL-ESS user meeting in Grenoble with its 500 participants. It was very successful to strengthen the neutron network and putting the current and future possibilities at the two European institutes in the spot light.

New SFT coordinators started their work for SFT Soft / Life (Esko), Chemistry and electronic phenomena (Dan) and Engineering (Premek). Valentina stayed on as SFT coordinator for particle physics. We have started to re-vitalise the SFT 'technoclogy and e-science' with Thomas Holm Rod taking on this task

With the BrightnESS2 grant awarded and starting in Q1/2019 we were able to start the recruitment for the 'scientific coordination and user office'. The 15PM provided by the grant do not cover the cost for 2019 (9PM) but also realising some savings in 2020 (6PM) when the recruitment had been planned initially. With this recruitment we shall be able to adequately support our engagements in respect to the BrightnESS2 WP2 and WP4, the ESS internal needs (including SFT and the DEMAX support service) but also SCUO-related share within the LENS initiative.

Discussions started on joint ESS MAX IV seminars series which should enable us to reach a critical mass for scientific seminars which had been a challenge for the previous ESS-internal SFT seminars.

Sample Handling and General User Labs (SULF)

Achievements

- SULF has become group within line organisation; Group leader M. Hartl
- Tendering process Lab fit-out concluded; CDR for glove boxes completed
- ESH to procure and provide off-the-shelf inventory system for chemicals but more ESH is still required.
- Agreement with CF on construction scope for waste water in E buildings
- Lab equipment arriving and progress on procurement of chemicals
- Awarded (small) grant for 1 yr pilot with local industry; starting Q1/2019

Enables scientific use of support facilities in E-buildings

Mitigates risks related to sample handling for (early) science.

Staff and Responsibilities:

Starting at November 1st, SULF has officially become a group in the Scientific Activities Division with Monika Hartl as group leader. Additionally, there have been noticeable changes in personnel at the end of Q4/2018. Katrin Michel is still working 100% for SULF with the main focus on the MV-lab, procurement and general laboratory safety. Athanasios Stathis, who was temporarily employed by SULF as project engineer, left us with the end of Q4. He supported SULF with 50% of his time establishing our confluence pages and staying on top of CF related issues. The remaining 50% of his time he functioned as interface to conventional facilities (CF) Melissa Sharp is still working "half-time" (40% for SULF) but has been transitioning back to being the interface to CF. She is expected to be back full time by January 2019 and will then be working 50% for SULF and 50% as interface to CF. She will be moving from the Neutron Instrument Division to the Scientific Activities Division/SULF in Q1/2019. Monika has transitioned completely from Target Division to the Scientific Activities Division. She is working 80% for SULF and 20% for safety and licensing as part of the core team.

Due to these changes, we will have a one-day SULF retreat in the beginning of February to clearly define roles and responsibilities within the SULF project. This is imperative as 2019 will be quite stressful as we prepare and organize the lab fit out in the E-buildings that will commence in December 2019. Furthermore, this will prepare the group for the next IKON meeting in February as the instrument groups become more and more interested in sample handling and laboratories.

SULF in-kind projects:

Our UK in-kind partner STFC published the tender for the laboratory fit-out late summer 2018. We had a Skype meeting for the tender evaluation at the end of November 2018. Our review comments were submitted early December and the final decision for the winning tender is expected early January 2019. The VAT issues affecting the lab-fit out have been mostly clarified. It seems that VAT taxation will be on installation work only, while the goods procured through our in-kind partner STFC are not taxed. Consequently SULF and our in-kind partners are working on optimizing the cost by shifting the installation work from STFC back to ESS as ESS is not subjected to VAT. Most of the next six months will be spent preparing for installation in January 2020.

Our in-kind partners from Tartu visited ESS late September for the critical design review (CDR) of the glove boxes for the radiological materials laboratory (RML). The tender for the procurement of the basic glove boxes went out as planned in late October 2018 based on the successful CDR. The delivery of the glove boxes to Estonia is planned for summer 2019 and the customization will be performed at the University in Tartu. The glove boxes will have to stay in Tartu for one year before they can be delivered to ESS to avoid VAT. This actually fits well with the SULF plans and so the milestone for the delivery has been shifted to summer 2020. We will then install and operate the glove boxes first in the E04 building until the RML in building D08 is ready.

Safety and training for the current and future chemistry laboratories**:**

H. Boyer (OHS group leader) has established an "Area Co-ordinators Satellite Sites (OHS) Meeting" which took place in November 2018 for the first time. This meeting is trying to capture the requirements and demands of the satellite sites such

as Medicon Village (MV), Utgård and Embla. It will occur on a regular basis and Katrin from SULF will be participating with Monika and Melissa joining from time to time as needed. After the first satellite meeting in November, we are still not sure how our concerns will compete with the complexity and demands of safety on the ESS construction site. While it seems that OHS is now more aware of SULF needs, manpower at OHS is clearly too low.

