STAP Panel – Chemistry and Life Science Support

Fall 2024 – Panel members: Andrew Church (STFC), Tamim Darwish (ANSTO), Jeremy Lakey (University of Newcastle), Anne Martel (ILL), Thomas Shea (ESS), Gavin Stenning (STFC), Stewart Parker (STFC), Luke Daemen (Chair, ORNL)

CLS continues to develop increased cross-training and knowledge exchange with MSPS. The panel also notes good, improved communication and interactions with instrument teams. CLS has clearly initiated the transition from installation/construction toward first science. CLS is a solid team effort.

SULF

ESULF made excellent progress with D08 (furniture, electrical) with mechanical/gases/water under evaluation. The E04 and D04 labs are operational. The RML is in non-rad operations pending rad approval from authorities. SULF also identified lab space for cell culture and sample storage/handling. CLS is on track to deliver access to lab space for first science/first users.

Basic supplies are available and most equipment is operational in E04 and D04: LN2, freezers, fume hoods, instrumentation (new CHN analyzer).

SULF also continues to provide analytical support to various ESS construction/commissioning activities, more recently investigating oil for the He cooling loop. This work helps maintain the labs in a ready, operational state while provide rapid feedback to the remaining construction and installation activities at ESS. Monika, Katrin, Ghazaleh, and Nick are a great (if overworked!) team.

Concerns/recommendations:

The SULF team has valid concerns about space for safe chemical storage, as well as chemicals availability and cost. This will be important to support sample preparation at ESS. A well organized chemical inventory with easy access and a good selection of basic supplies and chemicals is essential. In this respect, the SULF budget does not appear to have increased since last year and remains below par compared to other neutron facilities.

Besides budget, personnel is the most important resource for CLS to accomplish its mission. Staffing levels remain low given the amount of work performed by the CLS team. The need remains for more support personnel for first beam/first science and the transition to a user program.

Good progress has been made regarding the sample storage facility that was a bare shell earlier in the year. This is really good work, but still more needs to be done (e.g., ventilation).

Do not underestimate the work that remains to be done: a funded plan is needed now. The STAP also wants to emphasize that sample storage (samples check in, bar coding, inventory, sample holders emptying/cleaning, sample disposal/shipping) will require a full time employee at a minimum.

Questions to the STAP:

Sample and chemical handling and storage:

Software and efficient processes and procedures have been developed at other neutron facilities for chemical inventory/storage, as well as sample handling. These can be shared with ESS. SULF would benefit from a visit to ISIS or SNS/HFIR for a few days to watch the process and collect documentation.

Stock and cost of chemicals (including D2O):

Specialized, expensive chemicals should be the responsibility of the users and/or individual beam lines. A stock of chemicals that can reasonably be expected to be useful to multiple users or ESS staff should be maintained by SULF. This includes mineral/organic acids and bases, salts, organic solvents and reagents, gases, and liquid nitrogen as one might expect to find in the average chemistry department at a research university. Small amounts of D2O should be available. Large quantities (> 1 L) should be supplied by users.

DEMAX

DEMAX continues to demonstrate excellence with biodeuteration and crystallization, as well as with chemical deuteration with a successful call for proposals and an increasing list of publications (62 molecules delivered/36 proposals supported).

The transition from Medicon Village and integration of the team into D04 is another success for CLS in general and the DEMAX team in particular. Increased interactions with NMX, LOKI and other beam lines demonstrate DEMAX's dedication to the transition to first beam/first science.

The STAP also notes very significant efforts by the team to go after grants, push publications, and seek scientific collaborations.

DEMAX is actively working on recruiting a biodeuteration scientist (2025) to relieve Zoe at LP3. This is a positive development.

Miscellaneous accomplishements: Kudos for working out various approaches to reduce D2O consumption. The new GC/MS will improve DEMAX productivity

Concerns/recommendations:

Staffing levels remain low given the workload on Anna, Jia-Fei and Zoe.

Contracts expiring in 2025/2026 will adversely affect DEMAX operations (Medicon, LP3, ILL,…) -In particular, DEMAX cannot afford to lose NMR access. This is a single point of failure for DEMAX/Chemical deuteration. Contract renewals and/or new solutions must be sought now.

Questions to the STAP:

Commercial availability of deuterated lipids:

It makes sense for DEMAX to focus on deuterated lipids that are not commercially available. If Larodan (or other companies) provides a range of lipids, it should be the users' responsibility to procure the essential materials needed for sample preparation. This is true of any sample, not just lipids. Users should buy commercially when available and collaborate with DEMAX (CLS in general) if no commercial availability or sample requires preparation on site.

Balance between supplying deuterated compounds and developing new, more efficient deuteration methods:

The DEMAX focus needs to remain on user support. Requests for new deuterated molecules provide an opportunity to develop new techniques. Improving synthesis techniques to provide higher deuteration levels, better yields, faster preparation, or more cost-efficient approaches is certainly laudable as time and manpower permit. SNS and ISIS rely on students and postdocs to pursue such goals.

SCSE

The D04 workshop is operational and Alice and Harald are making impressive progress in the organization and development of SCSE with increased, regular interactions with beam line teams, completing projects with in-kind partners, and initiating new projects to develop sample environment for reflectometry and chemistry in particular.

The continued involvement of SCSE with sample environment teams at other neutron sources and attendance to relevant workshops and conferences is another positive development. Alice's participation on the organizing committee of ISSE is to be commended.

SCSE initiated the development of low pressure gas handling manifolds for adsorption experiments at multiple beam lines. This includes ISORB: a new stick for in situ high pressure gas adsorption (with new intern)

The STAP is also pleased to hear that SCSE is increasingly involved with controls and instrumentation -a positive development compared to the situation 6 months ago.

Miscellaneous notable accomplishements: Development and testing of the humidity chambers and electrochemistry cells from Estonia (in kind partner). New collaboration on combined ellipsometry/IR project (in kind partner Linkoping U. Sweden) to support FREIA and ESTIA. Automation of static troughs for FREIA (with postdoc at Lund U.).

Concerns/recommedations

A team of two (Alice, Harald) is insufficient to support the transition to first beam/first science or to support soft matter/chemistry sample environment at multiple beam lines during operations. Is there a plan in place to replace Hannah Burrall?

A large fraction of sample environment under development seems to be focused mostly on reflectometry, and the the SCSE budget appears to be supporting mostly reflectometry. This makes sense for now (tranche 1 Instrument), but the increased involvement of SCSE in the projects listed above (to support chemistry sample environment in particular) ought to be reflected progressively in future budgets.

Questions to the STAP:

Development of sample environment for chemistry, battery research, energy materials, etc…

As much as possible, procure commercial equipment or duplicate/adapt equipment already available and tested at other neutron facilities. Catalysis, gas sorption, batteries, and energy materials will almost certainly remain critically important areas of research for ESS for the foreseeable future. A plan should be developed based on the demand at other neutron facilities. Cells for in operando battery studies, flow cells/pressure cells for catalysis, in situ gas sorption at a minimum are needed to support high-impact science at ESS. Other sample environment equipment such as photochemistry, electric fields, simultaneous Raman or x-ray, etc,… are nice to have but used only by a small fraction of users and should not be a priority for the first few years of ESS operation.