Sample Environment STAP Report – April 2016

Executive Summary

The Sample Environment (SE) team is responsible for setting up support laboratories, providing and maintaining a pool of sample environment equipment, and assisting with the integration of non-pool equipment into the ESS working environment. The guiding strategy for the team is to concentrate on providing full support for the first eight instruments to be built. The team have clearly outlined the training needs required, and provided a prioritised equipment list. However, the panel feel that more clarity is needed over exactly what total package of equipment will be available to users from the different sources (the SE pool, laboratories, and directly from the instruments). In general, the instrument teams need to provide more feedback to the SE team.

The budget for equipment purchase is very tight, considering that eight instruments must be catered for, especially considering the rapid turnaround times expected due to the increased flux at ESS. To ensure that early experiments are successful, the STAP recommends that the primary aim of the Sample Environment team should be to make sure that basic Sample Environment needs are met. To do this, the team needs to be able to start serious practical studies and training now, and to sort out safety issues well in advance of operation. They need to be involved in the floor planning of the experimental halls and individual instrument areas. The team is very enthusiastic and motivated and can achieve the stated objectives with the right support and infrastructure.

Key Recommendations

- Establish a clear and transparent procedure for determining which equipment is to be provided by individual instrument teams and which is to be provided by the SE team. All decisions should be documented.

- Funds for developing the current test laboratories should be released now, and some of the proposed technical support should be recruited immediately. This will help leverage additional support from other facilities.

- The budget, as it stands, cannot cover certain expensive pieces of equipment that have been cited as scientific highlights in the Technical Design Report and the Instrument Scientific Cases, without compromising the ability to provide basic support for eight instruments. The STAP suggests that a separate pot of money be established that interested parties (e.g. instrument teams, the Sample Environment team, other partners) may bid for, to fund these singular pieces of equipment.

Sample Environment (SE) Strategy

The ESS has defined 15 of the first 16 instruments, and will soon be defining the first eight to be built. Some of these instruments will include sample environment as a key part of their design, particularly for equipment that is tailored to that one instrument. Some equipment will be easily shared between different instruments, either across multiple classes (the 'pool') or within a given instrument class ('mini-pools').

The SE team will purchase, maintain and support the pool equipment, as well as providing support for integrating non-pool equipment into the ESS control systems. They also define standards for utility supplies and space requirements. Instrument teams will be encouraged, where feasible, to make their equipment available for use by other instruments. The SE team will also set up and equip the necessary support laboratories.

At present, the split between instrument-owned and SE group-owned equipment has not been defined. This needs to be resolved quickly, in time for the Scope Setting meetings for each instrument. The decision-making process needs to be transparent and clearly documented. The STAP are happy to advise on specific questions where desired.

The SE group has prepared prioritised lists of equipment that define a comprehensive reference suite for a well-founded neutron scattering laboratory (see Appendix B). This list needs to indicate whether or not a particular piece is being supplied through the pool, provided by an individual instrument but included in the pool, or is instrument-specific and excluded from the pool. This information will be forwarded to the Samples and Users STAP.

The stated strategy of the SE team is to prioritise support for the first eight instruments; the STAP agrees with this approach. Therefore, at the moment, the question of balance between different user communities is defined by the nature of the eight initial instruments. For this reason, the SE team should remain flexible in assigning funds between the four identified areas (TEFI, FLUCO, PREMP and MESI)[1]. The current proposed split is: TEFI 3.8 M€, FLUCO 2.6 M€, PREMP 3 M€, and MESI 2 M€. The STAP judges that, to be successful, the first experiments scheduled on each instrument should start with well understood SE to ensure a good first set of results.

The equipment purchasing and integration programme needs to match the construction schedule closely, in order to come on stream at the right moment for the initial instruments. The plans proposed by the SE team at present provide a good reference suite, but the STAP is concerned that there is not enough duplication of commonly used pieces of kit, especially as experiment changes on a daily basis are anticipated for many instruments. With 8 instruments, the SE team would conceivably be supporting 8 separate pieces of SE on instruments and 8 in preparation for rapid installation the next day. The SE pool (of both equipment and trained personnel) must be large enough to support this to avoid unhappy users or postponed experiments. Instrument technicians will need appropriate cross-training to carry some of this workload.

With the proposed budget, SE equipment purchases are limited to basic kit. Two (non-exclusive) options for dealing with this were discussed by the STAP:

- Requiring instruments that will use common pieces of kit (e.g. Orange cryostats/PTR cryostats) to supply one to the pool.

- Borrowing equipment in the first instance from other institutes. This would serve double duty for training, and to set up the ESS SE team as credible partners. It might also help to leverage staff secondments from other institutes.

