Science Activities

Chemistry and Life Science Support & Material Science and Physics Support.

General Comments

The separation of the sample environment teams into two groups may provide additional barriers to success. The global provision of gas handling from the Chemistry and Life Science Support team (CLS) cuts across pressure systems and their provision and support from the Materials Science and Physics (MSP). MSP provides the only machining capabilities in the supervised zone, currently with 2 FTEs trained to use the equipment. The workflow for providing this service to all of the SE teams as well as other interested parties in the Science Directorate has not been defined. The working through of operational workflow is vital if the SE teams are to deliver success. SE systems are now as important as the instruments and systems, responsibilities and ownership could fall between two stools in the model presented.

Recommendation – ESS should consider a single sample environment group. A review of SE requests and publications in other facilities will expose the complexity of SE provision in an era when researchers want to replicate their home laboratory on the instrument.

Chemistry and Life Science Support (CLS)

General comments

The Chemistry and Life Science Support group has access to a remarkable amount of lab space, including the handling of activated materials. The labs are very well equipped with the necessary instruments for preparing and characterizing soft matter and life science samples. Additionally, they cover the complete set of approaches for deuteration of matter. However, the inclusion of optics support here was not well justified, especially because the assigned tasks are more related to materials characterization than optics.

Is the Proposed Organizational Structure Fit for Purpose?

No. See note regarding the separation of the SE in to two teams

The Chemistry and Life Science Support group is divided into (i) Sample Environment for soft matter and life science research, (ii) Deuteration and crystallization of samples, and (iii) Neutron optics. While the organizational structure for (i) and (ii) is generally fit for purpose, as mentioned above, (iii) requires more motivation to be justified for SSO, especially as part of the Chemistry and Life Science Support group.

Is the Full Scope Required for Successful Operation of All Aspects of ESS Properly Identified?

Sample Environment: The current plans for the sample environment cover the majority of aspects needed for successful operation. There might be a need to explore possibilities for offering correlative characterization beyond current utilization. It wasn't entirely clear if the process of developing and installing new user equipment is well understood and established. The interface between different groups or teams needed for mechanical or software solutions also lacks clear definition. Ownership of devices and responsibility for their proper operation were not always well defined. The provision of gas systems for all sample environment seemed an afterthought and was not well thought through.

Deuteration and Crystallization Lab: The decision to cover chemical and biological deuteration approaches, as well as lipids, is a unique feature that should be fully exploited. The potential demand from the MOFs and batteries community should be monitored. Also, it should be anticipated that there will be an increased demand for samples as well as more demanding samples in the future. However, it's evident that some of the work relies on external cooperation, which may not always be

available in the future. ESS must ensure that alternative solutions and collaborations are established in time. The crystallization lab seems to be sufficiently equipped.
The other staffing in DEMAX (deuteration and crystallization) appears low compared to the amount of deuteration activities that will be required in steady state. More synthetic chemists and biological scientists in the deuteration activities appear to be required to meet the anticipated demand in steady state operation.

Optics Support: This team appears not to have a real customer base. The Optics Support primarily engages in materials characterization, and it's unclear how this team is involved in the maintenance of guides or if its involvement is necessary for future developments. Moreover, there are other technical groups that could potentially handle the guides if needed. Consideration should be given to reallocating this responsibility.

Are There Opportunities for Consolidation and Increased Efficiency That We Have Not Yet Recognized?

From the discussions, it was not entirely clear how the vast amount of support available for the Chemistry and Life Science Support group will be coordinated. Implementing a ticket/diary system and designing a single point of entry for any requirements related to problems or demands could streamline this process. Connection to experimental beamtime needs to be made. There are enough staff to achieve this in close collaboration with instrument scientists and instrument associates. A clear process for prioritization should be established.

Are the Resources (Labor and Non-Labor) That Have Been Identified for the Defined Scope Reasonably Estimated?

For the Chemistry and Life Science Support group, there is some overlap with other groups or teams, particularly with the Materials and Physics Support group. Personnel can be shared to improve efficiency. The necessity of the Optics support should be carefully assessed. The budget for non-labor costs appears to be quite generous, especially the capital costs which were not fully justified – new equipment should be reviewed by the science teams to keep alignment with the needs of the instrument user base.

