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SOURCE

Webcast for SAD update related to slides #1-18 (password: STAP2020):
http://vrelay.esss.lu.se/replay/showRecordingExternal.html?key=2kmtoFqxJaYZlVy

audio comments are available on TEFI and PREMP systems on slides #19-29

Update from the Scientific Activities Division for Diffraction STAP

Highlights from scientific coordination & user office, laboratory & sample services, sample environment

PRESENTED BY ZOË FISHER AND ARNO HIESS

2020-04-21

Agenda

1 Team

2 Scientific Coordination and User Office

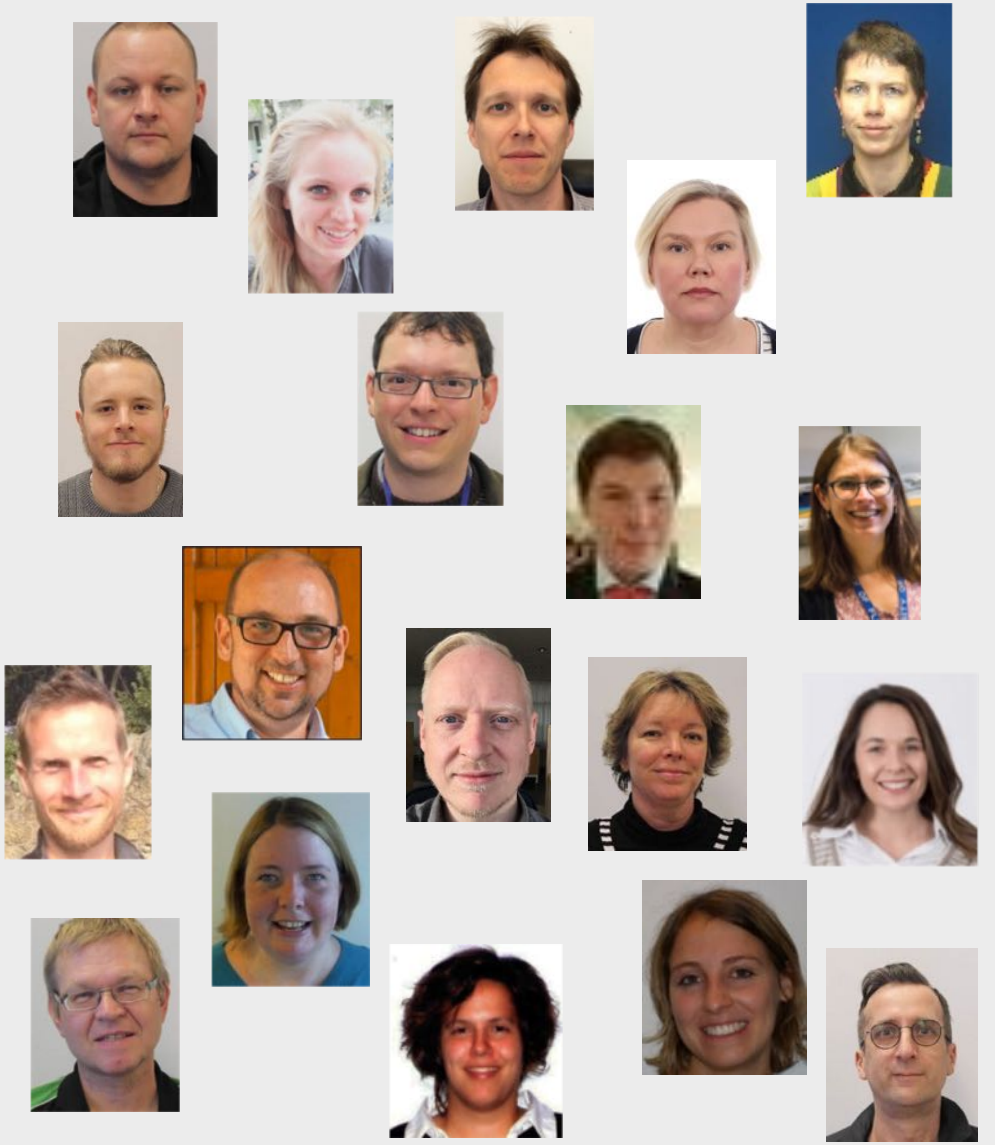
3 Deuteration and Macromolecular Crystallisation

