SAN FRANCISCO BAY NUTRIENT MANAGEMENT STRATEGY

Updates to Moored Sensor Program Calibration and Data QAQC Procedures

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Summary

The San Francisco Bay (SFB) Nutrient Management Strategy maintains an extensive array of *in situ* data sondes for water quality monitoring as a part of its Moored Sensor Program (MSP). This report describes new calibrations for three of these sonde types. It also documents a major procedural change for data storage and QAQC. In total, this report addresses four aspects of data processing:

1) **Correction of historical data collected by HydroCat multiparameter sondes**

The MSP maintains a network of multiparameter sondes that collect high-frequency (15 min) continuous monitoring data of several key water quality parameters in SFB. Historically, the primary multiparameter sonde used by the MSP has been the YSI EXO 2, a high-quality instrument that is also used by the United States Geological Survey (USGS) for water quality monitoring in the SFB-Delta region. However, from Jan 2018 – August 2022 the MSP piloted the deployment of SeaBird HydroCat (HC) sondes at the San Mateo Bridge (SM) and Coyote Creek (COY) monitoring sites. After several years of deployment, the HC sondes were judged to be less reliable than the EXOs, leading to their retirement. In this report, we describe a set of two side-by-side deployments between a HC and EXO 2 at SM and COY. From these deployments, we created a series of calibrations that we used to correct past HC chl *a* and turbidity data for better comparison with EXO 2 data.

2) **Calibration of SUNA V2 NO_x data**

Another data sonde maintained by the MSP is the SeaBird SUNA V2 nitrate + nitrite (NO_x) sensor. The MSP currently has SUNA V2s deployed at three locations – Dumbarton Bridge (DMB), Shoal (SHL), and Alviso Slough (ALV). Throughout its deployment at SHL (Aug 2020-present) the MSP has been collecting discrete NO_x samples for comparison with SUNA values. In this report, we describe a calibration of SUNA data based on these discrete samples.

3) **Deployment of StarODDI salinity sensors for calibration of miniDOT DO sensors**

Beginning in Sep 2021, PME miniDOT (MD) DO sensors were added near the mouths of Alviso and Guadalupe Sloughs for better DO monitoring in Lower South Bay (LSB) sloughs. These sensors measure DO percent saturation and water temperature (T). Importantly, they do not measure salinity (S), which along with T, is required to accurately convert DO percent saturation to DO mass concentration (e.g. mg L^{-1}). S at the MD locations varies widely over the tidal cycle, so choosing a single value for S introduces substantial uncertainty when calculating DO mass concentration. To address this concern, beginning in April 2023 Star-ODDI S sensors were co-deployed with MDs at Alviso and Guadalupe. In this report, we describe the Star-ODDI data pipeline and how these data are used to convert DO percent saturation to mass concentration. We also describe an S correction based on nearby EXO 2 data for the period before the Star-ODDIs were deployed.

4) **Shift to Aquarius software for QAQC**

Historically, the MSP has used Python scripts developed in-house for QAQC of MSP data, with master data files stored in .CSV format on SFEI servers. To manage the growth of datasets resulting from site expansion and the addition of telemetry, in 2024 the MSP transitioned EXO 2 data QAQC and storage to the Aquatic Informatics Aquarius platform. Aquarius was designed for high-frequency environmental data from programs like the MSP, promoting more streamlined data QAQC and better fidelity of stored data. This section of the report describes the transition to Aquarius and the resultant changes in QAQC procedure and data storage.

1. Introduction

The Moored Sensor Program (MSP) is a Nutrient Management Strategy (NMS) funded effort to monitor water quality in San Francisco Bay (SFB) using continuously recording high frequency (15 min) moored sensors. The MSP sensor array consists of 13 primary sites, 2 secondary sites, and 3 retired sites deployed throughout the Central, South, and Lower South Bay sub-embayments (Fig. 1; Montgomery et al. 2025). All 13 primary sites and 2 of the retired sites utilize YSI EXO 2 sondes, which continuously record a suite of water quality parameters including dissolved oxygen (DO), chlorophyll *a* (chl *a*), turbidity, salinity, temperature, and dissolved organic matter. The 2 secondary sites utilize PME miniDOT (MD) DO sensors. At three of the primary sites (Dumbarton Bridge – DMB, Alviso Slough – ALV, and Shoal – SHL), Seabird SUNA V2 nitrate + nitrite (NO_x) sensors are also deployed.

