



Monitoring the neutronic stability of the liquid methane moderator on ISIS Target Station 1

C Ridley

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STFC Author Identifiers (ORCIDs)

Author ORCIDs are provided where available.

Christopher Ridley



[0000-0002-3060-9656](https://orcid.org/0000-0002-3060-9656)

Monitoring the neutronic stability of the liquid methane moderator on ISIS Target Station 1

Christopher J Ridley

ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Didcot, Oxfordshire OX11 0QX, United Kingdom

Corresponding author: *christopher.ridley@stfc.ac.uk*

Abstract

The stability of the output from the liquid methane moderator on ISIS Target Station 1 is investigated through analysing close to 3 million μAmps of historical neutron data collected on the PEARL diffractometer over the period September 2015 to June 2021. The fundamentals of neutron moderation are introduced, and the requirements for moderator output stability for the diffraction instruments are discussed. It is found that while the thermometry of the moderator may indicate stability, the neutronic output from the moderator can indicate otherwise, if over-exposed to radiation with time. Analysis of the shift in peak-flux from the moderator over long durations suggests an upper critical limit for accumulative neutron irradiation between 250,000 and 300,000 μAmps , prior to degradation beyond an acceptable tolerance. The rate of change of degradation shows potential for continuous monitoring of the moderator output, to better inform decisions on operation and replacement of the moderator. Implications for understanding the new methane moderator assembly, post the major refurbishment of TS1, are discussed.

Introduction

The ISIS Neutron and Muon Source (ISIS) delivers neutrons through directing bunches ($\sim 10^{13}$) of high-energy (~ 800 MeV) protons at a dense tungsten target and repeating this process every 20 ms. This produces intense bursts of very high energy neutrons through the spallation process; the majority of which are too high in energy for the types of measurements being performed at the facility. Instead, these high-energy neutrons are moderated to lower energies through passing through an additional medium, a moderator [1].

Moderators are used at both spallation and reactor sources and are designed to interact strongly with the high-energy neutrons, whilst minimising neutron capture/absorption which act to reduce the flux of neutrons reaching the instruments. Fast neutrons collide with the moderator material (typically a material with a large scattering cross-section and low absorption cross-section), reducing their energy, or ‘thermalising’ with the moderator. Once moderated, the energy spectrum of the thermalised neutrons produced can be approximated following the statistical analysis of an ideal-gas, on a Maxwell-Boltzmann distribution, where ϕ_{mod} is the flux of moderated neutrons (in arbitrary units), E is the energy of the neutron (J), T is the temperature of the moderator (K) and k_b is the Boltzmann constant ($1.380649 \times 10^{-23} \text{ JK}^{-1}$):

$$\phi_{mod} = \frac{E}{(k_b T)^2} \cdot e^{-E/k_b T} \quad (1)$$

This function shows a maximum at the point where $E = k_b T$.

Many neutrons will only be partially thermalised by the moderator (‘epithermal’ neutrons), and many more will leave the moderator in a direction away from the desired beam port. To help counteract this inefficiency, these neutrons may be partially reflected back into the moderator for further moderation. This is achieved through surrounding the moderator with a reflector assembly (often beryllium or graphite).

Aside from the temperature of the moderator, there are many design parameters used to control the profile shape and intensity vs. energy of Equation 1: the choice of moderator material, the size and geometry of the moderator and reflector assembly, the inclusion of an additional absorbing foil within the moderator (‘poisoning’) to control the width of the pulse [2,3] and controlling the wavelength range over which the reflector is effective (‘coupling’) [4]. As such, the output wavelength range and pulse-width are tuned. These have a fundamental effect on the achievable measurements and are therefore carefully controlled to ensure repeatability over long timeframes.

The time spent by the neutron in the moderator broadens the initial pulse width¹, and the reflector effectively broadens this further, having implications for the wavelength range produced, and ultimately the time-resolution of the instrument [2]. The range of wavelengths produced, and the time-resolution dictate the types of measurements for which the neutrons are suitable.

ISIS Target Station 1 (TS1) has two decoupled/poisoned water moderators which sit above the target assembly and a coupled liquid hydrogen moderator and decoupled liquid-methane moderator which sit below the target assembly [3].

¹ The time distribution of neutrons of a given wavelength crossing the front face of the moderator.

Overview of the TS1 liquid-methane moderator

Of particular interest to this report is the decoupled liquid-methane moderator on TS1, which has historically operated at a temperature of 110 K. Exposure to high radiation causes the methane in the system to breakdown, forming hydrogen gas, ethane and long-chain hydrocarbons within the mixture [1, 5]. These alter the neutronic performance of the moderator, and the smooth operation of the cryogenic cooling of the moderator system. To extend the lifetime of the moderator, the 'charge' of methane within is refreshed periodically (usually once every 24hrs); this causes short term temperature disruption to the system. Every 6 to 7 months, the moderator is replaced in its entirety, as it no longer becomes possible to clear the impurities from the system, and the performance of the moderator is irreparably damaged. The storage, and eventual disposal of these highly irradiated waste moderator assemblies poses operational risk and considerable cost to the facility.

Part of the TS1 project [6] (2021 -> 2023) focussed on extending the lifetime and improving the serviceability of target and moderator operations on TS1. This also provided an opportunity to alter the moderator performance for a few instruments on the target station, where desirable. As part of this major project, a water pre-moderator was included between the target and the methane moderator. The concept was to reduce the flux of extremely high-energy neutrons hitting the methane moderator directly, the intention being to reduce the decomposition rate of methane in the system, and to extend the working lifetime of the moderator.