There have been renewed discussions in fall 2018 about a suitable chemical inventory management system and how to fit this into the ESS business software system. We had several meetings between the stakeholders (with SULF being the owner of most chemicals) and the OHS group, procurement and IT. On December 19th, 2018, we reached consensus that ESH will buy an “off-the-shelf” chemical inventory management system for the next two years which will give the inventory working group time to evaluate how to incorporate a suitable system into the ESS business software. This procurement needs to be pushed through fast as we are out of compliance with the legal requirements in Sweden without it. This effort in fall 2018 was strongly supported by OHS and due to that we were able to push it to a decision within a few weeks. On the other hand, we are still waiting on several issues that we have asked OHS to address and that have not been resolved. The OHS group still has to meet with Medicon Village (MV) personnel so that we can start using our glass blowing setup (waiting time > 1 year) and so that we are allowed to restart the compressor in the hydrogen lab (waiting time >6 months). Especially the restart of the compressor that we were able to use for 3 years before the sudden shutdown is crucial as work for the ESS project in collaboration with Target Division has come to a standstill. On a positive note, we have received the license to use mercury for our electrochemistry setup. This is a license that SULF applied for with the NSS safety officer and that has to be renewed every two years. This is not anticipated to be a problem as we can apply for the license ourselves and thus we can plan for it.

The safety paperwork concerning the use of the RML is in review by the ES&H group. We will follow up to see why we have not received comments yet.

The examples above clearly illustrate that we still do not get as much assistance as we need from ESH and we still have to spend a lot of time following up on issues. This is blocking our progress. We will try to work with confluence/jira web tools to make ESH aware of the topics and their urgency and at the same time illustrate the need for more support.

The training for the SULF members currently includes electrical safety, “ATEX” (flammables, every 5 years) and “hot works” (soldering, Bunsen burner, glass blowing, every 5 years). It is planned to have the SULF members also trained as “dangerous goods officers" (every 5 years). This is a training necessary to be allowed to transport dangerous goods within the ESS site and from ESS to the outside world. While ESH and logistics are planned to be the ones transporting and shipping chemicals, we believe it is crucial to have this capability within SULF. A very recent experience has shown that retirement or leave of personnel can lead to the situation that there is no dangerous goods officer left at ESS. While this currently is only an inconvenience, this could, were we running a user program, seriously affect operations as transport of chemicals between buildings on the ESS site by ESS personnel would be illegal.

CF interaction for on-site laboratories (auxiliary buildings):

SULF is continuing to attend the bi-weekly CF meetings and work on tasks as they arise. We have established confluence pages which allow us to keep track of issues at the interface to CF. These confluence pages contain some history as well as current status of tasks so we can assure that anyone can follow-up on items. We are continuing with the design reviews for the D-buildings.

The electrical distribution panels for the E-buildings have been procured and are on-site awaiting installation by SKANSKA. The waste water from the auxiliary buildings has been discussed again between CF, ESH and SULF/NSS. The water tanks in the basements are small and solutions for online monitoring and sampling were sought after. In December the decision was made that CF will design for two small tanks in each basement with feed-troughs for monitoring equipment and sampling. One of the tanks will be in use while the other one will await sampling. ESH and SULF will meet to discuss the monitoring possibilities and frequencies for radiological materials and chemicals. The main area of conflict between SULF and CF is still building D07 that is missing from several documents now as the design is on hold. The E buildings are well on their way and progress is clearly visible (see pictures below).

Progress in the E buildings is steady. The ventilation system for the fume hoods (left) is in place for most rooms and lab gases and utilities (middle left) are installed for all large labs. Some of the smaller rooms have been equipped with the suspended ceiling (middle right) and we could confirm that the tiles are removable with little effort. The crane in the sample environment workshop in E03 is ready.

Procurement of consumables and equipment

After all our procurement problems in Q3/2018, our orders are mostly arriving on time for Q4/2018. The framework agreement with one of the vendors that we were having difficulties with will be terminated as the shipping requirements established in the contract with ESS clearly could not be fulfilled. This opened up the discussion on how to make frequent but usually small orders from suppliers easier for SULF/DEMAX. We have discussed the possibilities to have “blanket orders” which would allow us to have one approved purchase request over a determined amount of money for a certain company. We could then start ordering up to that amount without having to go through the chain of approval for every single order. This will reduce the time spend on each order significantly for all concerned. There will be follow-up meetings with procurement to establish this process.

We have continued to buy equipment and chemicals for the laboratory according to our plan. We received a UV/VIS setup and have sent out the FT-IR for tender in December. We have contacted vendors for other large scale equipment as well as for bulk procurement of small scale equipment (stirrers/heating plates/water baths). We are preparing for another large order of basic chemicals in Q1/2019.

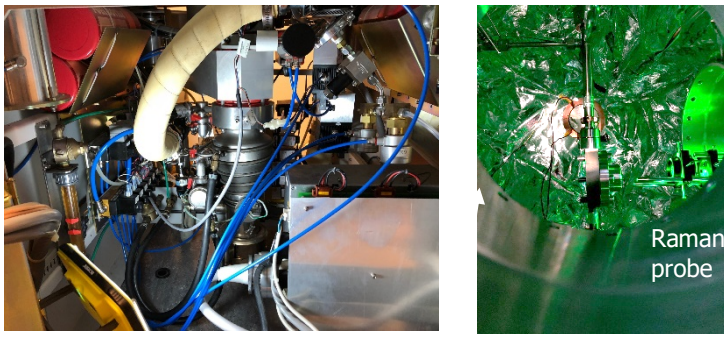
Once the lab-outfitter has been determined for the laboratories that are part of the in-kind project, we will establish a sole source justification for using the same outfitter for the remaining laboratories and workshops such as the SLIME lab and sample

environment laboratories. This concerns only certain equipment such as fume hoods, overhead extractors, special furniture for which we should use only one supplier for ease of maintenance and operations.