4 User Laboratories and Sample Services

5 Sample Environment

1

Team

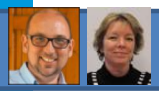


SAD Team

performing operational functions as part of Science Directorate

Line organisation matching operational functions – 17 FTE;

Some leverage via external grants; Anders matrixed 50% from data management division DMSC



Scientific Activities Division

DEMAX
Deuteration & macromolecular Crystallization Group

SULF
Sample and User Labs Group

SCUO
Scientific Coord. and User Office

SAMPLE ENVIRONMENT GROUP

TEFI
Temperatures and Fields

PREMP
High Pressure & Mech. Process.

FLUCO
Fluids incl Gases, Vapor, Compl. Fl.

MESI
Mechatronics & System Integr.







On-going recruitments:

- Group Leader for Sample Environment
- Mechanical Design Engineer for Sample Environment – matrixed from TD/NSS project division
- Postdoctoral Research Fellow ‘dynamics of cyanobacterial membranes’ (HFSP grant).
- Deuteration Chemist – 1 yr maternity coverage

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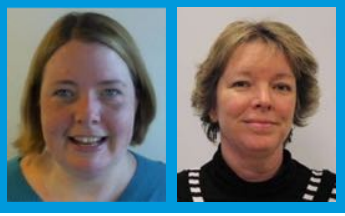
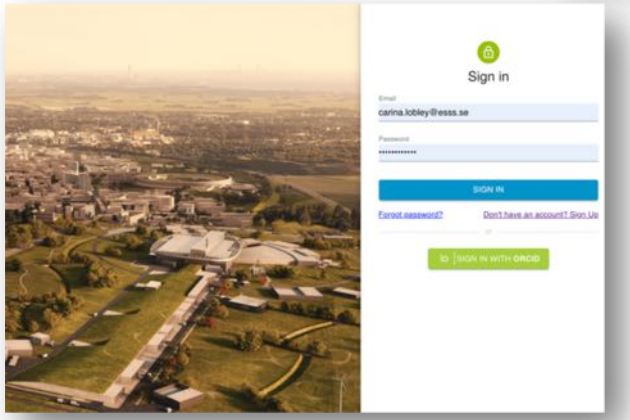
Scientific Coordination and User Office





Scientific Coordination and User Office

Achievement	Enables
User policies on evaluation / access and publication drafted, (to be) presented to SMT, STAP, SAC, Council	Implementation of procedures and guidelines for future user programme
Supporting 2nd DEMAX pilot call exploiting DMSC-developed User Office Software	'Hot commissioning' user programme and providing feedback on software features needed
Mapping of required SCUO functions / responsibilities: ▪ (On-site) user services ▪ Easy reporting against (ESFRI-recommended) KPIs ▪ Industrial access incl. industrial advisory board	Centring ESS activities on user needs and streamlining required ESS resources for successful user programme

Challenge	Mitigation
Emerging scientific events: • ESS Science Day 2020 cancelled • SXNS postponed to 2021 • **ESS-ILL user meeting in autumn at risk depending on COVID-19 developments**	**With stakeholders watching situation and adjusting the plan**
Mid-term planning for user engagement and on-site user services not a priority (yet) for ESS stakeholders	Multi-stakeholder activity requiring additional care (communication) in work-from-home environment