The YSI EXO 2 is the only multiparameter sonde currently utilized by the MSP. However, Seabird (SBE) HydroCat (HC) multiparameter sondes were previously deployed in place of EXO 2s at the Coyote Creek (COY) and the San Mateo Bridge (SM) stations from Jan 2018 – July 2020 and Jan 2018 – Aug 2022, respectively. During these deployments, the HCs were judged to be less accurate and reliable than EXO 2s based on comparisons with discrete samples, leading to their retirement. Of particular concern were chlorophyll *a* (chl *a*) values, which were consistently lower at HC locations than at nearby EXO 2 locations, and turbidity, which the HC measures with a different unit (Nephelometric Turbidity Unit - NTU) than the EXO 2 (Formazin Nephelometric Unit – FNU). Early in their deployment, the HCs at both COY and SM were co-deployed with EXO 2s to test agreement between these sensors. In this report, we describe a correction for HC chl *a* and turbidity data based on these past co-deployments. This correction represents a one-time calibration of historical HC-collected data. Correcting HC data allows for better comparison of chl *a* and turbidity data at SM and COY to other stations and time periods. Please note that we evaluated the other parameters collected by the HC (dissolved oxygen, temperature, salinity), and found sufficient agreement with EXO values such that no further correction of these data is necessary.

The SUNA V2 is a state-of-the-art sensor for continuous *in situ* measurements of NO_x. It works by calculating the strength of the absorption of ultraviolet light along a spectral range associated with the presence of water column NO_x (Johnson and Coletti 2002). However, different dissolved compounds such as bromide can interfere with this absorption signal, and site-specific calibrations of SUNA measurements with discrete samples of NO_x are often needed. The MSP currently has SUNAs deployed at DMB (Jan 2021-present), ALV (Oct 2023-present), and SHL (Aug 2020-present). Discrete water quality samples have been collected at SHL since 2018 and at ALV and DMB since 2023. In this report, we detail a new correction for SUNA data that accounts for the calibration of SUNA measurements with discrete values of NO_x.

In Sep 2021, MDs were added near the mouth of Alviso (ALV DO) and Guadalupe (GUAD DO) sloughs to augment DO monitoring in the Lower South Bay (Fig. 1). MDs measure DO percent saturation and water temperature (T). However, both T and salinity (S) are needed to accurately convert DO percent saturation to DO mass concentration [mg L^{-1}]. When offloading DO data the MD software asks for a single S value that is applied to an entire deployment. As Alviso and Guadalupe Sloughs experience large tidal ranges in S, using a single value over a month-long deployment is not adequate for accurate DO mass concentration estimates. To ameliorate this concern, the MSP purchased Star-ODDI S sensors for co-deployment with MDs at ALV DO and GUAD DO. The addition of Star-ODDIs allows for an accurate