The user labs need support technicians to keep the labs running but the activities of the associated laboratory support scientists are not clear. Two laboratory support scientists for handling safety, and more sophisticated exploitation of the equipment as well as ensuring resilience would seem to be sufficient as opposed to the 5 FTEs suggested.

Rent on the DEMAX facility seems odd since no other ESS-site based group has listed rent, or separate charges for waste disposal in their operations budgets. (the Bench Fee for use of the Lund University labs for biological deuteration is fully justified) Rent should only be needed if DEMAX is located offsite.

Materials Science and Physics Support (MSPS)

Is the proposed organizational structure fit for purpose?

No. See note regarding the separation of the SE in to two teams
However, the scope is clear. The polarization activity is separate to the rest of the scope. Planning for resilience was demonstrated. There is major inter connectivity between soft matter and chemistry/gas sample environment and to a lesser extent sample characterization before and after experiments. The provision of gases to experiments is assigned to Chemistry and Life Science support(CLS) team which will be integral to many Materials Physics experiments – issues of responsibility are likely to arise.
The panel notes that the current plan provides a research engineer for each major class of sample environment. In practice, certain types will be more in demand than others and many SE systems require multiple techniques as noted above, this level of research engineer appears top heavy. Weighting has happened for the technicians, and cross-training was emphasized, but this should also be considered for the research engineers. This was also an area where documentation was given as the driver for many engineers.

Is the full scope required for successful operation of all aspects of ESS properly identified?

The scope presented was clear, although the expectation of leaving simple sample environment systems for the instrument associate/instrument teams to pick up and install was stipulated both for SE and polarization cells. For the polarization cells, it is easy to lose the polarization state, and in our opinion, non-expert installation of any technical equipment will not be efficient in the long term.
Recommendation – Technical teams should be professional service providers and own the service until it is installed and working.

Are there opportunities for consolidation and increased efficiency that we have not yet recognized?

To maintain resilience investment in multiskilling and cross-training between the technical staff would be advised to minimize single point failures.
This group operates and controls the only mechanical workshop in the supervised zone, benchmarking for machining requirements across the whole facility has not identified that considerable machining is required at short notice when running a user program. It was clear that operational tasks which include unexpected requirements have not yet been thought through.
Recommendation – A fact finding tour to facilities to explore the organigram and unpick the provision and delivery of SE in ISIS and ILL would greatly benefit planning.
The interactions with ESH&S were not discussed in general; the experimental risk assessment system needs to function for a research-focused user facility.

Are the resources (labor and non-labor) that have been identified for the defined scope reasonably estimated?

FTEs look appropriate but only if full-service mode is instigated and 24/7 on call. The need for 6 research engineers is doubtful – these FTEs should be experienced technicians. Benchmarking with ISIS did not reveal full helium recovery system support, full on call for each area of support and full-service mode for 30 instruments. However, consumables and investment budgets are considered to be a little thin considering the equipment base for steady state operations and the cost of helium replacement.
As a point of organization recharging instrument budgets for SE consumables is messy. The SE teams should have all the items they need to deliver everything and this is why this budget looks light. Chasing for the cost of the clamp or gas fitting is a huge waste of time and effort.

The labor costs are split almost equally between research engineers and technicians, the motivation for the number of research engineers was given as the need for documentation and training of technical staff. It is probable that the number of technical staff needs to increase and the number of engineers reduce. The work plans for the team involve cross-training to ensure resilience. One of the research engineers will be dedicated to off-beam use of some of the mechanical processing equipment. The non-labor costs are split into operations and capital investment. The operations costs include the liquid helium to cover the losses from the recovery system. The liquified helium for experiments is supplied by the liquefier in the accelerator directorate. The cost of Helium is very variable, but could potentially constitute a very significant portion of the consumables budget quoted for the Temperature and Fields activity. The capital costs requested are 380 k€ / year for new sample environment, with bids to the Science Division capital pot for larger items possible, as well as participation in seeking external funding.