Increasing SULF capabilities

As mentioned in previous reports, SULF is currently trying to support local neutron scattering users with synthesis of neutron scattering samples. This helps SULF to test equipment and operations in MV, to apply for grants which can be used to buy scientific equipment and to establish a neutron scattering user community that is aware of the possibilities offered by the laboratories. We are currently working closely with F. Ossler from Combustion Physics at LTH and A. Gonzalez-Perez from Swedish Water Research AB on joint research. SULF was successful in receiving the one-year pilot project with local industry (Swedish Water Research AB). We have started to work on the project and are buying chemicals as well as other consumables. We are using MV lab to synthesize the samples and characterize them with our equipment. We are currently in discussion on how to apply for a larger grant as well as how to extend the industrial collaboration into the area of life science.

To deepen our local collaboration, we are currently commissioning the Scanning Electron Microscope that belongs to the Materials group. This marks the start of establishing one laboratory for ESS in collaboration between SULF and other groups/divisions. We have also supported Yannick Bessler at the FZ Jülich by assisting in setting up the ESS Raman system with their cryostat. They will test the hydrogen flow and ortho to parahydrogen conversion in a mock-up model of the ESS hydrogen moderator. SULF will continue to contribute to the effort of online monitoring of liquid hydrogen which is an ESS collaboration established with SNS and JPARC.



Commissioning of the Scanning Electron Microscope has begun in the TA-1 lab (Materials Group) on site (left). ESS Raman system incorporated in the cryostat from FZ Jülich to measure Raman signal of liquid hydrogen (right).

6 month plan SULF:

The detailed plan for the next 6 months can be found below divided into the various SULF topics. There will be a SULF retreat on February 7th, 2019 to organizing which SULF member is leading which task.

in-kind project progress:

Jan-March, 2019:

- Decide together with our UK in-kind partner on the details of the lab-fit out and what amount of the in-kind money will be transferred back to ESS for lab installation to avoid VAT tax. Renewal of the technical annex between ESS and STFC will follow this decision.
- Invite the lab-outfitter and our UK in-kind partner for a kick-off meeting at ESS. Arrange for the NSS installation engineer to attend to start detailed planning of goods delivery, goods storage, site-access, training/safety and other installation-related topics.
- Contact the in-kind partner from Tartu to follow up on the status of the tender and the procurement process of the basic glove boxes.

April-June, 2019:

- Establish a regular and frequent channel of communication with the lab-outfitter and our UK in-kind partner to assure efficient planning of the installation commencing in December 2019/January 2020.
- Visit the in-kind partner in Tartu or have a Skype meeting to discuss the plans for the modification of the basic glove boxes for the RML.

Safety and training for the current and future chemistry laboratories

Jan-March, 2019:

- Continue with bi-monthly satellite-site area coordinator meetings.
- Monika to attend “Initial training for dangerous goods officers" at the end of January.
- Follow up the procurement request for a chemical inventory management system and participate in the tender process for the software.
- Remind OHS to follow up on what needs to be done to allow the use of the compressor in the hydrogen lab at MV and to allow glass blowing.
- Follow up with the radiological protection group on the review of the two RML procedures.

April-June, 2019:

- Implement chemical inventory system to comply with legislation.
- Monika to meet with the Radprotection Group leader Sigrid to talk about future ways of collaborating efficiently for general safety and the SSM application.
- Follow up with training to see if the chemistry lab training has been incorporated into the official database.
- Establish a confluence/jira page with the ESH/OHS group to communicate SULF needs and deadlines and to illustrate the urgent need for safety personnel

CF interaction

Jan-March, 2019:

- Continue with the bi-weekly CF meetings and work on tasks as they arise
- Continue with detailed design review of D-buildings
- We will update ESS Safety and Sample Workflow for Instruments-Reference Document for WBS 13.6.X.7.1 (ESS-0040840) with detailed information on the containment and conventional ventilation for instrument specific laboratories as we receive them from CF. This document will contain technical information and requirements such as piping size, end point connection, HEPA filters as well as rules and regulation for the use of these ventilation systems. It will be ready before IKON.

April-June, 2019:

- Start discussions with the lab outfitter about drawings for the labs in E04 not part of the in-kind contract, e.g. the engineering lab SLIME. Work with the other workshops and align common goals to make the fitout as cost efficient as possible.
- Start discussion about procurement for electrical distribution boxes for the D-buildings
- Discuss monitoring/sampling equipment with ESH/CF for waste water tanks in basement of auxiliary buildings

Procurement of consumables and equipment

Jan-March, 2019:

- Keep our SULF procurement list up to date. It contains the chemicals that we plan to always have present in the lab. It includes the CAS number, the order number, the amount present, and the price.
- Buy second large order of chemicals to establish a set of commonly used chemicals that do not expire. Follow the SULF procurement list when ordering chemicals. This list was created by SULF with input from other user labs.
- Buy an FT-IR machine

April-June, 2019:

- Buy third large order of chemicals to establish a set of commonly used chemicals that do not expire. Follow the SULF procurement list when ordering chemicals. This list was created by SULF with input from other user labs
- Establish sole source justification for lab-outfitter to have contractor for laboratories that are not part of the SULF in-kind.

Increasing SULF capabilities

Jan-March, 2019:

- Work on grant for water research; hire a temporary technical assistant for 2 months from grant money;
- Continue discussions with ESS internal groups interested in using the user labs to find common ground and possibly joint procurement of larger equipment
- The grant decision for HFSP will be announced and we will proceed with procurement and hiring if successful.

