BrightnESS²

Bringing Together a Neutron Ecosystem for Sustainable Science with ESS

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Deliverable Report

D2.8 Report on lessons learned from engineering and deuteration pilot

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3. List of Abbreviations and Acronyms

DEUNET	Deuteration Network
ESS	European Spallation Source
ILL	Institute Laue-Langevin
NQL	Neutron Quality Label
STFC	Science and Technology Facilities Council
WP	Work Package

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4. Executive Summary

Work Package 2: 'Strategy to deliver neutrons for Europe and beyond' aims to define the best way to provide neutron instrumentation, associated characterisation methods and analysis tools in a strategic and coordinated fashion to the European neutron user community and beyond. This work package encompasses neutron instrumentation and methods as well as support functions that can increase the efficiency and impact of neutron usage if utilised in a cohesive, innovation way.

Two pilot projects focussing on engineering and deuteration services have demonstrated how collaborative method development between neutron facilities can be beneficial, scientifically and economically. Spending time to establish novel or efficient methods or procedures extends the capabilities of neutron facilities, enabling high-impact scientific experiments. Doing so in a harmonised fashion increases user confidence across the neutron landscape, providing researchers with the confidence to use the most applicable instrument, sample or laboratory regardless of which neutron facility they are located in.

5. Introduction

Work Package 2 aims to define the best way to provide neutron instrumentation, associated characterisation methods and analysis tools in a strategic and coordinated fashion to the European user community and beyond. Broadly, WP 2 should establish a common strategy for future neutron capability, in alignment with the needs of the user community; and explore and implement new ways of working for the most efficient use of neutrons.

Towards this end, two pilot projects were designed to demonstrate such new ways of working: an engineering science pilot which would produce an experimentally-validated Neutron Quality Label for residual stress, and a deuteration pilot focused on strengthening soft matter and life sciences research by establishing robust and efficient methods of producing complex deuterated lipid samples.

The engineering pilot aimed to further promote and raise the confidence of industry in residual stress measurement using neutron diffraction. Although the technical development and standardisation of neutron diffraction for residual stress analysis have been performed through previous projects (VAMAS TWA20, RESTAND) and a standard has been published (ISO 21432:2019), industrial users have voiced a perceived disparity of 'measurement quality' and lack of standardised procedures between different neutron strain scanners. This plays a significant role in preventing neutron diffraction residual stress mapping to be an established tool for industry.

The engineering pilot addresses the stated problem by strengthening the network between the participating neutron facilities for residual stress measurement, including developing a standard for instrument benchmarking and a template for experimental reporting. The two activities led to the establishment of the *Neutron Quality Label* (NQL), which acts as a quality assurance of the output from the participating neutron facilities. The pilot also highlighted the instruments' interchangeability through a demonstrator industrial experiment, representing the sustainable academic and industrial access to neutron facilities for residual stress measurement in the future.

The deuteration pilot aimed to demonstrate the value of efficient and cohesive workflow between support labs such as those producing deuterated samples, and beamlines at neutron facilities. The framework for such a workflow is already in place, in the form of the Deuteration Network (DEUNET), a collaborative effort between labs across Europe and the world, with a focus on deuteration science. Collaborative projects can be carried out between deuteration labs at neutron facilities; and the facility where a sample is produced is not necessarily the same facility where it is investigated using neutron experiments.

A user survey carried out by the DEUNET in 2017 revealed that some of the molecules that would prove to be the most useful for the neutron scattering community are lipid-based materials. The deuteration lab at STFC routinely synthesises deuterated lipids for the neutron scattering community, but reported that the range and complexity of the lipids requested meant that fulfilling the community's needs was a challenge. The deuteration lab at ESS recently began using biological catalysis (using enzymes) to produce complex molecules, and it was proposed that these methods could be applied to the synthesis of complex deuterated lipids, which would facilitate more, and better, neutron experiments in the fields of soft matter and life science.

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6. Lessons Learned

1. Method development increases capability and increases efficiency

Although method development has clear scientific and financial value to neutron facilities, many facilities find that user demand is so high that method development is difficult to prioritise. However, investing resources in method/procedure developments is worth the effort if new methods are more efficient and/or produce better and/or more reliable results. These can be a huge time-saver in the long run while at the same time increasing the usage and confidence of users of the neutron techniques.

The methods developed in the pilot tasks *Deuteration* and *Engineering* within the BrightnESS² project have, respectively, produced products that are not commercially available using novel and robust methods, and produced procedures which ensure the quality of results from neutron experiments.