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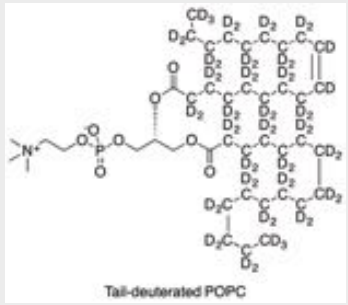
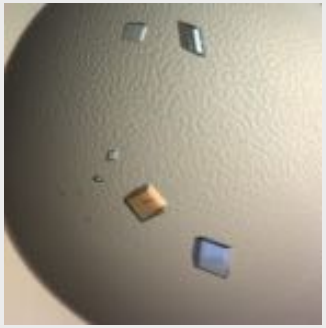
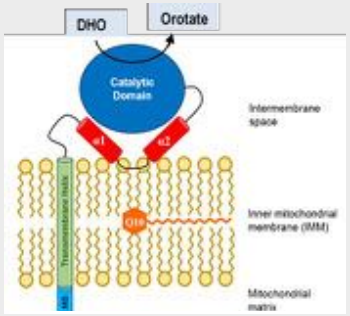
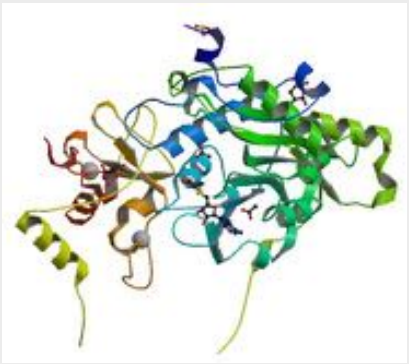
Deuteration and Macromolecular Crystallisation









Deuteration & Macromolecular Crystallisation

Achievement	Enables
Priority access for COVID-19 projects building on established capabilities and pilot user calls	**ESS team supports fighting health-related societal challenges.**
1st pilot call: successfully concluded on 16 accepted proposals; last materials being worked on as planned 2nd pilot call: 17 proposals received and now evaluated via user office software supported by SCUO & DMSC	Hot commissioning user programme and refine SCUO software, supported neutron user community for access to deuterated materials & crystals in life science, chemistry, soft matter, enabled scientific research in our key (future) user community to ensure first science
Collaborations and grant activities: • SINE2020 and iNEXT successfully concluded • Brightness2 and 2x VR incl. PhD student progressing • Coordination of DEUNET and LENS PA 'health'	Expands scientific capability to support users and scientific research (11 publications in 2019-2020), work synergistically with other facilities and attracts funding

Challenge	Mitigation
Understaffed in key positions to support user proposals while growing to be ready for First Science lacking in life science/biology expertise	Recruitment for maternity coverage on-going, but need to recruit to meet demand for first science: • 2nd synthetic chemist for small organic molecules (LoKI, Skadi, C-SPEC, Estia) • biodeuteration/life science specialist (LoKI, NMX, Estia, ODIN, C-SPEC)
Ensure long-term home for chemical deuteration labs	Renew lease for MV space for 5 year term beyond 2023