As discussed above, the output from the moderator is sensitive to a number of factors. From an operational perspective, the variable of particular concern is the temperature stability. As described by Equation 1, the temperature of the moderator determines where the peak in thermalised neutron flux sits. However, the temperature doesn't necessarily reflect the overall condition of the moderator. Significant methane degradation may occur before the normal operation/temperature-stability of the moderator is impacted. The moderator is routinely monitored from a diagnostic perspective, through observing flows/pressures/temperatures but the neutronic performance is assumed to be repeatable based on temperature stability alone and isn't officially monitored.

Stability requirements

The methane moderator on TS1 services 5 instruments on the south-side (PEARL, HRPD, ENGIN-X, GEM and MARI), and currently 2 operational instruments on the north-side (SANDALS and ALF) of the target station. PEARL, HRPD, ENGIN-X, GEM, SANDALS and ALF are neutron diffraction instruments, while MARI is a spectrometer. A critical component of performing quantifiable diffraction experiments, is related to data normalisation.

For the crystallography instruments, there are two important considerations when it comes to normalisation. 1) The flux delivered to an instrument has a wavelength dependence described approximately by Equation 1, so the intensity of a diffraction peak measured at peak flux will be larger in raw counts than one measured at the very tail of the flux distribution. This difference in intensity is not due to the sample but is due to the incident beam being inhomogeneous in intensity. 2) The instrument's detectors have a finite efficiency. This efficiency is variable across different elements of the detectors due to differing active components, and electronics etc. As such two neighbouring pixels on the same detector-bank may show very different count-rates and may have different responses to each other as a

function of neutron wavelength. Peak intensities provide extremely powerful information in analysis of diffraction data. Among other properties, accurate peak intensities provide information on atomic positions, sample composition and magnetic properties. As such, erroneous normalisation can lead to severe misinterpretation of the data.

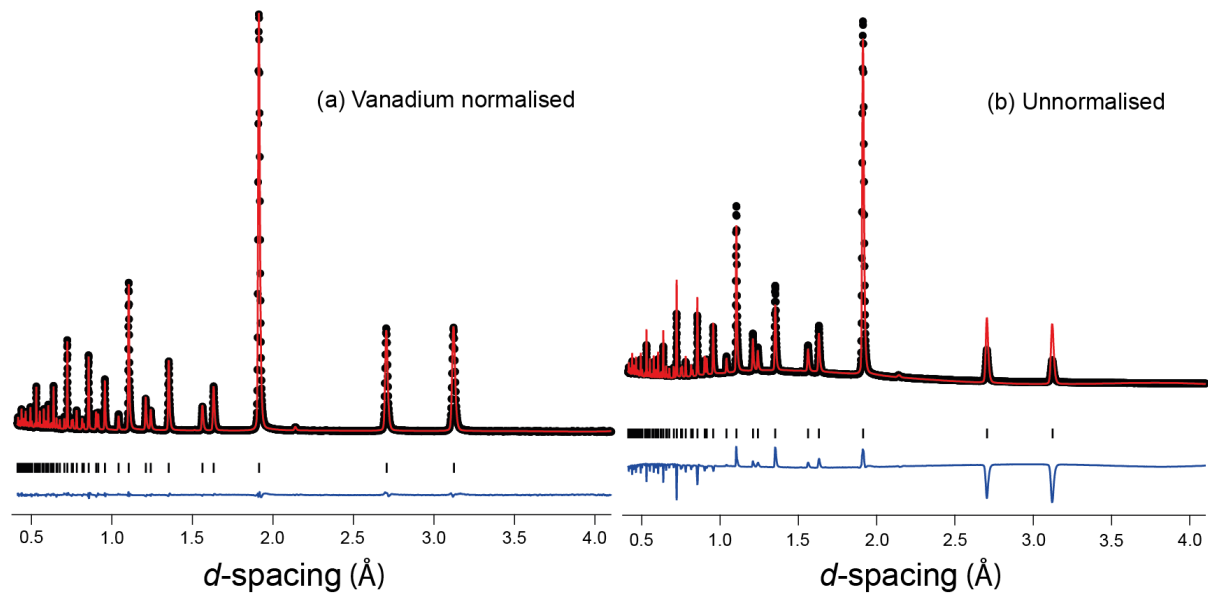


Figure 1: Diffraction data collected from PEARL diffractometer (port S9 on TS1). NIST standard (SRM674a) CeO_2 powder loaded in 6mm diameter vanadium can, collected in cycle 23/4. Run numbers 118000-118007 (total $\sim 1100 \mu\text{Amps}$). (a) data normalised against 10mm diameter vanadium-sphere data, (b) same data unnormalized against vanadium data. In both figures, the raw data are represented by black symbols, the Rietveld fit to the data is the red line, the blue line is the residual to the fit. The black tick marks represent the expected peak positions based on the cubic symmetry of the sample (sg. $Fm\text{-}3m$, $a=5.4119 \text{ \AA}$).