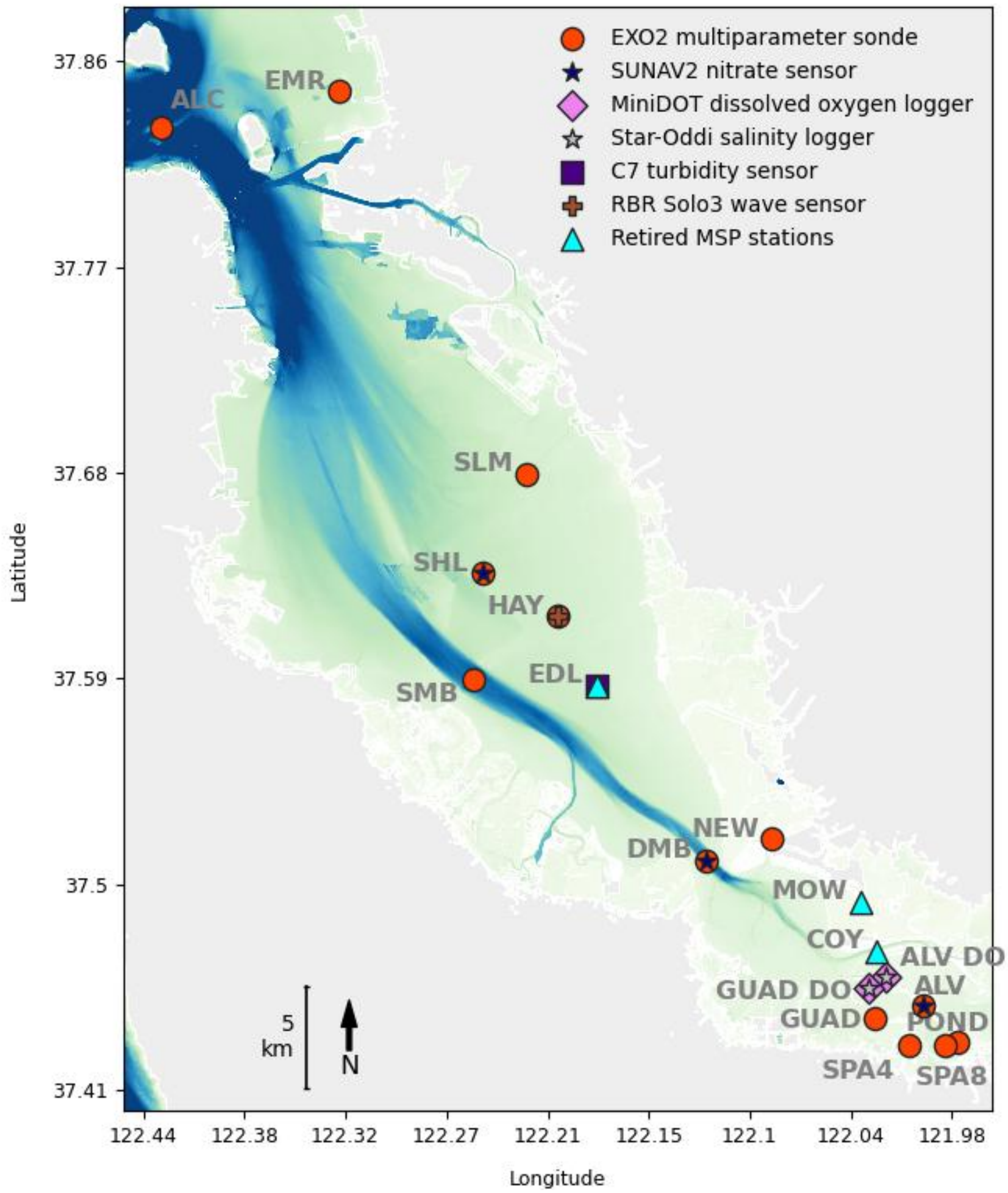

Figure 1 - Map of FY24 MSP water quality sites and instrument types, including YSI EXO 2 multiparameter sondes, SUNA V2 NO_x sensors, PME miniDOT DO sensors, and Star-ODDI salinity sensors. Seabird (SBE) HydroCat multiparameter sondes were deployed in place of EXO 2s at Coyote Creek (COY) and the San Mateo Bridge (SM) from Jan 2018 – July 2020 and Jan 2018 – Aug 2022, respectively.

salinity correction for DO concentration estimates at the 15 min measurement frequency of the MDs. In this report, we describe the deployment of new Star-ODDI S sensors and their QAQC procedure. We also detail a new level of MD data that includes an S correction.

Prior to Oct 2024, data collected by the MSP underwent a rigorous QAQC procedure whereby data was processed through various hierarchical levels (L0-> L1 -> L2, etc). The precise number of data levels depended on the instrument, but for all sondes the lowest data level L0 represents collated raw (untreated) data, while the highest level (L1, L2 or L3) is what the MSP recommended for data visualization and scientific analysis. The QAQC pipelines for each instrument were run using a series of Python scripts created and maintained by SFEI. The scripts became so extensive that only experienced coders could manipulate the code, while the procedures in place were extremely time consuming for MSP staff. Additionally, master data copies were stored as .CSV files that were constantly overwritten, resulting in poor data fidelity and limited reproducibility of past file versions. To address these concerns and streamline data QAQC, in Oct 2024 the MSP began using the Aquarius data management software suite. In this report, we detail the transition from Python scripts and .CSV data storage to use of Aquarius, and describe new MSP QAQC procedures.

In summary, the purpose of this report is to document four changes to the calibrations and QAQC of MSP sondes (affected sites shown in parentheses):

1. Correction of past SBE HC data using calibrations derived from side-by-side deployments with YSI EXO 2 sondes (SM and COY).
2. Creation of L3 data level for SUNA V2 NO_x that incorporates calibration of field results with discrete NO_x samples (SHL, DMB, ALV).
3. Co-deployment of Star-ODDI salinity sensors with PME MD DO sensors at Alviso and Guadalupe Sloughs and creation of a new L3 data level for MD data that includes a salinity correction (ALV DO, GUAD DO).
4. Change in QAQC and storage of EXO 2 and SUNA data from tiered data levels (L0, L1, etc.) and in-house Python scripts to use of Aquarius data software (all sites).