There are two major benefits to highlight considering the achievements of both pilots:

1. Scientific value: these pilots have made otherwise impossible experiments possible (deuteration pilot) and have demonstrated the usefulness of alignment of instruments/facilities so research continues throughout shutdowns, or so the most appropriate, available instrument is used (engineering pilot).
2. Monetary value: these pilots demonstrate ways to increase the efficiency of beamtime and increase confidence in the use of our installations and methods at neutron facilities.

Engineering Pilot

The engineering pilot successfully developed a common calibration procedure (method) to quantify the positioning accuracy of neutron strain scanning instruments. This facilitates **benchmarking of instruments performance** and, together with the demonstrator experiment using an industrial sample, highlights the **interchangeability** between the instruments. Additionally, by facilitating performance assessment, the procedure allows beamline scientists to make further **improvements** on the current and future instruments.

The procedure has been integrated into a so-called *Neutron Quality Label (NQL)* together with a master report template. The NQL has been established to raise awareness and confidence within the whole neutron scattering and engineering communities, with a particular emphasis towards increasing industrial uptake for residual stress measurement.

Deuteration Pilot

The deuteration pilot project demonstrated that spending time to establish novel, robust and efficient methods of producing challenging deuterium-labelled molecules is worth the effort as it can **improve** the efficiency of beamtime by facilitating **more** neutron experiments using **superior** samples. Enzymes are highly specific biological catalysts that are capable of, for example, distinguishing between two positions on a molecule, where chemical agents cannot; in this project enzyme catalysis was exploited in a new method of producing complex deuterated lipids.

The method facilitates access to biologically-relevant lipids which are challenging to produce using traditional chemical synthesis. The method has been published (DOI: 10.1021/acsomega.0c02823). The modularity of the method meant it could be extended: three new deuterium-labelled lipids were produced and supplied to collaborators for use in neutron experiments for research in the fields of biology, pharmacology and human health.

2. Collaboration ensures quality and reliability

Developing methods and procedures that are beneficial to neutron facilities is even more advantageous when it is coordinated between facilities. Harmonised procedures on neutron instruments or within support functions is likely to increase confidence in using different instruments or support services interchangeably. The user community frequently combines data obtained from instruments at different facilities; or uses combined techniques (such as complementary measurements with the specificities of the instruments for the same method e.g. TOF and monochromatic, or deuterium-labelling with SANS for contrast-matching). Promoting horizontal/transversal synchronisation across neutron facilities would enhance not only a more complete scientific research output but also the exchangeability of users during long reactors shut downs, securing a continuous use of neutron instruments and research output.

Engineering Pilot

Stronger networking between four neutron strain scanners at MLZ, ILL, ISIS and NECSA with different specifications (resolution, flux, energy selection, etc.) allows users to access a wider range of capabilities through a single contact point (**www.neuss.com**). This consequently makes the technique easily reachable for industrial and academia researchers alike.

With better understanding about instruments capability in between the facilities, the scientists can advise potential users on the most suitable method/instrument for any given case, therefore maximising the beam time efficiency. As the instruments follow the common protocol developed in the pilot, the quality of the output from each instruments is ensured. This assurance is manifested in the proposed NQL @trademark 2021, which also allow other instruments to join. Instrument interchangeability, as proven in the pilot, allows greater availability of neutron strain scanners for both academic and industrial users. With the aim of sustainable industrial services, this is especially critical during shutdown periods of neutron facilities.

Deuteration Pilot

Long-term collaboration within the DEUNET offers the possibility to dissociate the location of synthesis completely from the location of the neutron experiments. Perhaps the best neutron instrument for the purpose is at ISIS (UK), but the methods for sample production are housed at ESS (SE). As with the instrument interchangeability discussed for the engineering pilot, this disassociation provides greater availability and flexibility for users.

Learning from the engineering pilot, the group of deuteration laboratories at neutron facilities (part of the Deuteration Network, DEUNET, www.deuteration.net) could, in the future, look to align on quality assurance of the deuterated samples produced and supplied. Currently, the analysis and quality control of samples produced at the different laboratories is not consistent across facilities. Doing this would provide beamline scientists with assurance of the quality of the deuterated sample and ensure beamtime is well-utilised. This was discussed at the most recent DEUNET meeting, 7-8 July 2021 and all of the represented neutron facilities agreed that it would be beneficial to collaborate on standardising quality certification of the deuterated materials produced for neutron experiments.

7. Conclusion

These pilot programmes reinforce that **collaborative method development** is a valuable use of time for highly-specialised neutron facilities and their support services, such as deuteration laboratories.

The demands placed upon neutron facilities are ever expanding, and facilities ought to spend time establishing robust methods and procedures which increase the efficiency of neutron experiments, improve user confidence, and enable high-impact science. If method development can be performed *collaboratively*, this is ideal – as users will have confidence in the validity of their experimentation regardless of the facility where the experiment is performed (or where the sample for their experiment is produced).

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