To counter these two issues, diffraction instruments normalise the detector efficiency through measurement of a standard. The ideal standard for this is a strong isotropic scatterer, i.e. ideally a large incoherent scattering cross-section, with small coherent and absorption cross-sections. Vanadium is routinely used, as it shows weak diffraction peaks, but scatters very strongly incoherently. As vanadium scatters isotropically, dividing the raw detector counts against a vanadium measurement corrects for both the moderator profile, and the detector efficiency. On PEARL these data are collected from a 10 mm diameter vanadium sphere. To ensure accurate intensity normalisation, these data are also corrected for neutron absorption/attenuation of the sphere itself.

To illustrate the effects of this, see Figure 1, which shows a powder-diffraction dataset collected on the PEARL diffractometer, with and without vanadium normalisation applied. The sample used to demonstrate the effects of normalisation is a NIST diffraction standard (CeO_2 , SRM674a), which is crystallographically well-defined, with a tightly constrained structure (i.e. there are very few free parameters to refine in the model against the data). It is clear from Figure 1 that without normalisation there are extremely large misfits in the data. For a more crystallographically-complex sample, the structural model would have a much larger number of free parameters to refine against the data. The nature of least-squares fitting would lead to these parameters shifting so as to minimise the difference curve, resulting in unphysical structures, e.g. cases where atoms may start to overlap etc.

Figure 1 demonstrates an extreme example (with and without normalisation), a more realistic concern is that the vanadium normalisation effectively changes during a measurement, or during a cycle of operation. Small changes in intensity can still lead to

erroneous results, while being less obviously spotted, as the refined structures may appear physical. On PEARL it takes typically 12 hours to measure the vanadium sphere. This is done at the beginning of the cycle and is assumed to be correct throughout the ~30 days of the user-cycle. To validate this, the instrument data acquisition software monitors the temperature of the methane moderator, and vetoes (pauses data-collection) if the temperature strays outside a predefined temperature range. The range of acceptance on PEARL is currently set as ± 2 K around the stable base temperature (nominally 110 K). The choice of tolerance on this temperature is largely historic, as *any* degree of shift in the temperature of the moderator results in a change in the normalisation; in usual operation, the temperature of the moderator only oscillates gently within 0.5 K of the base temperature. However, some degree of tolerance is required, as there are noticeable shifts in the base temperature achievable depending on the level of beam current being delivered to the target.

In summary, providing that the vanadium normalisation data are collected in the same conditions as the data collected for subsequent samples, then the normalisation is considered valid. Typically, collection times on the instruments range from 30 mins to 24 hours, so stability over long timeframes, and consistency through a full cycle are imperative for the crystallography instruments.

Monitoring the neutronic stability of the moderator

PEARL is an instrument well-suited to collecting information on the neutronic performance of the moderator, as it measures the full frame of neutrons delivered per pulse (i.e. has no choppers), has no complex neutron optics, and measures the maximum divergence flux delivered from the moderator (it uses the full view of the moderator face). In addition to this, PEARL has three incident beam monitors (at a distance of 11.13, 11.18, and 12.01 m from the moderator), which have been position-calibrated against a natural uranium foil, providing accurate information on the energy of the neutrons detected. These monitors have not been normalised for efficiency but are remarkably stable over very long periods of time. In addition to this, PEARL collects datasets in blocks no longer than 1 hour long; historically this was so as to prevent data corruption from sample-environment failures. This means that PEARL has 1 hour time-resolved data collected from the moderator over full cycles, going back to at least 2011. As such, this large body of data collected on PEARL provide a powerful diagnostic tool to understand neutronic stability, and to benchmark past moderator operations against the changes made during the TS1 project.

Figure 2 shows an example of the monitor data collected, measured at the same time as the vanadium data collected in Figure 1. The data, over the range of thermalised neutrons, can be fitted to Equation 1, which would estimate the temperature of the moderator to be closer to 100 K, rather than 110 K. This discrepancy is most probably related to the fact that the monitor is not accurately normalised for energy efficiency, and so may provide a slightly inaccurate absolute measure of the peak profile. However, the monitors are highly stable, and so these data can be used for meaningful relative changes between measurements.