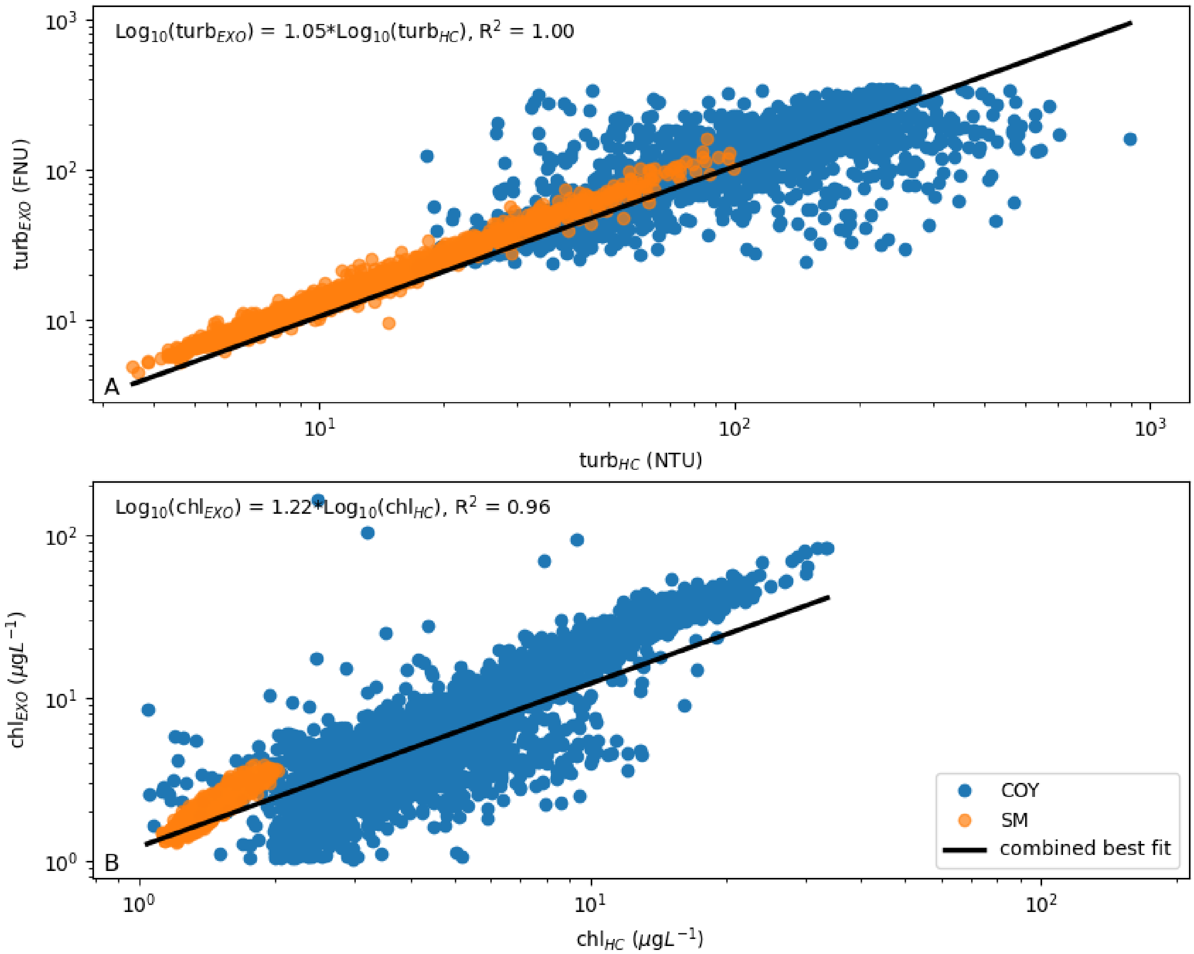

Figure 2 - Best fit relationships between EXO and HC for turbidity and chl *a* measurements.

2. Calibration development and changes to data QAQC

2.1 HydroCat and EXO 2 co-deployment

Co-deployments between an EXO and HC took place from Jan 23 - Feb 18, 2018 and Nov 30, 2018 – Jan 31, 2019 at SM and COY, respectively. Values of chl *a* and turbidity tended to be substantially higher at COY than SM. At both sites, chl *a* measured by the EXO tended to be greater than that measured by the HC, while turbidity measurements were more variable. Please note that data at SM were affected by significant fouling after Feb 7, 2018, so these data were omitted from the calibration.

Given that the sondes at COY collected far more data during the calibration period than at SM, COY and SM datasets were merged to create one global calibration for each scalar to ensure a sufficient range of calibration values for both sites. This calibration was created using a least squares linear fit to the log_{10}-log_{10} transformed data in the script 'HC_perform_correction.py'. The final calibration curves are shown in Fig. 2. The best fit relationship for turbidity was: $log_{10}(turb_{EXO}) = 1.05 * log_{10}(turb_{HC})$ (R^2 = 1.00). The best fit relationship for chl *a* was: $log_{10}(chl_{EXO}) = 1.22 * log_{10}(chl_{HC})$ (R^2 = 0.96). A time series showing example EXO data plotted against both raw and corrected HC data is depicted in Fig 5. For this figure please note the different y-axis scales between the two sites, particularly for chl *a.*

All chl *a* and turbidity data collected by the HC COY and SM have undergone a one-time change performed on the historical L3 data. When re-transforming values from log-log space we applied a bias correction factor (BCF) as described by Volaric et al. (2025). These data have been imported into Aquarius and merged with EXO measurements in the appropriate datasets. Original, unaltered HC data remain in Aquarius as "historic raw". Although we did not identify any other issues with data collected by the HC, if future SFEI staff wish to calibrate additional parameters we recommend that these new calibrations be added to the script 'HC_perform_correction.py', and the resultant datasets uploaded to Aquarius

