Bottle-calibrated dissolved oxygen profiles from yearly turn-around cruises for the Ocean Observations Initiative (OOI) Irminger Sea Array 2014 – 2022

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Project
» Collaborative Research: The Annual Cycle of the Biological Carbon Pump in the Subpolar North Atlantic (OOI Irminger BCP)

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Abstract
This dataset contains bottle-calibrated dissolved oxygen (DO) profiles collected from Conductivity Temperature Depth (CTD) casts on turn-around cruises performed yearly to maintain the Ocean Observations Initiative (OOI) Global Irminger Sea Array (60.46°N, 38.44°W). DO profiles were used in conjunction with oxygen bottle measurements (Winklers) to produce a post-cruise oxygen-calibrated CTD product for scientific use. Bottle-calibrated CTD salinity products were used to produce post-cruise oxygen-calibrated CTD profiles starting in 2018 (Year 5). This document contains overviews of CTD data collection and processing and post-processing oxygen sensor calibration method. Reports for each cruise include a summary of relevant cruise events, oxygen sensor calibration results, and issues/problems associated with oxygen data collected on each cruise. This dataset has been created for end-users that require field-calibrated oxygen data products that are currently not provided by OOI through its standard data dissemination.

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Coverage

Spatial Extent: **N**:62.7715 **E**:-28.6567 **S**:41.5838 **W**:-69.3613
Temporal Extent: 2014-09-08

Dataset Description

The Ocean Observatories Initiative (OOI) is a long-term NSF-funded program that deploys autonomous sensors on both moored and mobile platforms at multiple locations, including the Global Irminger Sea Array

(60.46°N, 38.44°W) (Trowbridge et al., 2019). The OOI program conducts yearly turn-around cruises to the Irminger Sea Array to recover and redeploy moorings and gliders deployed year-round at this site. During these cruises the OOI program routinely conducts Conductivity Temperature Depth (CTD) casts and collects water samples from Niskin bottles on the CTD rosette for discrete sample analysis. These turn-around cruise data are critical for validation and calibration of the data from sensors deployed year-round and also provide a valuable dataset in and of themselves (Palevsky et al., 2023).

The complete collection of shipboard data and cruise documentation from these cruises is available from an OOI-managed document storage system called Alfresco (see related publications, cruise data), following the path: OOI > Global Irminger Sea Array > Cruise Data > {Cruise ID}. This dataset uses CTD data collected by the OOI program during the first 9 turn-around cruises of the Irminger Sea Array, alongside supplementary samples collected for this project during the AR30-03 and AR35-05 cruises (see related dataset Palevsky et al., 2023) to produce calibrated, quality-controlled oxygen depth profiles.

Methods & Sampling

CTD casts were performed using a ship-provided SeaBird 911plus CTD and deck unit configured to measure pressure, temperature, conductivity, oxygen current, and other variables. Rosettes were equipped with primary and secondary pumped CTD sensor packages to measure pressure, temperature, and conductivity in duplicate. A SBE43 dissolved oxygen sensor was integrated into the pumped flow path of the primary CTD sensor package. During AR35-05 (Year 6; August 2019) and AR46 (Year 7; August 2020), Aanderaa oxygen optodes were also integrated into the CTD rosette due to issues with the SBE43 (2019) and circumstances interfering with routine discrete sample collection and analysis (2019 and 2020), described in greater detail under “Problems/Issues”. Sensor data were acquired by an SBE Deck Unit providing demodulated data to a personal computer running SEASAVE acquisition software. Calibrations for CTD sensors were performed by the manufacturer before the cruise.

Data Processing Description

SeaBird processing

CTD data are processed using SeaBird data processing software. The raw 24 Hz CTD data are converted from HEX to ASCII, lag corrected, edited for large spikes, smoothed according to sensor, and pressure averaged for final data quality control and analysis. Table 1 summarizes the order in which SeaBird Modules were processed and the inputs applied during each module.