April-June, 2019:

- Meet with local industry “Arcadia AB” to discuss potential life science experiment with neutrons followed by potential grant application.
- Prepare for one of the large SINE 2020 proposal calls.
- Support the Materials Group/Target Division with materials characterization in the MV laboratory for their Beryllium Reflector Project and their Irradiation Campaign for polymers.
- Take part in a Raman experiment at JPARC and assist with setting up the Raman system.

Deuteration and macromolecular crystallisation (DEMAX):

Achievements

- DEMAX has become group within line organisation; Group leader Z. Fisher
- DEMAX has concluded its construction scope; moves into operation in 2019
- DEMAX continues to profit from grants; published two papers
- Extended collaboration with Japanese and Australian colleagues
- DEMAX is ready start deuteration support services in 2019
- Very good progress on software for DEMAX support service.
- Challenges remain with too much travel (away from lab), negotiating service agreement cost with LU and (to lesser extend) vendors on consumables.

Enables providing operation of deuteration and macromolecular crystallization support service

Mitigates risks related to being unable to show scientific impact in soft matter research and life sciences.

Staffing:

Starting at November 1st, DEMAX has officially become a group in the Scientific Activities Division with Zoë Fisher as group leader. Anna Leung was hired on as our deuteration chemist in a full-time, permanent capacity. Hanna Wacklin-Knecht has transitioned to work full time in DEMAX from Neutron Instruments Division and is funded by both SINE2020 and DEMAX. Both Hanna and Anna work on the chemical deuteration support pillar of DEMAX. Zoë continues on the biodeuteration and crystallization side with the aid of a 0.5 FTE technician from the LP3 on a research contract basis. This is a 24 month agreement and we aim to extend it at least 12 or maybe even 24 months. Oliver Bogojevic, who completed a six-month project in the chemical deuteration lab as part of his Masters degree in Biotechnology at Lund University, returns to the chemical deuteration lab for an 8-month period to complete his work on enzyme catalysis and immobilization for deuterated lipid synthesis, a key extension of the DEMAX capability to purify biological lipids from cell cultures, and an important alternative to chemical lipid synthesis.

Activities, external funding:

Since the last STAP meeting held in March 2018, DEMAX staff and activities have continued as usual. We continue to benefit from third-party funding, specifically SINE2020 work packages 5 and 6 that are partially supporting Anna, Hanna, and Zoë. SINE2020 will continue until September 2019. DEMAX successfully participated in 6 Interreg-funded projects (MAX4ESSFUN). These were very useful as they served as practice rounds for real service requests and allowed us to test access modes and procedures for biodeuteration and crystallization (external) projects. We recently learned that BrightnESS2 is funded and this will provide 10 PM to DEMAX starting in January 2019 to continue the method development started in SINE2020 WP5.

Publications:

DEMAX published a methodological paper in large crystal growth optimization [Katarina Koruza, Bénédicte Lafumat, Maria Nyblom, Wolfgang Knecht, Zoë Fisher (2018) "From Initial Hit to Crystal Optimization with Microseeding of Human Carbonic Anhydrase IX—A Case Study for Neutron Protein Crystallography", Crystals 8(11), p.434; doi:10.3390/cryst8110434]. There is another manuscript in preparation on the lactic acid project and will be submitted soon [draft: Leung AE, Raba A, Beckerle K, Allgaier J, Wacklin-Knecht HP "The enzymatic synthesis of perdeuterated D- and L-lactic acid-d4 and polymerization of their lactides to polylactic acid"].

Initial Operations:

We will start initial operations by soliciting a limited number of service requests in 2019, in order to set up and optimize the workflows to process proposals and produce materials on demand to a schedule. We are preparing to issue our first call at the end of February as presented to the SAC and STAP meeting (Q4/2018) and will also ask for Expression of Interest" (EOI) and Letters of Intent (LOI) as strongly suggested by the STAP. We will leave the call open for 6 weeks before closing it and starting the review process. There will be two levels of review: The Technical, Safety, and Feasibility Review panel will perform the first level of review to triage requests in terms of DEMAX being able to execute possible tasks in a safe way with the equipment and expertise we have. Requests that pass this review will be sent for scientific peer review. All panel members have agreed to serve and represent a broad range of scientific knowledge, from biological deuteration, to chemistry and protein crystallography. We will notify applicants of the outcome of their requests within a month or so.

There is a resource from DMSC working on developing User Office Software for use by DEMAX initially and the prototype looks very good. The initial functionality is quite basic but applicants can register, enter all relevant/required information for deuteration and crystallization experiments online, as well as attach images and PDF of their proposals. There is also a basic possibility to enter review and score for our internal tracking purposes and we hope to make the available to reviewers in the future as well. We hope to learn a lot through this pilot period and will have chances to improve the processes and software as we go along. From our internal (admin) log in there is also a basic possibility to enter reviews, comments, and a score for our internal tracking purposes and we hope to make this available to reviewers in the future as well. We hope to learn a lot through this pilot period and will have chances to improve the processes and software as we go along. For collecting reviewer comments and scores we will use an Excel sheet and then will manually input the information into the web system. We will also conduct a survey at the end of the period (ie Survey Monkey or Google Forms) to collect customer feedback after each service request cycle as per the STAP's recommendation. DMSC is also very interested what user may say about the software interface and we will come up with the questionnaire together.