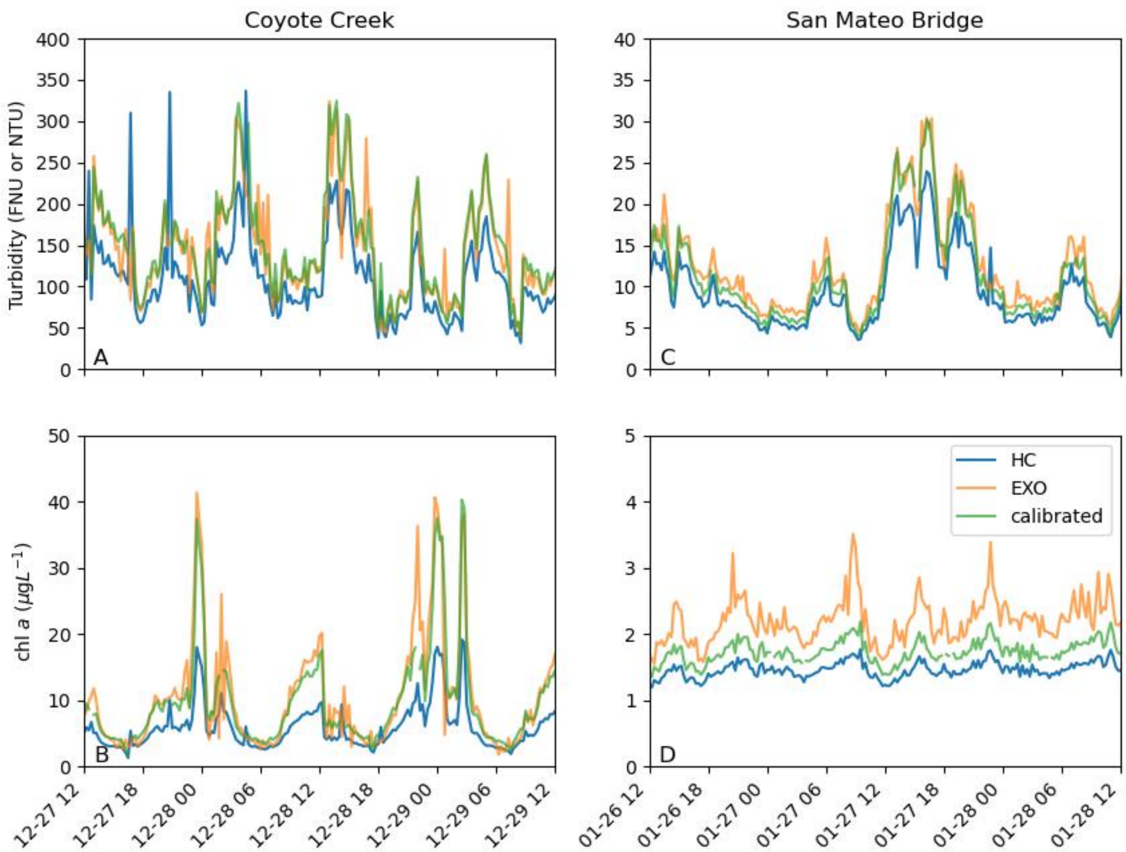

Figure 3 - Time series of turbidity and chl *a* measured by EXO and HC at SM and COY stations during test deployments. Both turbidity and chl *a* tended to be greater as measured by the EXO vs. the HC. Turbidity is in FNU for the EXO and NTU for the HC.

2.2 Discrete NO_x sampling

Calibration of SUNA data from discrete samples occurs in the Python script 'SUNA_Processing_AQI.py', which will also eventually be used to prepare the data for import into Aquarius. This script imports T+S corrected SUNA data (described in Art and Mourier 2022) and the discrete sample results from the SHL site. A least squares linear fit is performed between the discrete data and the T+S corrected SUNA data with the same time stamps as the discrete results (15 min resolution). For this best fit, outlier datapoints (defined as those with absolute residual values greater than twice the standard deviation) are removed.