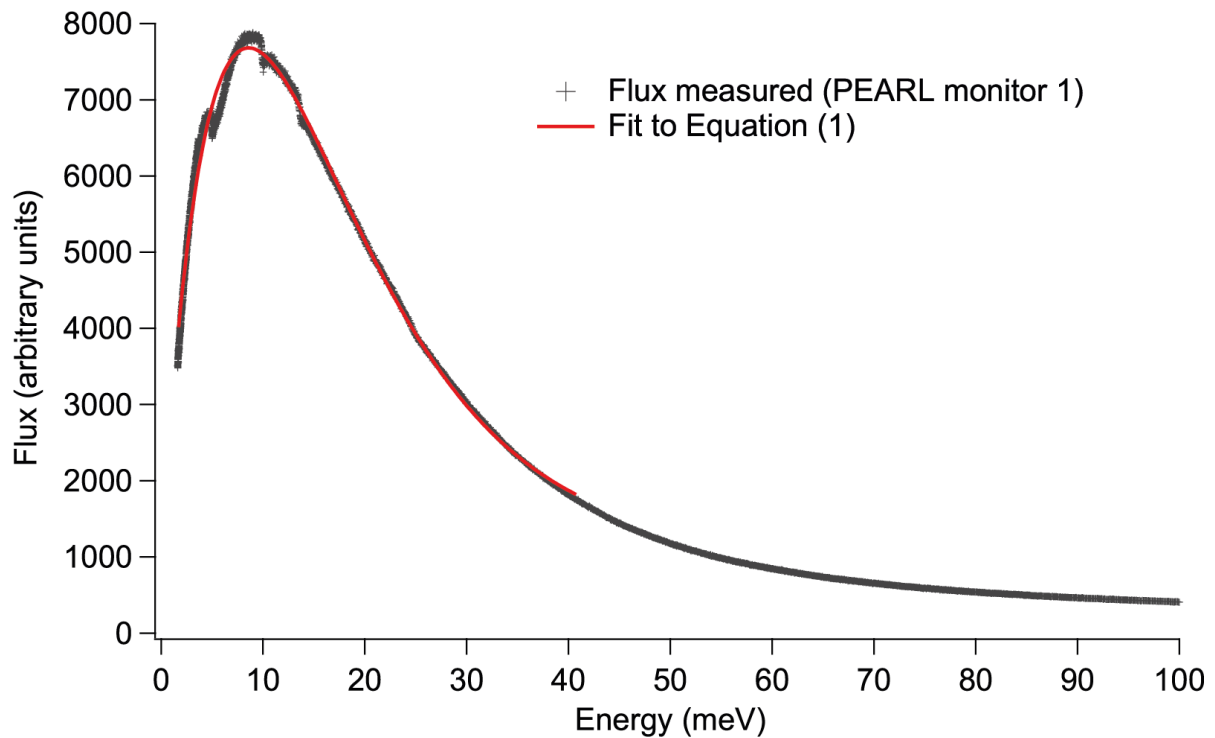


Figure 2: Data collected from the PEARL incident beam monitor, located approximately 11.13m downstream from the methane moderator, on port S9. The black markers are the measured data, normalised by bin-width, and the red line represents a scaled fit to Equation 1. The fit extends over the region of thermalised neutrons but is unable to match the epithermal regime. The resultant temperature from the fit is estimated to be 100 K.

Stability from cycles 15/2 → 21/1 (pre-TS1 project)

Quantifying changes in the overall pattern is non-trivial, though could be achieved through a series of convolutions, but a prime indicator of stability is the position of the peak in the Maxwellian distribution. This is highly sensitive to the overall temperature of the moderator, and to the composition of the methane moderator.

The fitting procedure is very simple. For each completed measurement on PEARL, the spectrum relating to the primary incident-beam monitor is loaded, and then the overall levels are normalised by proton beam-current. For robust positional information on the peak flux, the data are fitted in time-of-flight using a simple Gaussian peak shape. The process is automated, enabling the fitting of a large number of datasets. It should be noted here that these data represent measurements where the data acquisition software **isn't vetoing** on the temperature of the moderator. In other words, the methane moderator is believed to be delivering a stable output according to the thermometry. The fitting is performed within Mantid [7], the code for which is included in the Appendix.

To gain an historical understanding of the stability of the methane, all runs measured on PEARL between cycles 15/2 and 21/1 (inclusive) were reduced in this way. Totalling over 25,000 runs, the full dataset represents close to 3 million μ Amps of neutron data and is shown in Figure 3.