4

User Laboratories and Sample Services

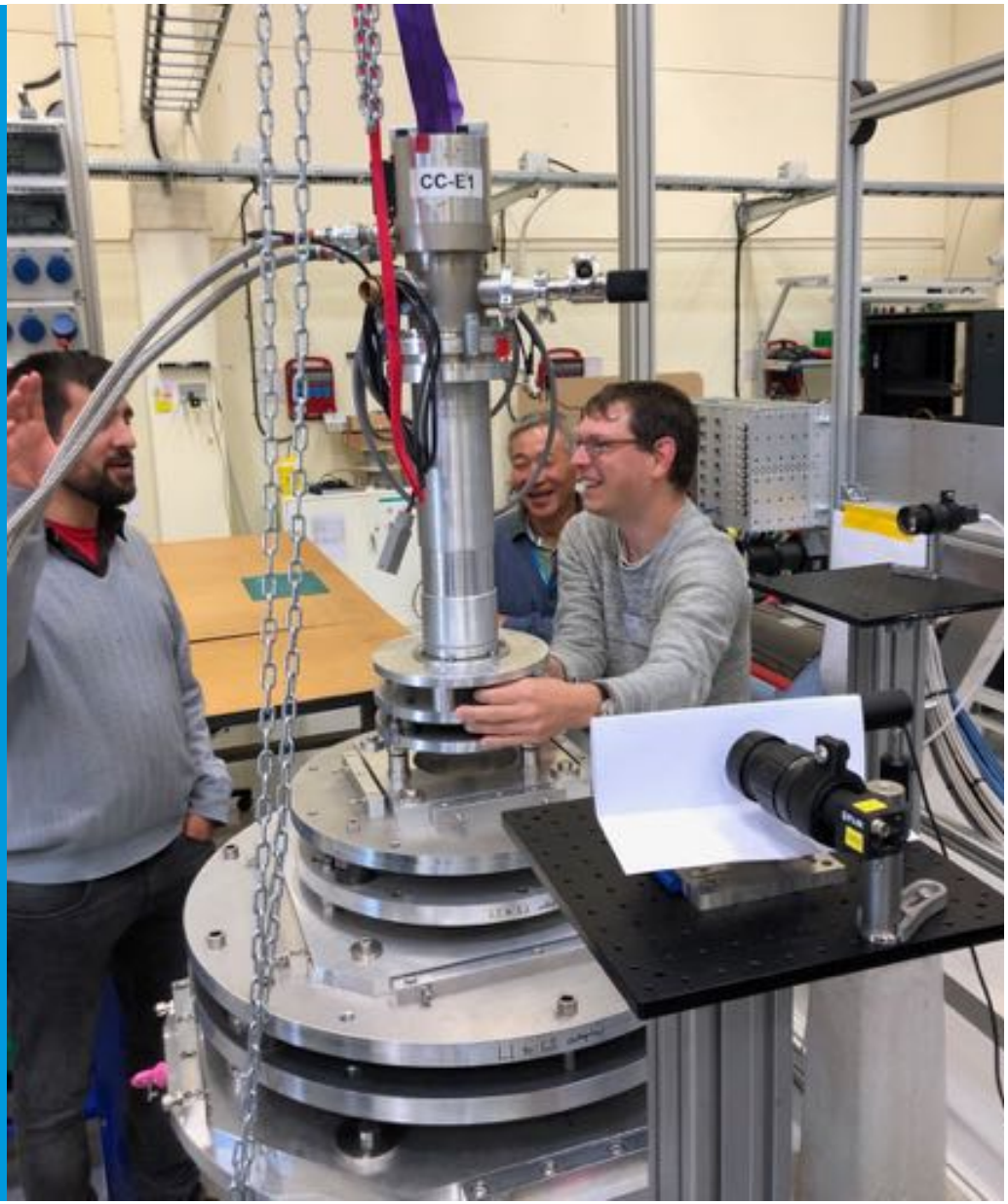
User Laboratories and Sample Services

Achievement	Enables
Area coordination of construction and declassified spaces in E03/E04. Following successful IRR, fit-out of laboratory (80-90% complete) and technical workshop spaces (started) ahead of schedule.	**Installation of laboratory equipment and glove boxes (temporary); commissioning of on-site chemistry and life-science services for hot commissioning and first science.**
Analytical support to ESS construction project: Ortho-/para-hydrogen, luminescence screen beam diagnostics, bunker / target concrete analysis, radiation-hardened grease, beam dump water analysis	Essential for TD/ SD engineers to advance ESS construction project and ensuring ESS project delivery
PostDoc recruitment for HFSP grant started	boosts life science and soft condensed matter expertise and equipment, e.g. DLS instrument.

Challenge	Mitigation
Related to COVID-19 crisis (in-kind) installation team has been ordered back to UK and fit-out of on-site E03 / E04 laboratories has stopped.	• **Partner revising installation plans (~3m float) as well as updating as-built documentation** • **Revise schedule to advance ESS self-performed infrastructure installation** • **Information on access for D buildings required**