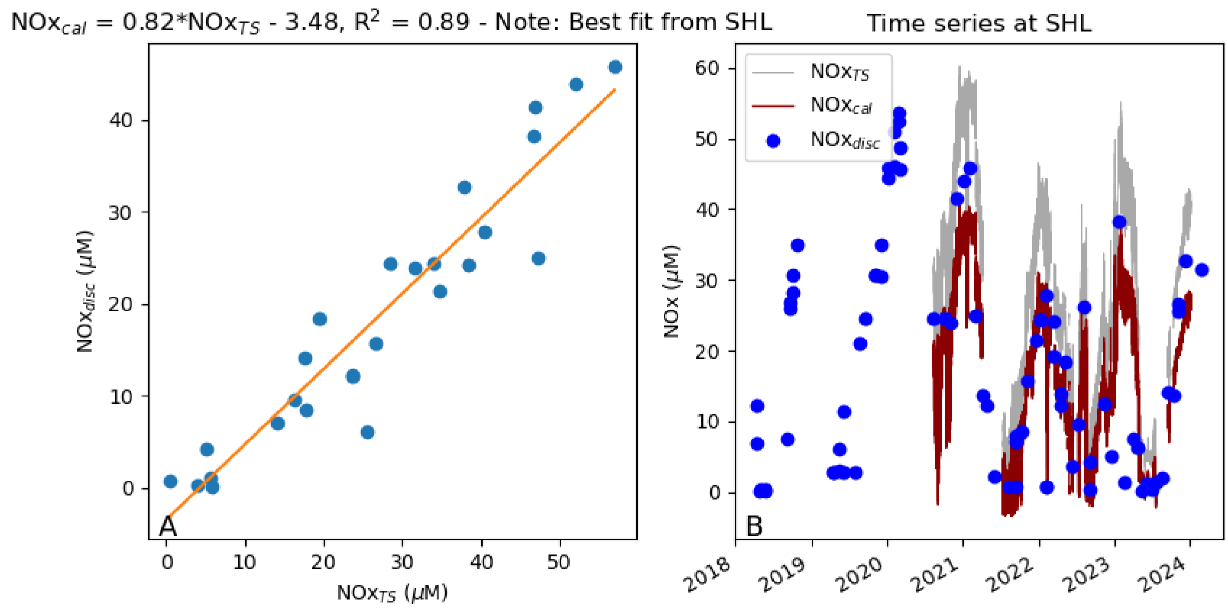

Figure 4 – (A) Best fit discrete vs. T/S corrected SUNA data relationship, used to calculate final NO_x data for Aquarius import. (B) Time series depicting NO_x concentration from discrete samples (NOx_{disc}), T and S corrected SUNA data (NOx_{TS}), and final calibrated SUNA data (NOx_{cal}).

At the time of this report, there are not sufficient discrete NO_x samples at either DMB or ALV for an accurate calibration, so the calibration for SHL is used to correct SUNA data at all three sites. Once there are more than 10 discrete samples at DMB and ALV, this methodology will be revisited, and either site-specific calibrations will be developed or data from all sites will be grouped to define a global calibration. Following this one-time calibration of historic DMB and ALV data, further updates to SUNA calibrations resulting from ongoing discrete sample collection will not be applied retroactively so as not to alter historical data. In other words, after this one-time calibration, newer SUNA data may undergo a slightly different discrete sample calibration than older data as more discrete samples are collected.

The current relationship for calibrated NO_x (NOx_{cal}) based on T+S corrected SUNA data (NOx_{TS}) as of this report is: $NOx_{cal} = 0.82 * NOx_{TS} - 3.48$. This best fit relationship, as well as time series of the various NO_x data at SHL, are depicted in Fig. 4. The resultant data from this script are saved in the file "[site]_[date]_AQI.csv"

2.3 Star-ODDI salinity sensors and miniDOT DO correction

MD deployment began in September 2021, while Star-ODDI S sensors were first deployed in April 2023. This means that there are nearly two years of MD data without 15 min S data. Once deployed, Star-ODDI sensors were attached to the same structure as the MDs so that both instruments sample the same volume of water.

We developed a two-tiered (L0, L1) QAQC pipeline for Star-ODDI S data, run using the Python scripts "Process_StarODDI_L0.py" and "Process_StarODDI_L1.py". The L0 script reads in the raw salinity data from an individual deployment and collates it with pre-existing L0 data in a file named "[site]_SO_L0.csv". "Process_StarODDI_L1.py" removes all data with S < 0.05 PSU, as it assumed these are periods in which the Star-ODDI is out of the water. This script also imports the Excel file "StarODDI_QAQC_Remove.xlsx", which contains user-defined periods of bad data, removing data from