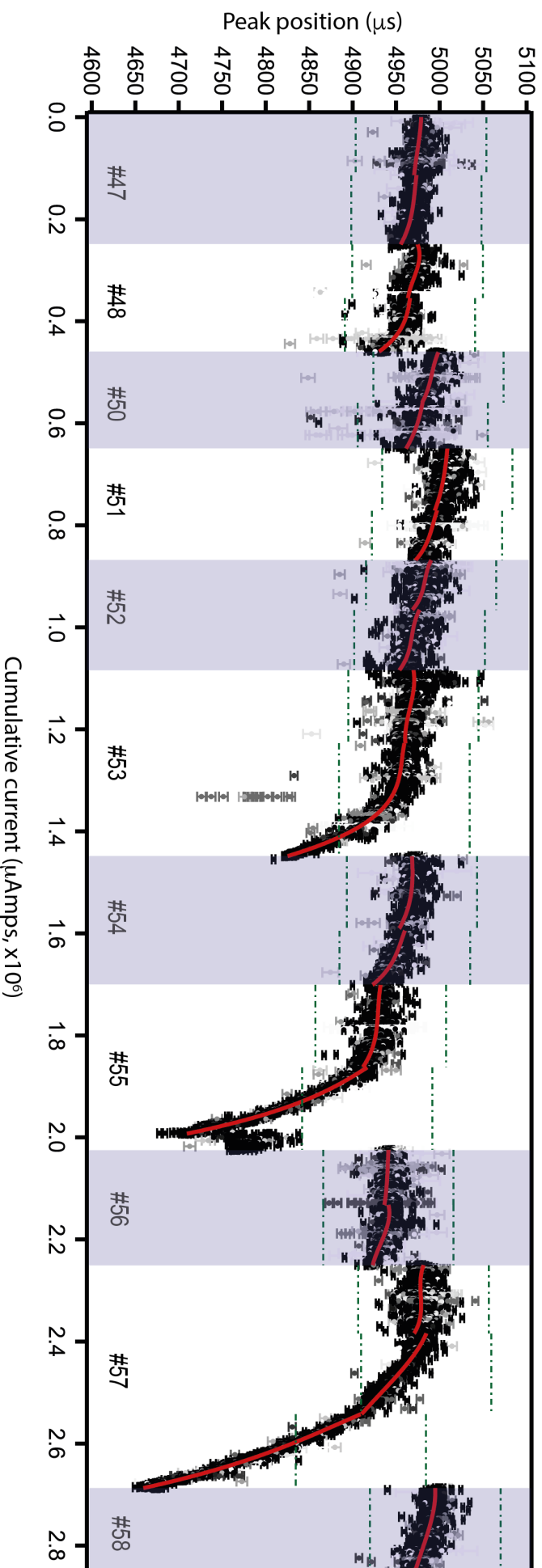


Figure 3: The position of peak-flux, in microseconds, as determined from the PEARL incident monitor data, as a function of cumulative current to the moderator. The data points represent the fitted values for each run, with the greyscale colouring representing the total number of μAmps delivered for that run; the darker the data-points the better the measured statistics on the monitor. The solid red line represents a weighted line of best fit to the data for each cycle, using a 4th-order polynomial. The horizontal, dashed-green lines represent the window of stability nominally accepted from the moderator within a $\pm 2\text{K}$ veto window through the data acquisition software; as the instruments are recalibrated at the start of the cycle, the absolute position of this window changes between cycles. The data are separated into blocks representing periods where the moderator has been replaced; the numbering of these blocks (47-58) is consistent with the numbering used by the ISIS Target Operations Group.

Rather than runs, or cycles, it now makes more sense to refer to the data in blocks referring to which moderator they were measured from (see numbering in Figure 3), as the effects of radiation damage are cumulative. In most cases, the moderator is delivering a consistent and stable output before replacement. As mentioned above, all of these data were collected within the veto limits according to the thermometry; the green dashed lines in Figure 3 represent the real window of stability represented by a +/-2 K drift in temperature. In all bar three moderators, the output sits comfortably within this window of stability. However, moderators 53, 55, and 57 show significant excursions outside this, while the temperature of the moderator was nominally within the veto limits. For moderator 57 the observed drift is equivalent to an increase in moderator temperature from 110 to 119 K.

Quantifying the impact of this magnitude of drift on the resultant science is very challenging. It is clear that the vanadium normalisation was to some extent invalid during these periods, though the extent of the error propagation is impossible to tell without data collected from well characterised standards at the start and end of the cycle. The diffractometers will not typically measure the vanadium standard more than once during a cycle, and so disentangling this systematic error from the measurements is impossible.

To better understand the observed drift in stability, the total number of μAmps delivered to each moderator can be considered, see Figure 4. Moderators 53, 55, and 57 received a significantly higher total beam current than the other moderators considered. The data from these three moderators suggest that an upper-critical total beam current before moderator degradation sits between 250,000 - 300,000 μAmps . This observation, with the fact that the output drifts towards higher energy, is consistent with what would be expected from a radiation-damaged moderator.

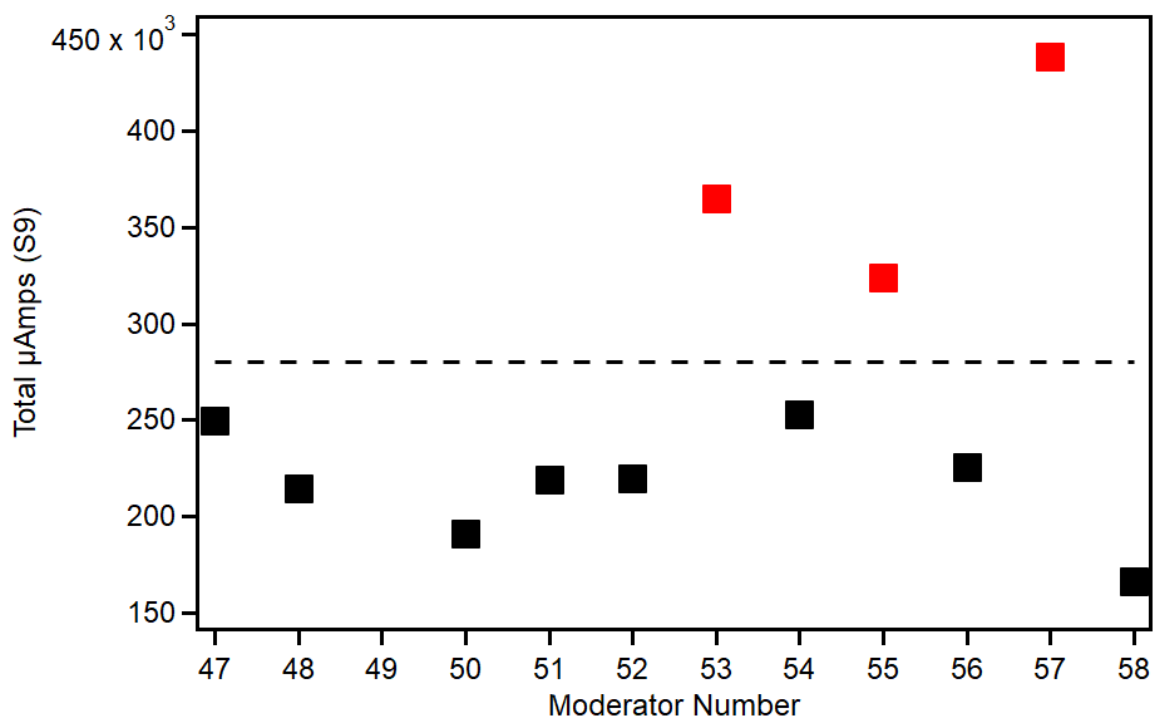


Figure 4: Total μAmps delivered to each of the methane moderators used in cycles 15/2 to 21/1 inclusive. Moderators 53, 55, 57 (marked in red) were found to have degraded significantly in performance, as discussed in the main text.