5

Sample Environment

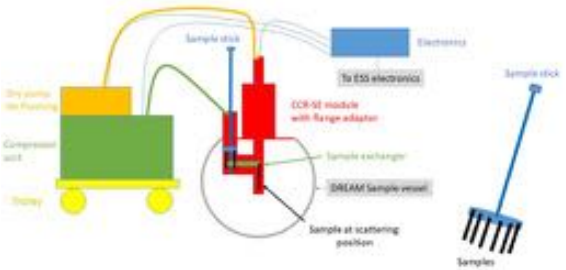


Sample Environment

Achievement	Enables
Standardised floor-mounted mechanical interface validated & ready for instrument implementation	**Eases change-over & operation of sample env. on all instruments; helps hot commission & first science**
Planning for E03 workshop fit-out and infrastructure incl. mechanical tools enclosure, hot works area, helium recovery ready to be executed	Fit-out once UK partner resumes on-site work; Installation machine tools and commissioning of first sample environment systems
All in-kind TAs agreed and all – but one –activated	Manufacturing for critical sample environment systems
High pressure blow-out tests performed; plans for on-site testing facility progressing	Safety assessment, safety validation and life-cycle management of high pressure equipment
PE high pressure system assembled with hydraulic system and specific anvils for MAGIC and DREAM	High pressure diffraction experiments on first instruments
Progress on instrument-specific sample environment: • CTV 8T magnet (MAGIC) and cryo-furnace (DREAM) • Kick-off SANS changer (LOKI) & solid-liquid (ESTIA) • Stress rig #1 available for control integration	Prioritised critical sample environment systems required for hot commissioning and first science
Mechanical and control Integration of wet cryogenic systems converging; 15T magnet ready for shipment.	Low temperature experiments; magnet essential for BIFROST first science
Communication protocol SECoP: SINE2020 project successful, ready for ESS implementation via ECDC/ICS	Standardised meta-data, validation of control develop. platform); cross-facility operation of sample env.

Sample Environment

Challenge	Mitigation
Related to COVID-19 crisis (in-kind) installation team has been ordered back to UK and fit-out of on-site E03 / E04 workshops has stopped	• **Revise schedule to advance ESS self-performed infrastructure installation** • **Information on access for D buildings required** • **Use of temporary workshops (Utgård, MV)**
Related to COVID-19 crisis in-kind partners in Estonia and France temporary suspended /reduced work	Follow up with partners to adjust delivery schedule.
Partial closure of vendor developing non-magnetic components resulting in uncertain dimensions and delays of spatial integration (CSPEC & DREAM tank)	Overcome pending recruitment of design engineer to quantify effect on critical parameters in instrument design and support spatial integration



SE Priorities for Imaging & Engineering

as required for hot commissioning and first science of different instruments

BEER

Platform	System	Details	partners
PREMP	Stress strain rig 1	100kN 'workhorse'	NPI
PREMP	Stress strain rig 2	40kN with rotation for imaging, torsion	NPI / MLZ / commercial
PREMP	Dilatometer		commercial

ODIN

Platform	System	Details	partners
PREMP	Stress strain rig 2	40kN with rotation for imaging, torsion	NPI / MLZ / commercial
PREMP	Gas / liquid cells	5 kbar gas / liquid cell	LLB

Some (pool) SE systems shown more than once – matching SE reference suite

Details on delivery schedule provided by later presentations.

SE Priorities for Spectroscopy

CSPEC

Platform	System	Details	partners
TEFI	6.5 T Magnet	Ex-HZB VM-2 +Dilution insert	ESS/HZB
TEFI	Cryofurnace	Inst. specific 6 pos. changer	LLB
TEFI	Wet cryostat	Standard Orange Cryostat	LLB
PREMP	Clamp + DAC uniaxial	2 GPa + low T	LLB, U Copenhagen
PREMP	Gas liquid cells	10 kbar gas/liquid cell	LLB
FLUCO	Humidity cell	Wide angular access	ESS/EE
FLUCO	Pump-probe	In-situ laser trigger	EE

BIFROST

Platform	System	Details	partners
TEFI	15T Magnet	Ex HZB VM1B +Dil.	ESS/HZB
TEFI	Wet Cryostat	Specific Orange Cryo 100mm	BIFROST
PREMP	Clamp, PE, DAC pressure cells	2, 20, 50 Gpa + low T	LLB, LLB, SNS

SE Priorities for Large Scale Structures

LOKI

Platform	System	Details	partners
FLUCO	SANS changer	Inst. spec.; (indiv.) thermalized, tumbler	ESS
FLUCO	(Stopped) Flow cells	Inst. spec.; incl. pumps	ESS, EE
FLUCO	In-situ techniques	Supplied via external grants	External / ops
TEFI	Low field magnet	HTSC warm bore or electromagnet	LLB
PREMP	stress-strain rig 3	5-10 kN versatile rig	LLB