Of course we hope for a good number of proposals (>20) and will prepare a detailed report at the end of Q4 on the outcome. Part of the challenge here will be to develop key performance indicators for DEMAX, and may include: total number of proposals received, number of proposals received in each category (bio, chem, crystals), unique users, mail-in/mail-out requests, in person visits to crystallography lab, amount of deuterated material produced (by category), number of proposals

services/completed/delivered, publications arising from DEMAX (e.g. method development papers or collaborations), number of neutron experiments performed using materials DEMAX prepared, and so on.

We are advertising the opportunity for submitting service requests next year through dissemination at national and international scientific meetings, topical conferences, and by talking to our colleagues on the instrument side. We also aim to present our current and planned capabilities at IKON16, AILM2018, ECNS2018, and at various SANS, reflectometry, and spectroscopy STAP meetings next year. We have a list of materials and services we will be able to offer in this first pilot call and will complete the cycle within a 6-7 month window. We will cater to a balanced set of requests that test our methods, equipment, and further develop our expertise. With this in mind, we will focus on successfully servicing a reasonable number of requests.

Premises, rent & service agreements:

As far as premises go, we are fine for the coming years. ESS has just renewed our lease on the MV labs for a 5-year period. Space is tight but SULF staff are expected to moved out towards the end of 2019. At this point DEMAX will take over the rent payment and the lab will only be occupied by DEMAX staff. For the Biodeuteration & Crystallization activities, we are in year 3 of our 5-year agreement with LP3/LU and recently negotiated fees and services for the coming 2 years. DEMAX has set up agreements with a local MV company (Red Glead) to pay for access and usage of the NMR spectrometer, with the Karolinska Institute for intact protein mass measurement with ESI-MS, and with the department of chemistry at Lund University for mass spectroscopic analysis of small molecules. These are very fruitful interactions and saves us a lot of effort and cost.

Procurements, equipment:

The procurement of the Parr reactor has been a very positive thing for us as it is constantly in use for chemical deuteration. Most of the equipment is in place and we have a few minor procurements in the 20-25 kEuro range that will happen in Q1/2019.. Budget planning for initial operations is underway and we are ready to implement our spending plan once a financial tool for operations is ready to use at ESS. SULF will take a lot of the shared basic lab equipment currently available in the MV lab when they move out, including the fridge/freezers, centrifuges, analytical balances, vacuum furnace, tip sonicator and so on. DEMAX has prepared a prioritized list of things to replace and our estimate is about 50 kEUR for all of it.

Events:

From the last SAC meeting it was clear that due to the intense focus on instrument construction, not all instrument STAPs are fully aware of the activities of DEMAX and have not made specific comments on how the instruments & users will benefit from deuteration and crystallization services. To address this DEMAX was invited to present at the last SAC meeting. The presentation was well received and the SAC was very positive and supportive of DEMAX activities and development. At the ILL-ESS user meeting in October, DEMAX had a strong presence with talks and posters. Later in the year, Anna and Zoë visited deuteration facilities in Japan and Australia. The meetings went very well with a lot of international interest on our deuteration

activities. Several collaborations have emerged as well as making closer ties to our colleagues over there.

Conclusion:

DEMAX is well-positioned and has entered initial operations as planned in Q1 / 2019. Having software support from DMSC is a large step in the right direction. With our current projects, lab spaces, staffing, and equipment we are well-equipped to serve users in the soft matter, chemistry, and life science neutron research fields. We would like to emphasize that our capabilities match the scientific scope of the first ESS instruments and being ready in time is necessary to enable early scientific success – not only for DEMAX but also for the beamlines.

Sample Environment

Achievements

- Improved interactions with instrument teams throughout detailed design phase (TG3 reviews) and via workshops with instrument classes to define requirements for each specific sample environment system
- Floor mounted sample environment stack was eliverd , assembled and is now being tested.
- Collaborative externally funded FlexiProbe project (BMBF Germany) successfully concluded by external partners providing unique capabilities for 'fluids'.
- Conceptual design for integration of high pressure cells successfully completed.
- Collaborative VR funded project on uniaxial stress extended to involve more partners.
- Detailed plans for instrument sample environment for mechanical processing established with BEER instrument team.
- Experiments on V20 at HZB to benchmark MxStas background simulations and to commission the Huggins sub-cryostat (in-kind Roskilde University) with neutrons.
- Semi-automatic helium pumping crate for wet (orange) cryostats completed.
- SINE2020 funded SECoP project to establish standard protocol progressing well and now supported at ESS.
- Sample environment integration team (MESI) taking active part in Beamline Controls Team. Prioritization plan helps to keep track of sample environment projects in a situation of scarce integration resources.

Enables building up sample environment capabilities for the first 8 instruments

Mitigates penalizing early science by not providing the right parameters for exepriments

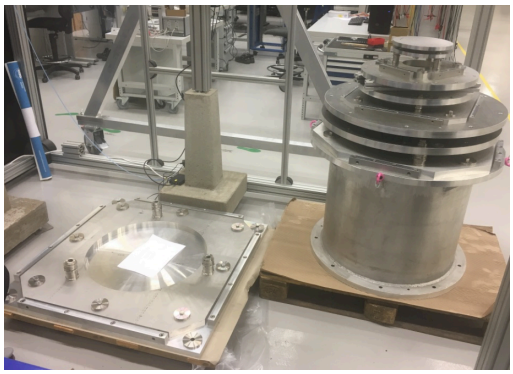
Sample Environment Staff

Richard Ammer started as technician within the sample environment team aminly supporting the TEFI platform. The sample environment technician Pontus left ESS but the recruitment of a replacement has no concluded (Lauritz starting Q1/2019). We shall continue in 2019 to add technical resources to the sample environment team as planned.