Cycles 23/1 onwards (post-TS1 project)

The first complete cycle post TS1 project was cycle 23/1. Performing a similar analysis to that done for previous cycles, the data from the monitors are shown in Figure 5. The estimated total beam current to moderator from cycle 23/1 to 23/4 (inclusive) is 225,000 μAmps . The moderator to this point is seen to behave stably, well within the expected stability window. A small step in peak output is observed after approximately 100,000 μAmps , between cycles 23/2 and 23/3; this is due to a change in the operating temperature of the moderator, from a base of 110 K up to 112 K. This was done to experiment with the stability of the ancillary equipment for recharging the moderator. The observed shift in output (approximately 45 μs), is consistent with what would be expected for a 2 K increase in temperature, according to Equation 1.

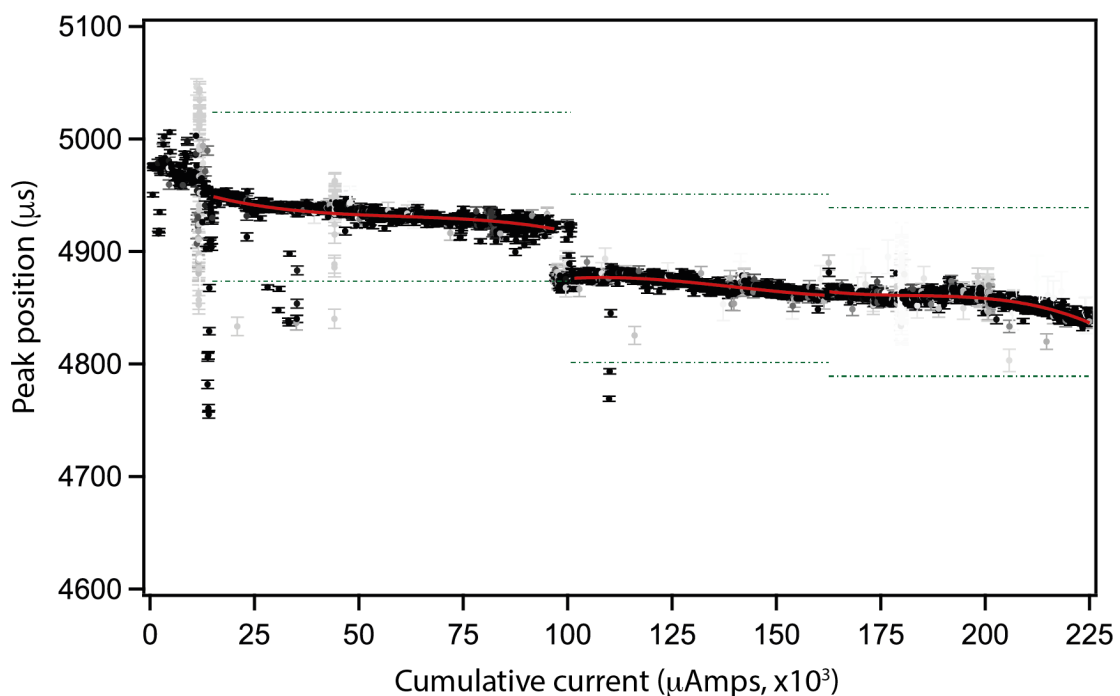


Figure 5: The position of peak-flux, in microseconds, as determined from the PEARL incident monitor data, as a function of cumulative current to the moderator. The data points represent the fitted values for each run, with the greyscale colouring representing the total number of μAmps delivered for that run; the darker the data-points the better the measured statistics on the monitor. The solid red line represents a weighted line of best fit to the data for each cycle, using a 4th-order polynomial. The horizontal, dashed-green lines represent the window of stability nominally accepted from the moderator within a $\pm 2\text{K}$ veto window through the data acquisition software; as the instruments are recalibrated at the start of the cycle, the absolute position of this window changes between cycles. All these data were collected from a single moderator. The first data points are from cycle 23/1, and these have not been fitted due to a limited number of data-points, and highly unstable methane temperatures. A few of the data points in the cycle 23/2 are clear outliers, as some were collected with the temperature veto turned off.

Discussion and future outlook

Analysis of pre-TS1 project data has shown that the stability of the old moderator system was largely acceptable, though on three occasions over this period the lifetime of the moderator was exceeded, and this resulted in large shifts in the peak output of the moderator. Retrospectively, it is extremely difficult to quantify the effects of these drifts on the measured diffraction data. It is, however, promising that we have demonstrated the sensitivity of PEARL's incident beam monitors to the effects of methane degradation under irradiation, and the fact that these data are collected in sequence with normal operation of the instrument, is a great strength.

Whether the addition of the water pre-moderator has had the desired effect of extending the lifetime of the moderator remains to be seen. Post cycle 23/4 the moderator has been changed, so it will take several further cycles of monitoring before any conclusions can be drawn.