ESTIA

Platform	System	Details	partners
TEFI	Low field magnet	2T HTSC warm bore magnet	LLB
TEFI	Flow cryostat	Instrument specific	PSI
FLUCO	Solid Liquid Cells	Instrument specific	ESS

SE Priorities for Diffraction

DREAM

Platform	System	Details	partners
TEFI	Cryofurnace	Instr. specific; multi-position changer	LLB
TEFI	Wet Cryostat	Standard Orange Cryostat	LLB
TEFI	Magnet	Asymmetric 8T + Dilution / ^{3}He	LLB
TEFI	Furnace	HT vacuum furnace	ESS
PREMP	Clamp, PE, DAC pressure cells	2, 20, 50 Gpa + low T	LLB, LLB, SNS
FLUCO	Gas Processing	Automated	EE

MAGIC

Platform	System	Details	partners
TEFI	Magnet	Asymmetric 8T + Dilution / ^{3}He	LLB
TEFI	Wet Cryostat	Instrument specific	LLB
PREMP	Clamp, PE, DAC pressure cells	2, 20, 50 Gpa + low T	LLB, LLB, SNS

5.1

TEFI Individual systems

8T Magnet for MAGiC, DREAM, *HEIMDAL*

Providing 8T, 1.6K (or 50/300 mK with ULT inserts)

1. System Overview and Deliverables

+15°/-35° vertical field wet cryomagnet

2. Schedule, Milestones and Reviews

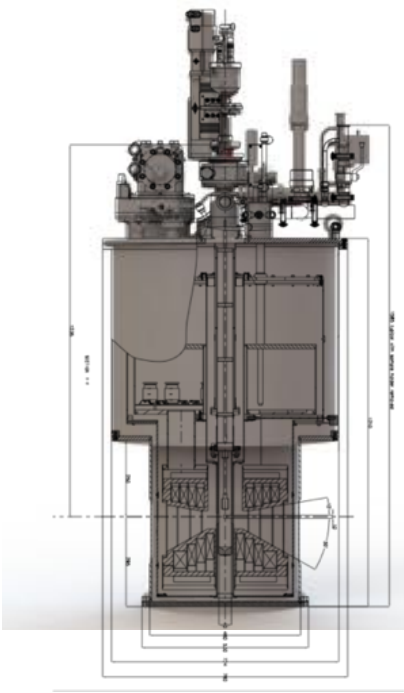
Call for tender review (CTV) complete.

Waiting in procurement queue at LLB, likely publication October

⇒ delivery late 2022/early 2023

3. Integration, Safety, Verification, Validation

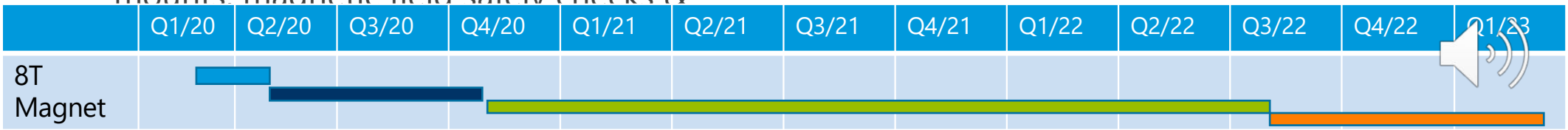
Requires mechanical integration with kin. mounts, magnetic field safely checks &



4. Achievements and Challen

Completing CTV!

Finite procurement bandwidth.



New ULT systems for ‘8T magnet + OC’

Providing ‘parameter range’ 50/300mK – 300K

1. **System Overview and Deliverables**

- 2 dilution systems
- 1 ^{3}He sorption

Matched to 8T magnet, usable in wet cryo.