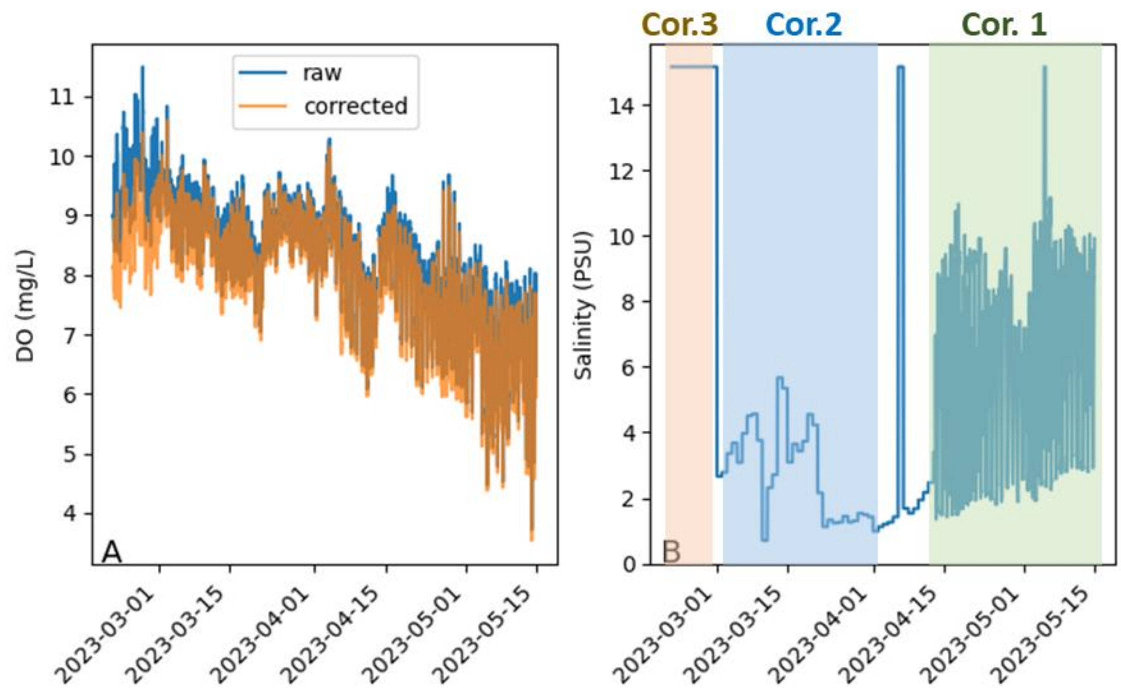

Figure 5 - Example miniDOT data from Guad station showing all three corrections applied to raw DO data (which assumes S = 0). Correction 1 uses 15 min Star ODDI salinity data. Correction 2 applies the daily mean S measured by the nearest EXO 2 sonde. Correction 3 applies the mean S measured over the entire Star ODDI deployment.

the L1 dataset during these times. The script then saves the updated L1 dataset under the file name "[site]_SO_L1.csv".

Calculation of DO in mg/L, corrected for S, occurs in the new script "Process_MiniDOT_L3.py", which creates a new L3 tier for MD data. This process follows the methodology detailed in Staehr et al. (2010). First, we calculate the concentration in mg L^{-1} of the 100% saturation concentration of DO (DO_{sat_mgl}):

$$DO_{sat\_mgl} = e^{C} * 1.423 \qquad \mathbf{1}$$

where C is a constant based on T [°K] and S [PSU]:

$$C = -173.492 + 249.6339 * \frac{100}{T} + 143.3483 * ln\ ln\left(\frac{T}{100}\right) - 21.8492 * \frac{T}{100} + S * \left(-0.033096 + 0.014259 * \frac{T}{100} - 0.0017000 * \left(\frac{T}{100}\right)^{2}\right. \qquad \mathbf{2}$$

DO in mg L^{-1} (DO_{mgL}) is calculated from DO_{sat_mgl} and the percent saturation measured by the MD ($MD_{\%sat}$):

$$DO_{mgL} = DO_{sat\_mgL} * MD_{\%sat} \qquad \mathbf{3}$$

S is defined in three different ways depending on the availability of Star-ODDI and/or EXO 2 data. When Star-ODDI data are available, S is defined as the temporally nearest Star-ODDI L1 datapoint (Correction 1). For times with no Star-ODDI data but with EXO 2 data, such as most periods before Star-ODDI deployment, S is defined as the daily average of the nearest EXO 2 sonde (Fig. 1) (Correction 2). For times with no Star-ODDI nor EXO 2 data, S is defined as the mean of the entire Star-ODDI dataset (Correction 3). Correction 3 occurs relatively rarely, approximately 10% of the time at both GUAD and ALV. While this is a rough estimate, it is more accurate than assuming S = 0 for the calculation of DO concentration from percent saturation. Raw and corrected DO data from GUAD DO, calculated using all three estimates of S, are depicted in Fig. 5.

Data level	Script	Actions
L0	Automated script	• Converts raw output files from instruments to CSV format with standardized column headers
L1	Automated script	• Removes data that fall outside set maximum and minimum thresholds for individual parameters • Removes data points that fall outside three standard deviations from the mean of a two-hour window centered around the point of interest • Removes data when instruments are out of water
L2	Automated script	• Removes data when sensor depth is < 0.5 meters • Re-enters data during periods of heavy freshwater inflow
L3	Manual	• Removes remaining false data that have been identified through manual review by an NMS team member, including that associated with sensor fouling • Re-enters data that were identified manually by an NMS team member as real but had been removed during automated processing

Table 1 - EXO 2 data QAQC steps prior to October 2024.

2.4 Aquarius QAQC procedures and data transition

After MSP data is collected, it undergoes several steps of QAQC before being considered finalized and ready for use in analyses and models. The QAQC steps involve both automated and manual assessment by MSP staff. Prior to October 2024, EXO 2 data was processed through a series of Python scripts that stitched the raw data files together, removed outliers, and performed other QAQC procedures. The previous QAQC steps for the EXO 2 data are outlined below in Table 1.