While the above analysis has been used to find instabilities in the moderator retrospectively, it is interesting to consider whether this technique could be used for in-situ determination of stability fluctuations. This has potential to be used to determine, for example, the requirement for additional charge changes towards the end of the operational lifetime of the moderator, or to make other predictions on the overall health of the moderator based on the rate of change under prolonged irradiation. Figure 6 shows the changes in gradient of the fit to moderators 53, 55, and 57. All three moderators dipped outside of tolerance at a similar rate of degradation (between -1.0 and -1.2×10^{-3} s/A). This information could be a useful diagnostic for future moderator health and will be subject of further investigation.

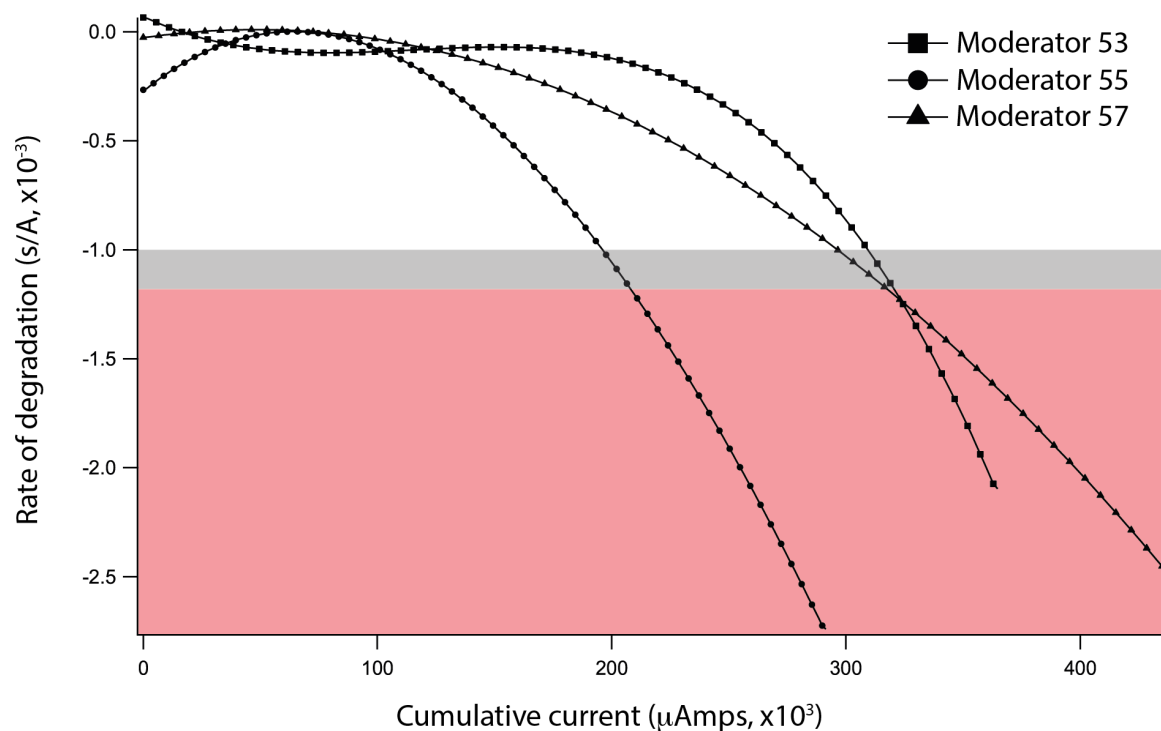


Figure 6: Rate of change of degradation as determined from differentiating the polynomial fit to the data shown in Figure 3, for moderators 53, 55, and 57. Each of the moderators in question fall outside of the tolerance window at a similar rate of degradation between -1.0 and -1.2×10^{-3} s/A (the grey shaded region). The rate of change in the red shaded region is outside the tolerance window for all three moderators.

Conclusion

PEARL's incident beam monitors have provided useful diagnostic insight into the stability of the liquid methane moderator on TS1. Analysis of close to 3 million μAmps of historical data has been performed to retrospectively inform on the health of the moderator. From this, an upper threshold of total beam current between 250,000 and 300,000 μAmps is suggested based on a ± 2 K window of tolerance on the moderator output. Note that this is based on the pre-TS1 project system, and further analysis of the post-TS1 project system with the inclusion of the water pre-moderator is required, though it is expected that this should extend the upper threshold, rather than reduce it.

The rate of change of degradation of the moderator at the point of exiting the tolerance window is found to be reproducible between the three failed moderators, at a rate between -1.0 and -1.2×10^{-3} s/A. Further work will be performed to understand how this could be used to inform future decision making regarding the operation of the moderator.

Data availability

The data used in this manuscript is freely available from the ISIS DataGateway (<https://data.isis.stfc.ac.uk/datagateway>) up to and including cycle 21/1. The data used for cycles 23/1 to 23/4 inclusive will be freely available after the initial embargo period of 3 years, as detailed in the ISIS data management policy (<https://www.isis.stfc.ac.uk/Pages/Data-Policy.aspx>).