General Integration Activities:

The sample environment team takes part in reviews (TG3) of the instruments when relevant. Exchange with instrument teams has also improved via workshops with each instrument class to define the specific requirements of each sample environment system.

The floor-mounted SEE stack prototype was delivered and initial assembly completed in Utgård. Delivery of k-mount components expected in 19Q4 to enable final installation and alignment.



Engineering project for detailed design of a test station for the flange-mounted system was initiated with planned completion in 19Q4

Progress on scanning alignment system included first testing of a laser-based prototype. A formal plan has been implemented in discussion with BCT on coordinated project to test system on V20 in 19Q2. As part of this, quotations of hardware (stages have been obtained). Challenges relating to handling the ESS pulse structure have been discussed and some solutions proposed (to be tested on V20). This includes providing an interface to the Motion Control Group (MC&A) at ESS and also handle contact with motion hardware providers.

The cryogenic testing in Utgård acted as a useful test case for developing and testing our risk analysis processes. In addition, safety signage was developed for activities in Utgård and the on-site PREMP DAC lab.

The sample environment team participate within the electrical power and grounding group currently finalizing the plans for the electrical installation at the ESS.

Fluids incl. Gases, Vapour, Complex Fluids (FLUCO):

FLUCO progress according to plan. Updated design of RUC sample changer has started, 8 positions, bigger free angle for outgoing beam (2 x 45 degree). Internal project of rotating sample cell magazine continues with the procurement of parts and manufacturing is finalizing state.

In kind projects with Tartu University, Estonia and FZ-Juelich, Germany :

1. Follow up for Laser pump probe, LPP2: Delay with accepted design due to funding problems at Tartu university
2. Gas process handling systems, definition about software delivery from the supplier has began. Preparation of integration started on participation of MESI, Supplier and Uni. Tartu is ongoing.
3. Humidity chamber for SANS , university Tartu. Design of cell started and market survey for humidity generator also started
4. Stopped flow unit for SANS , university Tartu. Procurement for stopped flow unit

started

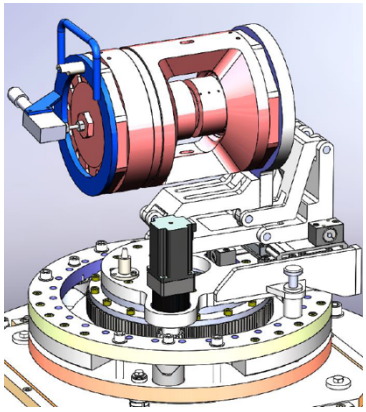
5. Gas blower unit for thermalizing applications , FZJ Germany
6. Rheometer for RheoSANS, FZJ Germany
7. Both, Gas blower and Rheometer, are now in the pending mode , because of cost reduction procedure at ESS. Shifted to OPS phase.

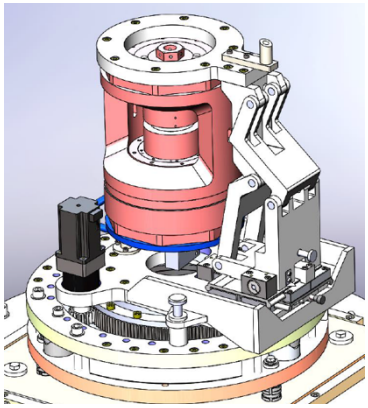
FlexiProbe project, BMBF w. 3 German Universities successful finished. Application for a follow up project for robotic sample changer is done at the German funding agency BMBF

High pressure and mechanical processing (PREMP):

High Pressure Activities

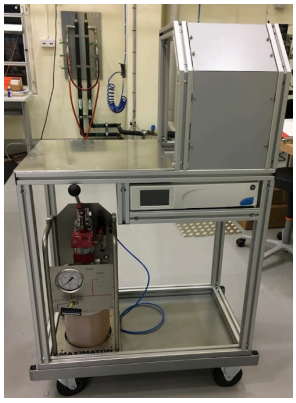
Systems integration: Work was completed on conceptual design for PE cell installation on the (Level 2) floor mount interface. The final concept facilitates loading of the cell and subsequent installation of all types of PE-cell in either horizontal or vertical geometry on any floor-mount instrument without realignment.





Detailed design is almost complete and quotations are being sought for manufacture and subsequent installation/testing during 19Q4 (hopefully before IKON16)

A portable pressure-control trolley has been designed and partially constructed. This device enables control of both hydraulic pressure (2000 bar) and gas pressure (<200bar) and will be used to test both integration with EPICs, mechanical interface and equipment installation logistics. Basic integration of pressure transducer and the PACE gas controller has been achieved by the MESI group.



A collaborative project (VR funded in collaboration with P. Deen; L. Ørduk Sandberg and M. Haubro) to develop uniaxial pressure cells was worked on including fabrication of new cell, cryogenic testing of load gauges (Utgård) and online neutron data collection at ILL.

