**Workshop on Sample Environment for**

**Large Scale Structures Instruments at ESS**

2018-11-27 to 2018-11-29

**1. Overview and Goals**

In November 2018, a workshop was held at the ISIS neutron source to discuss sample environment for the Large Scale Structures instruments (LSS) at ESS: LoKI, SKADI, ESTIA and FREIA. The meeting started with overviews from each instrument team of each science case and their prioritization of sample environment as to when it is needed: for hot commissioning; for early science (first 2 years); and for the longer term. The remainder of the workshop was divided into topical areas, with “session conveners” introducing the topics and leading the discussion.

The goals of the workshop were:

1) **Prioritisation** : Revisit sample environment prioritization for each instrument and determine if it is still valid

2) **Specification** : Identify top level requirements or identify needs for development

3) **Delivery Planning** : Identify the responsible party for delivery of each piece of equipment

4) **Schedule Alignment** : Check the delivery timeline is in alignment with the instrument needs.

**2. Participants**

**3. Instrument Overviews**

The summaries below are complemented by the slides from each instrument, which are included in the appendices.

**3.1 LoKI**

**3.2 SKADI**

**3.3 ESTIA**

**3.4 FREIA**

**4. Session Summaries**

The session summaries below are presented in the order they were discussed, with introductory presentations included for reference in the appendices to this report.

**4.1 near-Ambient Temperature & Humidity Control (including sample changers)**

Session Convener : Andrew Jackson

*4.1.1 Overview*

*4.1.2 Key Discussion Points*

*4.1.3 Identified Equipment and Equipment Specifications*

*4.1.4 Development Needs*

**4.2 Mounting & Movement: Stages, Motion Stacks, Mounting & ESS Requirements**

Session Convener : Judith Houston

**4.3 Solid-Liquid Cells, Flow-Cells & Associated Equipment (including sample changers)**

Session Convener : Tom Arnold

**4.4 In-Situ Techniques (strain, rheology, etc) and In-Line/In-situ supporting measurements (e.g. UV-Vis, pH, etc)**

Session Convener : Adrian Rennie

**4.5 Air-Liquid and Liquid-Liquid Cells (including sample changers)**

Session Convener : Ali Zarbakhsh

**4.6 High Temperature & Pressure**

Session Convener : Sebastian Jaksch

**4.7 Ex-Situ Support Equipment (lab equipment, SAXS/XRR, offline alignment etc)**

Session Convener : Judith Houston

**4.8 Magnets & Cryostats (including sample changers)**

Session Convener : Artur Glavic

**5. Alignment of Delivery Plans with Instrument Requirements**

**5.1 LoKI**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **SES** | **Phase** | **Date Needed\*** | **In SSS Plan** | **SSS Plan Date** | **Delivery Responsible** | **Budget Responsible** |
| Thermostatted sample changer for quartz cuvettes | HC | Q3 2022 | Yes | Q2 2020 | ESS | LoKI (const.) |
| Cell tumblers/rotating sample holders | HC | Q3 2022 | Yes | Q2 2021 | ESS | LoKI (const.) |
| Flow cell (including pumps) | HC | Q3 2022 | Yes | Q3 2021 | ESS | LoKI (const.) |
| Quartz cuvettes | HC | Q3 2022 | Yes |  | ESS | LoKI/SKADI (const?|) - though should be “consumable” from ops budget |
| Individually thermostatted cuvette rack | ES | Q2 2023 | Yes | Q3 2021 | ESS |  |
| Rheometer | ES | Q1 2023 | No |  | ESS | ESS (ops) |
| Stopped-flow cell | ES | Q3 2023 | Yes | Q3 2020 | ESS | ESS (ops) |
| Goniometer(s) | ES | Q3 2023 | No | No date | ESS | ESS (ops) |
| In situ techniques, as attachments to the flow-through cell | ES | Q1 2023 | No | No date | LoKI team | LoKI (const.) |
| Dismountable ‘sandwich’-style cells (ESS) | ES | Q2 2023 | No | No date | ESS | ESS (ops) |
| Stress/stretching rig (ESS) | ES | Q1 2023 | Yes | Q1 2023 | ESS | ESS (ops) |

**5.2 SKADI**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **SES** | **Phase** | **Date Needed\*** | **In SSS Plan** | **SSS Plan Date** | **Delivery Responsible** | **Budget Responsible** |
| Thermostatted sample changer for quartz cuvettes | HC |  | Yes | Q2 2020 | ESS |  |
| Cell tumblers/rotating sample holders | HC |  | Yes | Q2 2021 | ESS |  |
| Flow cell (including pumps) | HC |  | Yes | Q3 2021 | ESS |  |
| Quartz cuvettes | HC |  | Yes |  | ESS |  |
| Individually thermostatted cuvette rack | ES |  | Yes | Q3 2021 | ESS |  |
| Rheometer | ES |  | No |  | ESS |  |
| Stopped-flow cell | ES |  | Yes | Q3 2020 | ESS |  |
| Goniometer(s) | ES |  | No | No date | ESS |  |
| Dismountable ‘sandwich’-style cells (ESS) | ES |  | No | No date | ESS |  |
| Stress/stretching rig (ESS) | ES |  | Yes | Q1 2023 | ESS |  |
| Electromagnet? |  |  |  |  |  |  |
| High Field Magnet? |  |  |  |  |  |  |

**5.3 ESTIA**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **SES** | **Phase** | **Date Needed\*** | **In SSS Plan** | **SSS Plan Date** | **Delivery Responsible** | **Budget Responsible** |
| Sample Stack / Hexapod | HC |  |  |  | PSI | Estia (const.) |
| Warm Bore Magnet | HC | Q4 2022 | Yes | Q1 2022 | ESS (LLB) | ESS |
| Flow Cryostat | HC | Q4 2022 | Yes | Q1 2021 | PSI | Estia (const.) |
| Solid Liquid Cells + Changer | HC | Q4 2022 | Yes | Q1 2021 | ESS or ESTIA | Estia (const.) |
| Vertical 8T magnet (Estia == ~5T magnet) | ES | Q4 2023 | Yes | Q2 2022 | LLB | ESS |
| Free liquid | ES | Q4 2023 | No | No date | ? | ? |
| ”Very high field magnet” | Later |  | ? | ? | ESS | ESS |

**5.4 FREIA**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **SES** | **Phase** | **Date Needed\*** | **In SSS Plan** | **SSS Plan Date** | **Delivery Responsible** | **Budget Responsible** |
| Sample changer for standard air-liquid samples  (including material and volume options) | HC | 2024 |  |  |  |  |
| Sample changer for Langmuir troughs | HC | 2024 |  |  |  |  |
| Sample changer for solid-liquid samples  (including different sizes and adaptations) | HC | 2024 |  |  |  |  |
| Sample changer for air-solid samples | HC | 2024 |  |  |  |  |
| An in-situ technique to be confirmed | HC | 2024 |  |  |  |  |
| Improved Langmuir/Liquid trough sample changing | ES | 2025 |  |  |  |  |
| Improved solid-liquid cells & sample changing | ES | 2025 |  |  |  |  |
|  |  |  |  |  |  |  |
| Pool cryostats & magnets | ES/ Later |  |  |  |  |  |
| Additional in-situ & in-line techniques to be confirmed | ES / Later | 2025-onwards |  |  |  |  |
|  |  |  |  |  |  |  |

APPENDICES

APPENDIX A : LoKI Presentation

APPENDIX B : SKADI Presentation

APPENDIX C : ESTIA Presentation

APPENDIX D : FREIA Presentation

APPENDIX E : Session Introduction Presentations