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Appendix – Mantid script for data reduction

```
from mantid.simpleapi import *
import matplotlib.pyplot as plt
import numpy as np

Cycles2Run=['15_2', '15_3', '15_4', '16_1', '16_3', '16_4', '16_5', '17_1', '17_2', '17_3', '17_4', '18_1', '18_2','18_3', '18_4',
'19_1', '19_2', '19_3', '19_4', '20_2', '20_3', '21_1', '22_5', '23_1', '23_2', '23_3', '23_4']
Path2Save = r'C:\PathToSave'
Path2Data = r'X:\PathToData'
# Dictionary of cycle run numbers for PEARL
CycleDict = {
    "start_15_2": 90482,"end_15_2": 91528,
    "start_15_3": 91530,"end_15_3": 92430,
    "start_15_4": 92434,"end_15_4": 93402,
    "start_16_1": 93404,"end_16_1": 94515,
    "start_16_3": 94519,"end_16_3": 95629,
    "start_16_4": 95634,"end_16_4": 97530,
    "start_16_5": 97534,"end_16_5": 98469,
    "start_17_1": 98472,"end_17_1": 99474,
    "start_17_2": 99480,"end_17_2": 100574,
    "start_17_3": 100583,"end_17_3": 101505,
    "start_17_4": 101508,"end_17_4": 102939,
    "start_18_1": 102947,"end_18_1": 105079,
    "start_18_2": 105081,"end_18_2": 106253,
    "start_18_3": 106257,"end_18_3": 107151,
    "start_18_4": 107154,"end_18_4": 108579,
    "start_19_1": 108592,"end_19_1": 109798,
    "start_19_2": 109800,"end_19_2": 111030,
    "start_19_3": 111056,"end_19_3": 112080,
    "start_19_4": 112083,"end_19_4": 113280,
    "start_20_2": 113286,"end_20_2": 114296,
    "start_20_3": 114303,"end_20_3": 115227,
    "start_21_1": 115231,"end_21_1": 116442,
    "start_22_5": 116463,"end_22_5": 116478,
    "start_23_1": 116489,"end_23_1": 116646,
    "start_23_2": 116650,"end_23_2": 117456,
    "start_23_3": 117462,"end_23_3": 117960,
    "start_23_4": 117986,"end_23_4": 118728,
}
for cycle in Cycles2Run:
    reject=[]
    peak_centres=[]
    peak_centres_error=[]
    peak_intensity=[]
    peak_intensity_error=[]
    uAmps=[]
    RunNo=[]
    index=0
    start=CycleDict['start_'+cycle]
    end=CycleDict['end_'+cycle]

    for i in range(start,end+1):
        if i == 95382:
            continue
        Load(Filename=Path2Data+"\cycle_"+cycle+"\PEARL00'+ str(i)+
```

```

'.nxs', OutputWorkspace=str(i))
ws = mtd[str(i)]
run = ws.getRun()
pcharge = run.getProtonCharge()
if pcharge <1.0:
    reject.append(str(i))
    DeleteWorkspace(str(i))
    continue
NormaliseByCurrent(InputWorkspace=str(i), OutputWorkspace=str(i))
ExtractSingleSpectrum(InputWorkspace=str(i),WorkspaceIndex=index,
    OutputWorkspace=str(i)+ '_' + str(index))
CropWorkspace(InputWorkspace=str(i)+ '_' + str(index), Xmin=1100,
    Xmax=19990, OutputWorkspace=str(i)+ '_' + str(index))
DeleteWorkspace(str(i))
#Some constraints included to prevent divergence
fit_output = Fit(Function='name=Gaussian,Height=19.2327,\
    PeakCentre=4843.8,Sigma=1532.64,\
    constraints=(4600<PeakCentre<5200,1100<Sigma<1900);\
    name=FlatBackground,A0=16.6099,ties=(A0=16.6099)',
    InputWorkspace=str(i)+ '_' + str(index),
    MaxIterations=1000, CreateOutput=True,
    Output=str(i)+ '_' + str(index) + '_fit',
    OutputCompositeMembers=True,
    StartX=3800, EndX=6850, Normalise=True)
paramTable = fit_output.OutputParameters
#This catches some spectra where the alignment mirror
# was accidentally in place
if paramTable.column(1)[0] < 10.0:
    DeleteWorkspace(str(i)+'_0_fit_Parameters')
    DeleteWorkspace(str(i)+'_0_fit_Workspace')
    DeleteWorkspace(str(i)+'_0')
    DeleteWorkspace(str(i)+'_0_fit_NormalisedCovarianceMatrix')
    reject.append(str(i))
    continue
#This catches some fits where the fit constraints are ignored,
# allowing the peak to fall far outside the nominal range
if paramTable.column(1)[1] < 4600.0 or paramTable.column(1)[1] > 5200.0:
    DeleteWorkspace(str(i)+'_0_fit_Parameters')
    DeleteWorkspace(str(i)+'_0_fit_Workspace')
    DeleteWorkspace(str(i)+'_0')
    DeleteWorkspace(str(i)+'_0_fit_NormalisedCovarianceMatrix')
    reject.append(str(i))
    continue
else:
    uAmps.append(pcharge)
    peak_centres.append(paramTable.column(1)[1])
    peak_centres_error.append(paramTable.column(2)[1])
    peak_intensity.append(paramTable.column(1)[0])
    peak_intensity_error.append(paramTable.column(2)[0])
    RunNo.append(str(i))
    DeleteWorkspace(str(i)+'_0')
    DeleteWorkspace(str(i)+'_0_fit_Parameters')
    DeleteWorkspace(str(i)+'_0_fit_Workspace')
    DeleteWorkspace(str(i)+'_0_fit_NormalisedCovarianceMatrix')

combined_data=np.column_stack((RunNo, uAmps, peak_intensity,
    peak_intensity_error, peak_centres, peak_centres_error))
np.savetxt(Path2Save+'\peak_centres_'+cycle+'.csv',
    combined_data, delimiter=",", fmt='% s',

```