[1] TEFI = Temperature and Field; FLUCO = Fluids, incl. Vapours, Gases and Complex Fluids; PREMP = Pressure and Mechanical Processing; MESI = Mechatronics and System Integration.

Training Strategy

The SE team has clearly considered training needs, along with the needs for setting up equipment. The plans proposed are well thought out and clear. The STAP is concerned that the available manpower is limited and that this will be a serious concern in meeting all of the necessary benchmarks. We note that the MESI technical skill sets are somewhat different to those required for the other platforms.

The STAP was pleased with the training projects such as ESSIIP and the Utgård TBP lab. We encourage the SE team to look to equip these labs with borrowed equipment, to aid in leveraging seconded staff.

The STAP notes that it is important to have a test instrument available from Day 1 of operations equipped for checking crystals and sample alignment. It should also provide a good platform for testing SE and integration with the control systems.

To be able to reach benchmarks and use the next years profitably, money should be released now to equip these laboratories, and to employ technicians immediately. Procurement procedures for equipment and consumables need to be efficient and simple. The SE team is enthusiastic and motivated and can achieve what is required of them with the right support and infrastructure.

SE Development Strategy

The working environment is severely constrained financially. Work on novel techniques should focus on ESS-specific issues (e.g. small samples, high flux). Setting up the SE from scratch is already very challenging.

The STAP is pleased to see diamond anvil cell work high in the priority list of the PREMP responsible and recommends maintaining close contacts with the groups involved in these ongoing developments worldwide (SNS, J-PARC and ISIS), through regular visits, partnerships and beamtime applications. The STAP encourage the PREMP responsible to inform the high pressure community on the potential possibilities at ESS in suitable fora, such as high pressure meetings.

Reference Documents and Interactions with other Entities

The team has invested a significant amount of effort in developing clear reference documents as aids for the instrument teams. We would encourage the instrument teams to provide feedback to the SE team on the requirements. We also encourage the SAC to put due weight on these items in the Tollgate process, bearing in mind the time cost associated with non-compliance with the reference documents. Due to the shorter experimental data collection runs predicted at ESS, the number of SE equipment set-ups per day will be larger than at other facilities, so the process must be made as easy as possible.

This STAP also notes that a test instrument is now anticipated from the beginning of operations. We recommend that this instrument permit crystal alignment and sample testing for preparation prior to scheduled experiments, and that it also be equipped for testing sample environment.

Specific issues for the SE team :

The SE team clearly recognises the importance of training in handling the setup and integration of the various types of equipment to be used. This should also be reflected in the Gantt charts by marking in explicit time for cold commissioning.

The STAP is happy to see that Anders Pettersson is working closely with the DMSC (Data Management and Software Centre) and ISC (Integration and Systems Control) on integrating SE with EPICS. We note that lifetime maintenance needs for software must be considered at the equipment procurement stage, to avoid legacy and concomitant security issues.

The SE team should make sure that the MCA group provide paths for wiring to pass centrally through rotation stages, in the same spirit as the planned patch panels.

In the hall design, appropriate paths for heavy SE equipment must be provided around the halls. Roof heights and chicane dimensions should also be considered carefully in instrumental plans.

Access ports to the integrated control system for users bringing their own equipment should also be planned for. A short guidance sheet for these users should be prepared.

The STAP notes that sample management falls into the ambit of SAD. Management of irradiated samples will be by flexible zoning in the experiment hall; more detail on this needs to be considered by the Samples and Users STAP at their meeting. We note that at full power, samples will get very hot on some instruments, and appropriate procedures need to be developed for removal and storage of these samples.

Thanks

The panel would like to thank the Sample Environment team, in particular Malcolm Guthrie, Alex Holmes, Anders Pettersson and Harald Schneider for their detailed presentations and open discussions with the panel.

Elizabeth Blackburn 25/04/2016

Appendix to Sample Environment STAP Report

Equipment Lists for PREMP/TEFI/FLUCO with Priorities Noted

The Source for each item should be marked as Pool/Mini-Pool/Instrument/Lab accordingly. For FLUCO a prioritised pool list is supplied, based on the proposed SE budget, along with information broken down by instrument type with priorities to give a complete wish-list. If some of these items are not included in instrument specifications, this should be considered in re-assessing the FLUCO supply list, based on the priorities given.