This activity was expanded to include 3 VR-funded high-pressure projects with a goal of addressing SEE requirements for CSPEC, BIFROST, LOKI and SKADI. Lund and Stockholm Universities are involved.

Mechanical Processing

A meeting to formalize and detail plans for SEE equipment within the imaging and engineering classes was organized and held (attendance from BEER team, ODIN did not attend). Detailed plans for the key instrument-specific SEE on BEER were discussed and recorded.

PREMP attended the equivalent meeting for SANS and identified some requirements for a portable strain rig system.

A mechanical load gauge and readout were procured for load testing.

Temperature and Fields (TEFI):

Publications: We have submitted a paper describing the Huggins (Roskilde in-kind project) to the proceedings of the International Society for Sample Environment meeting 2018.

HZB test beamline experiment to benchmark MCSTAS background simulations: In November ATH participated in an experiment at the test beamline V20 at HZB, along with Mads Bertelsen and Martin Olsen from Copenhagen university, to benchmark Mads' recently developed Union Components add-on to MCSTAS. This software enables the simulation of multiple scattering and absorption in sample environment, which is often responsible for spurious signals (often known as 'spurions'). Union Components shows enormous promise, qualitatively reproducing recognizable multiple scattering signals, and providing valuable insight which has already influenced sample environment design. This experiment to verify its predictions for a very simple setup promises to build confidence in what will hopefully become a very powerful and widely used tool.

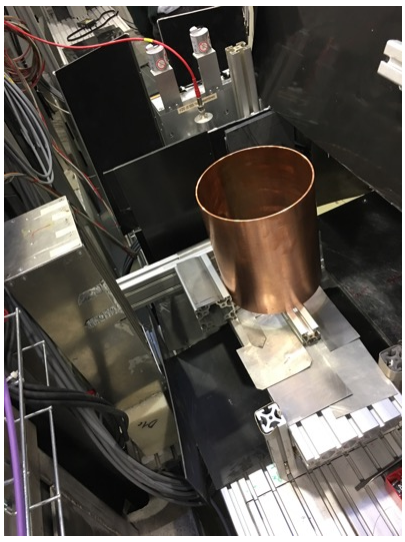


Figure: left: "Fake" sample environment for the verification of multiple scattering simulations. right: Copper cylinder in position on V20

Huginn operation on HZB test beamline: As part of the recent integration test on V20, the Huginn Peltier-based sub-cryostat was installed on a local HZB cryostat and could be remotely operated from Lund.

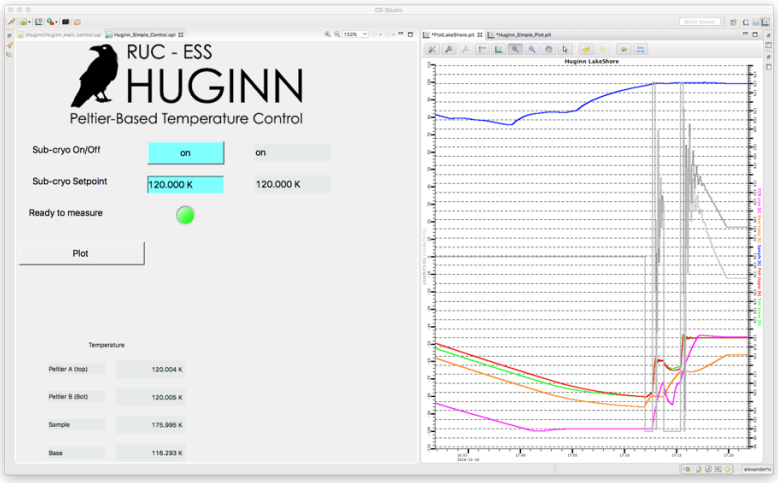


Figure: Screen capture from ATH's laptop in Lund, showing control screen and temperature histories in real time from HZB in Berlin. Note the much faster response times for the red and green traces (notwithstanding unoptimized PID control) compared to the pink – this indicates that the sub-cryostat provides genuine time savings when changing temperature in a cryostat for which it was not originally tested.

Semi-automatic Helium pumping crate for Orange cryostat: In cooperation with Andreas Hagelberg (MESI, see below) and with assistance from the vacuum group, we have set up a semi-automatic pumping cart for an orange cryostat (see photo). This consists of a number of automatic vacuum valves coupled to a Beckhoff PLC controller, along with two pumps and a vacuum gauge. The valves can be opened and closed and the pumps started and stopped manually with switches or programmatically using the Beckoff. This will initially be used to automate the sample space pump and flush sequence. Such automation is intended to improve reliability by ensuring consistency and avoiding potential operator error, as well as allowing monitoring of key signals for early detection of maintenance issues. At the same time MESI have been able to develop the PLC crate refining everything from cabling, cable labelling to power connectors and programming. It will potentially also develop into a tested for using small local screens for monitoring devices or even for local control (touchscreens). In the meantime safety assessments have been carried out which will allow the use of liquid cryogens regularly at Utgård.

Next steps Q1 2019

- Finalise and sign FR in-kind agreement and issue tender for 8T large aperture diffraction magnet
- Continue integration of orange cryostat, test with liquid nitrogen
- Meet with Diffraction and Spectroscopy instruments (along with PREMP) to refine sample environment suite for these instruments.

Mechatronics and Software Integration (MESI):

Temporary Workshops

The MESI at Utgård is very functional. The basic tools, components, benches, screens, chairs, heaters(…), softwares PC and PLCs are now available. However, there are still a lot to ask for regarding network infrastructure and stability (ICS responsibility), see ore in the interfaces section.