In October 2024, the MSP moved EXO 2 data QAQC and storage to a new quality control pipeline utilizing Aquarius environmental data management software. This software is also used by the US Geological Survey for data quality control and visualization. The transition to this platform allows the QAQC steps to be followed in a trackable way, with the advantage of automatically applied metadata, version control, and an interactive dashboard visualizing all applied data changes. The Aquarius platform keeps records of manual edits such as spike and biofouling removals, as well as offset corrections. To advance the metadata collection within the QAQC process further, we have implemented additional procedures such as adding notes and grades to the data within the software. Aquarius will eventually be the primary data repository of master copies for all water quality sonde data, with backups on Google Drive.

Raw EXO 2 data files are currently manually imported into Aquarius, however our goal is to soon import data using a Python script. Similar to the Python QAQC procedures, at least two staff members will review data before it is considered finalized in the updated Aquarius QAQC procedures. Table 2 describes the new Aquarius-based hierarchical levels of EXO 2 QAQC data review.

One difference between Aquarius and prior QAQC procedures is that the automated data removals for the EXO 2 data have been discontinued. Previously, L1 and L2 data that had automatically been removed were later found to be of acceptable quality and were added back in. To avoid this inefficient process, all data removals will now occur manually.

3. Implementation and future workflow

All new scripts and workflows mentioned in this report are now being used by the MSP team. As stated above, the chl *a* and turbidity corrections for HC data have already been performed. If in the future further corrections are deemed necessary for different HC parameters (e.g. DO, fDOM, S, etc.), they will be straightforward to calculate using the “HC_perform_correction.py” script. The results can then be uploaded and merged with the appropriate dataset in Aquarius.

The ‘SUNA_Processing_AQI.py’ script automatically updates the discrete calibration for nitrate at the SHL site as more discrete samples are collected. Although the calibration only considers discrete samples collected at SHL, once more discrete samples have been collected from DMB and ALV, this calibration should be revisited. Either DMB and ALV calibrations should be changed to site-specific discrete samples, or if all three sites have sufficiently equivalent calibration curves, all discrete samples should be grouped to create a global calibration across all sites.

Standard QAQC procedures for the miniDOTs will include processing Star-ODDI data to the L1 level before MD data is pushed to the L3 level. “Process_MiniDOT_L3.py” automatically uses EXO 2 or mean Star-ODDI S data to fill in gaps with no L1 Star-ODDI data, so if this script is run before Star-ODDI data has been fully processed, DO values will change once Star-ODDI QAQC has been completed. Another important note is that ‘Process_StarODDI_L0.py’ assumes the raw Star-ODDI data is stored in Excel files (.xlsx), so all data from these sensors should be offloaded in this format.

The transition of QAQC procedures for EXO 2 data to Aquarius has been successfully completed by the MSP. We are capitalizing on unique Aquarius features such as adding notes for each individual data point or time period, grading the quality of data, and documenting the level of QAQC to create a more robust and transparent QAQC process. Aquarius has the added benefit of being a secure data repository on a cloud-based server maintained outside of SFEI. In the future, we plan to add SUNA, MD, and StarODDI data to Aquarius to create a complete data repository for all MSP water quality datasets, although as of the time of this report these data are processed in Python as detailed above. The MSP also maintains three telemetered stations (SM, SLM, SHL) that retrieve sonde data throughout the day. These real-time data will eventually be automatically imported into Aquarius. Aquarius may also be used to store data not collected by MSP, such as USGS and NOAA data used in SFEI projects.

The MSP is constantly updating QAQC protocols to produce the highest quality data to allow for the synthesis and analysis of SFB water quality trends. In this report we detail four changes to our QAQC protocol to ensure that the data we use and share with regional partners is as accurate as possible.

Data level	Script	Actions
Raw	Semi-automated script and Aquarius data import	● Removes data on either end of the data file when the instrument was not in situ by using field note time stamps and a graph to manually correct the removal periods ● Interpolates data to the nearest 15-min interval ● Converts raw output files from instruments to CSV format with standardized column headers ● Confirms automated upload of data into Aquarius was successful
First + Second Review	Manual; two intermediate reviews	● Removes data points that are visually observed as irregularly spiky or fouled ● Removes data for periods when the instrument was out of water during deployment ● Applies drift corrections and offset corrections when identified ● Applies grades to low-quality data ● Applies Approval levels of ‘First Review’ and ‘Second Review’
Approved	Manual; final review	● Completed by senior level staff. Provides final data review and guidance on periods with irregular data identified during earlier review. ● Confirms drift correction and offset corrections completed accurately ● Applies Approval level of ‘Approved’ indicating finalized data

Table 2 - EXO 2 data QAQC steps post October 2024 using Aquarius.

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