Pressure and Mechanical Processing	Source
Priority 1	
Gas cells (up to 1 GPa) x3	
Clamp cells (up to 3 GPa) x2	
Paris-Edinburgh cell + seats and anvils x1	
Diamond anvil cells + stages x3	
Portable Raman system x1	
Portable stress-strain rig x1	Partial instrument contribution?
Priority 2 – currently out of budget	
Portable laser heating assembly x1	
Corrosive gas manifold x1	

Temperature and Field	Source
Priority 1 – for first testing and to decide which to use as general base of pool.	
Orange-type cryofurnace 1.5 – 600 K x1	
PTR cryostat 3-800 K x1	
IR furnace 300-1200 K x1	
Side-access PTR with robotic changer x1	
Priority 2	
3He sorption stick insert x1	
Dilution insert x1	
9 T vertical cryomagnet x1	
Peltier sub-cryostat insert x1	
3 T electromagnet x1	
Priority 3	
In-site susceptibility measuring insert	
6 kV electric field insert	
High temperature furnace 300 - 1800 K	
Priority 4 – currently out of budget	
11 T horizontal cryomagnet	
>20 T high field continuous magnet (horiz + vertical)	
40 T pulse field magnet	

FLUCO List	Source
For All Instruments – Priority 1	
Alignment goniometers, and slits	Instrument?
Laser for pre-alignment	Instrument?
Kinematic mounts for sample remounting	Instrument?
Proposed Pool	
Priority 1	
Laser pump probe	Pool - completed
Humidity chamber	
Thermalising blower	
5 Position Peltier for quick temperature steps	
Priority 2	
Stopped flow unit	
Gas process handling system	
Priority 3	
Rheometer	
In situ light scattering	
Priority 4 – currently out of budget	
Chemical process chamber	
Ultrasonic levitator	
In situ thermal analysis	
In situ gas adsorption	
SANS – Priority 1	
Sample changers (at least 2).	
Huber stage (x,y,z translation) This should be part of the relevant instrument but if it is considered SE then it should be a priority.	
Two tier sample changers (40 samples)	
Rotating racks	
Temp control/water baths (2 per instrument)	
Couette/other cells (plate/plate?)	
Quartz cells (Hellma 300)	
FPLC pump (protein aggregation)	
Titanium cells with windows (this permits saving money on Hellma cells).	
SANS – Priority 2 (specialised equipment)	
Furnace	Pool (TEFI) ?
Cryostat	Pool (TEFI) ?
High pressure 5 kbar	Pool (PREMP) ?
Stopped flow	Pool (FLUCO) ?

Linkcam (cooling/heating rapid) SANS and Reflectometry	
Stress strain DMTA	Instrument specific kit
Electrochemical capability	
Flow cryostat	
Electromagnet	Pool (TEFI) ?
Pressure cell (sapphire windows) → for CO2 Eastoe	
In-situ: UV-vis, IR	
SANS – Priority 3	
Rheometer	
Light scattering	
Liquid crystal set up	
Reflectometry (horizontal and vertical) – Priority 1	
Liquid/air troughs	
Temp control (water baths 2 per instrument)	
Solid liquid – mounts/blocks	
Liquid/liquid cells	
Humidity control/box	Pool (FLUCO) ?
LB trough for deposition/dipping	
HPLC pump	
LB trough for instrument	
Syringe Pumps	
Anti-vibration tables	
Reflectometry – Priority 2	
Shear cells/flow, 1-2 shear cell	
Shear cells/rheometer	
Electrochemistry: CV	
In-situ: FTIR	
Gas process handling system	Pool (FLUCO) ?
High pressure cell	
Reflectometry – Priority 3	
In situ Atomic force microscopy	
Polarised neutron reflectivity (noted)	
Laboratory Suggestions to Pass on to Samples and Users STAP	
LABORATORY Facilities – Priority 1	
Fume hoods - HNO3/Piranha/HF (2 dedicated?)	
Nanoparticle fume hood	
Chemical stores/stocks/waste handling/detergents	

Gas supplies and handling	
Glove boxes	
LABORATORY Facilities – Priority 2	
Cold room (bio lab)	
LABORATORY Equipment – Priority 1	
Spin coater	
UV lamp/ozone cleaner	
Plasma cleaner	
Vacuum oven	
Ultrasonic bath	
Precision balances	
UHQ water	
Paar densitometer	
DSC	
LABORATORY Equipment – Priority 2	
X-ray Reflectometer, X-ray Diffractometer	
Zeta sizer	
Tensiometer – e.g. Kruss	
Ellipsometer	
Brewster angle microscopy	
Fluorescence microscope	
QCM	
Tip sonicator to make vesicles	
LABORATORY Equipment – Priority 3	
Thin film deposition facilities	
DEUTERATION FACILITIES	