2. **Schedule, Milestones and Reviews**

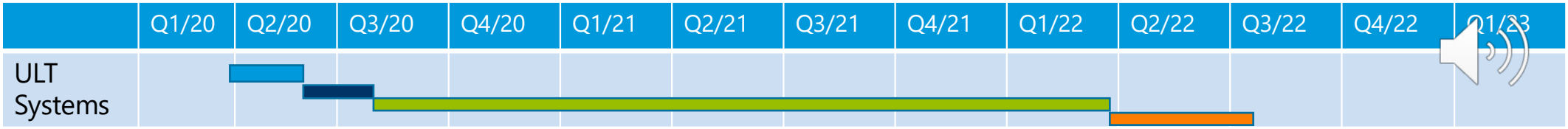
Have model tender docs from ANSTO CTV to be complete ASAP.

3**. Integration, Safety, Verification, Validation**

Must be compatible with other systems.

4. **Achievements and Challenges**

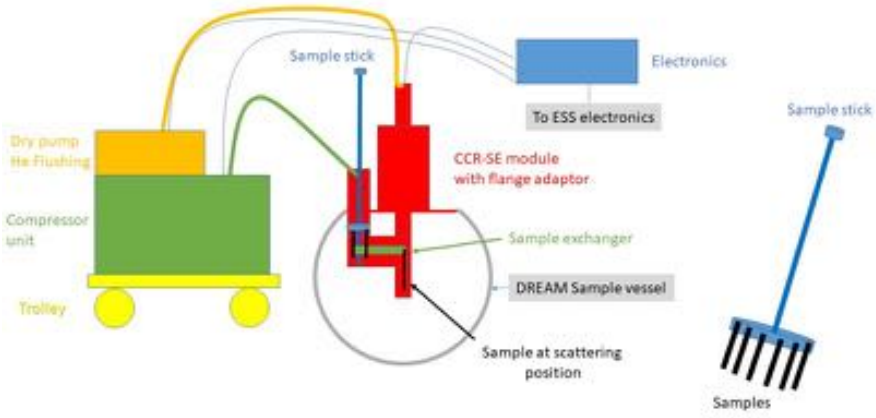
Technician Richard Ammer has participated in a number of dilution cooldowns.



'20 position Cryofurnace' for 'DREAM'

Providing 20 samples, 4 K-800 K at measurement position, sample storage at 90 K

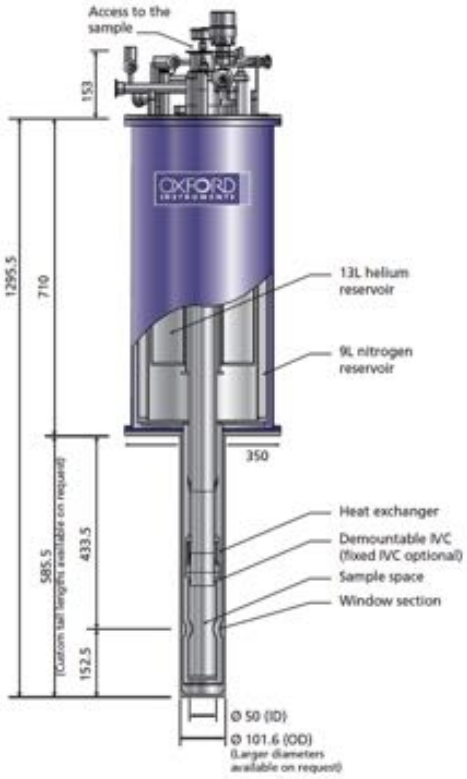
1. System Overview and Deliverables
   - Instrument specific multi position dry cryofurnace
2. Schedule, Milestones and Reviews
   - Part of DREAM instrument schedule
   - CTV complete
3. Integration, Safety, Verification, Validation
   - Fits with top loading
4. Achievements and Challenges
   - CTV passed
   - Very ambitions specs - need a plan B



‘Wet cryostat’ for ‘MAGiC’

Instrument specific cryostat providing 1.5K-300K

1. System Overview and Deliverables
   - Orange-type or Variox wet cryostat system
2. Schedule, Milestones and Reviews
   - Not yet fixed
3. Integration, Safety, Verification, Validation
   - Mechanical integration with XYZ coils and kinematic mount
4. Achievements and Challenges
   - JCNS has Variox available for donation.