Developments

With an equipped workshop for integration and mechatronics, work is becoming a bit easier and a bit more efficient. Collaboration projects with the rest of the SE teams are on-going. As most projects now still are “first time” projects, regarding staff or area of technology, progress is slow, but very valuable.

The SE Instrument cave Patch panel prototype has been finalized and there is now a matching inside/outside panel to be mounted in the mock-up cave. This prototype enables evaluation and usability test of the patch panel design (as defined in ref doc) to be used for connection of SES. It is now ready for testing with real SES.

SECOP project (SINE2020)

SECoP project is progressing well. Some question marks regarding support from divisions within ESS (DMSC, ICS) have mostly been sorted out. DMSC agrees to initially provide support, on the Experiment Control Systems ECS) side, to enable demonstrating the SECoP functionality at ESS. When the SECoP project is mature enough, discussions on if/how/when to implement it will be held. ICS have in initial discussions allowed for a more flexible approach, increasing the possibilities on how to implement SECoP at ESS and thus enabling nicer solutions. Work at MESI is ongoing and a clearer design has been defined. The work has now also been spread more in MESI to improve work situation. There is still a lot of work to be done. In 2019 MESI need to make an intense effort to launce a SECoP implementation for ESS.

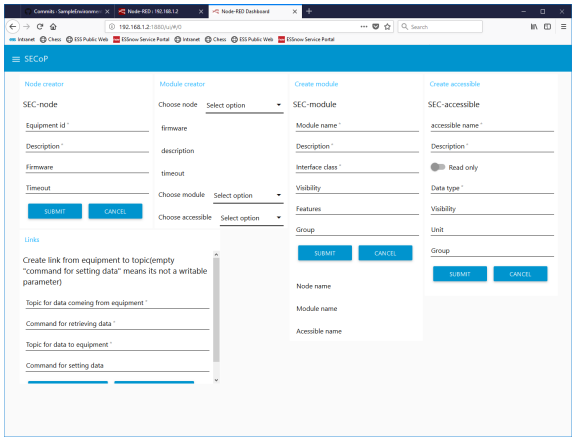


Fig: GUI for making and modifying a SEC node. NodeRed software is used for quick testing of functionality and behaviour of the implementation.

Integration

The prioritization plan helps to keep track on sample environment integration projects. They serve as important input to the Beamline Controls Team (BCT). However, as EPICS and EPICS infrastructure resources (ICS) are still very limited and the projects being worked on have been unexpectedly time consuming. This have now started to lead to integration projects being flagged as delayed and not meeting the setup deadlines (this is now at least visible, and documented).

Some of the process and software used by ICS in deploying a integration software module (mainly EPICS IOC) have been shown to be not suited for sample environment, slow and time consuming to work with. With the limited resources this have led to further delays and importantly available integrations not being used. To improve this situation until ICS provide better systems and resources MESI will try to provide a local solution (including providing a local MESI server).

In discussion with MC&A and ICS, MESI have also provided a first version of a “standard integration requirements” text. This text is to be used to specify the equipment’s communication to be available and also requirements on motion systems, when procuring SE equipment. This was triggered when MESI was involved early in TEFI’s magnet in-kind project.

A simple pressure sensor was connected to EPICS. This is the starting point of a larger pressure control system to be developed and planned to be usable for multiple pressure control systems.

Interfaces with:

BCT(Beamline Controls Team): The BCT is slowly coming into place and MESI is changing its way of work to include BCT. Some new topics that now will be handle by BCT are Handling and access of calibration files/data and Defining responsibilities and planning of the instruments utility supplies.

DMSC: New projects for integration will be started in 2019 Q1. As DMSC now have resources working at Utgård at least once a week this interface works even better.

ICS: Resources provided by ICS for integration is still very limited. Some integration project are now delayed. MESI is trying to inform SE on status continuously. MESI will also try to handle some of the ICS tasks (EPICS integration

and deployment) to reduce the effects. Focus is currently still for ICS to finalize some of the on-going projects.

Plans

MESI will be part of BCT and help to develop and realize it as a team and will increasingly use BCT as a forum to drive integration issues (issues relevant for many of the technology teams, e.g utgård network, calibration file/data handling, alarms, configurations hanlding, etc). MESI will try to minimise effects from lack of ICS resources, mainly by doing the work ourselves with our own tools.

DOCUMENT REVISION HISTORY

Version	Reason for revision	Date
1.0	New Document	24 March 2015
1.1	Update Jan-Jun 2015	07 June 2015
1.2	Update Sept 2015	29 Sept 2015
1.3	Update Jan 2016	17 Jan 2016
1.4	Update Q1 2016	04 April 2016
1.5	Update Q2 2016	22 June 2016
1.6	Update Q3 2016	10 Oct 2016
1.7	Update Q4 2016	16 Jan 2017
1.8	Update Q1 2017	09 April 2017
1.9	Update Q2 2017	15 June 2017
1.10	Update Q3 2017	5 Oct 2017
1.11	Update Q4 2017	14 Jan 2018
1.12	Update Q1 2018	10 April 2018
1.13	Update Q2 2018 (summary only)	03 July 2018
1.14	Update Q3 2018 (STAP input)	24. Sept 2018
1.15	Update Q4 2018 (new format w. bulletpoints)	14. Jan 2019