Variox

‘Wet cryofurnace’ for ‘DREAM’

Pool cryostat providing 1.5K-600K

1. System Overview and Deliverables
   - Orange-type wet cryofurnace
2. Schedule, Milestones and Reviews

To be fixed – ready by first science milestone

3. Integration, Safety, Verification, Validation
   - Top loading
   - Needs special tail materials.
4. Achievements and Challenges
   - Tail materials may not be compatible with spectroscopy. V/TiZr vs Al

Vacuum furnace for DREAM

Pool HT vacuum furnace RT - 1300 K

1. System Overview and Deliverables
   - ILL type vacuum furnace
2. Schedule, Milestones and Reviews
   - To be fixed – ready by first science milestone
3. Integration, Safety, Verification, Validation
   - Needs special tail materials.
4. Achievements and Challenges
   - Furnace expertise needs building

5.2

PREMP Individual systems

Clamp cells for DREAM, MAGIC, CSPEC, BIFROST Provides < 2GPa and <1K

1. System Overview and Deliverables (ref ESS-1545382)

- Clamp devices will follow LLB and Sine2020 designs
- 0.3cc vol
- TiZr <1 GPa* and CuBe < 1.5 GPa*
- Training to enable in house construction of cells

2. Schedule, Milestones and Reviews

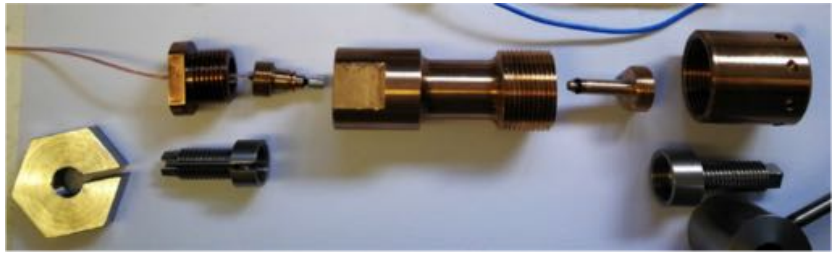
- see NIK 3-7 slide later

3. Integration, Safety, Verification, Validation

- Primary installation via cryostat stick (design pending)
- Safety/Quality see later slide

4. Achievements and Challenges

- TA (almost) at signing stage. Target: 24th April
- Main challenge is if this slips due to COVID



Sine 2020 developed clamp cell (WP7 report)

GAS/LIQUID cells for DREAM, MAGIC, CSPEC, BIFROST… Provides < 1GPa and <1K

1. System Overview and Deliverables (ref ESS-1545382)

- Gas/Liquid cells follow LLB and Sine2020 designs
- two std volumes: 0.5 cc and 1.0 cc
- TiZr <0.5 GPa*, Al < 0.4 GPa*, BeCu 1.0 GPa
- Training to enable in house construction of cells
- 1.0 GPa He gas compressor

2. Schedule, Milestones and Reviews

- see NIK 3-7 slide later

3. Integration, Safety, Verification, Validation

- Primary installation via cryostat stick (design pending)
- Safety/Quality see later slide
- Verification/validation requires Pressure Testing Facility

4. Achievements and Challenges

- TA (almost) at signing stage. Target: 24th April
- Main challenge is if this slips due to COVID

PE cells for DREAM, MAGIC, BIFROST
Provides < 20GPa and <4K

1. System Overview and Deliverables (ref ESS-1545382)

- PE cells: 1x VX5 (AW819), 2x VX1 tonne (BeCu)
- CCR-based cryostat for PE
- Gas-loader for PE (also suitable for DACs)

2. Schedule, Milestones and Reviews

- see NIK 3-7 slide later

3. Integration, Safety, Verification, Validation

- FAT conducted for RT mount for PE cell (Q1 202
- Low T mounting part of cryostat design
- Safety/Quality see later slide

4. Achievements and Challenges

- TA (almost) at signing stage. Target: 24th April
- Tender completed for hyd. pump: Vinci system
- Parallel project to increase angular aperture
  AM