- DATCNV: Convert the raw data (.hex) to pressure, temperature, conductivity, and dissolved oxygen (V) to a file with a .cnv extension. Use default hysteresis correction
- BOTTLESUM: Writes out a summary of the bottle data to a file with a .btl extension
- ALIGNCTD: Advance Oxygen raw [V] by time determined by processing relative to pressure
- WILDEDIT: Checks for and marks ‘wild’ data points: first pass 2.0 standard deviations; second pass 20 standard deviations
- CELLTM: Conductivity cell thermal mass correction; alpha = 0.03 and 1/beta = 7.0
- FILTER: Low pass filter pressure and depth (DO [V]) with a time constant of 0.15 seconds to increase pressure resolution for LOOPEDIT
- LOOPEDIT: Mark scans where the CTD is moving less than the minimum velocity (0.25 m/s) or traveling backward due to ship roll.
- BINAVG: Average data into 1 or 2 db pressure bins to match bottle-calibrated salinity files (when available)
- SPLIT (u or d): Split .cnv file into upcast and downcast files. Files are appended automatically with leading u or d

Post-processing SBE oxygen calibrations

To produce the best possible oxygen measurements, post-processing procedures were modeled after methods described in Uchida et al. 2010. The following Seabird-recommended calibration equation was used to calibrate the SBE-43 oxygen sensor data:

O2= SOC(V+ Voff)* Oxysol(T,S)*(1 + A*T + B*T2 + C*T3) * eE*p/(273.15 +T) (Equation 1) where O2 is the CTD oxygen [µmol/kg], V is the output voltage signal processed with the SBE default hysteresis correction [volts], Oxysol is the oxygen saturation [µmol/kg], T is temperature [deg C], S is salinity [psu], and P is pressure [dbar] (SBE Application Note 64-2). Coefficients for the oxygen calibration slope (SOC); voltage offset at 0 (Voff); temperature-related calibration coefficients of A, B and C; and pressure-related E term were determined initially from an 18-point factory calibration and provided by the manufacturer (Appendix A). Voff, A, B, and C are constant over the sensor life while values for SOC and E can be optimized using discrete water samples measured analytically for dissolved oxygen, and commonly referred to as Winklers.

Calibration coefficients for SOC and E were optimized by applying a non-linear least-squares fit to Winkler samples while calibration coefficients for A, B, C, and Voff were held constant. Oxygen sensor hysteresis due to pressure effects on the sensor membrane was improved by enabling the Seabird default hysteresis correction (Edwards et al. 2010; SBE Application Note 64-3). The optional response time correction, or tau correction, was determined to add excessive signal noise in relatively stable, deep portions of the water column; and, therefore, was not applied in the calibration equation.

While using this approach, a non-linear functional fit of Equation 1 was first attempted using one set of coefficients for the entire data set (whole cruise). Model fits were iterative with outliers discarded. Outliers were determined as values more than three scaled median absolute deviations from the median.

With outliers removed, residuals between CTD values and water sample values were then examined as a function of pressure, temperature, oxygen concentration, and cast number (≈ cruise time). An examination of the residuals as a function of cast number was used to 1) identify episodic events resulting in abrupt changes in SOC values, and 2) determine potential drift in SOC over the course of the cruise. After examining the residuals, cast numbers were grouped if necessary to minimize the residuals with an attempt to limit the number of groups used per cruise. New calibration coefficients were then determined for each group.

If a linear drift as a function of cast number (cn) or cruise time (dt) was determined for a group, a linear correction of the SOC drift was applied to the group while keeping other coefficients constant. The linear drift as a function of cast number/cruise time was then incorporated into the calibration equation, replacing SOC in Equation 1 as a function of cruise number/cruise time as:

SOCcn/dt = SOC1 + F*cn/dt (Equation 2)

where *cn* or *dt* is the cast number [-] or time since first cast [d], respectively. *SOC1* is the initial *SOC* value, and *F* is the rate of *SOC* change per cast number or day since first cast.

A nonlinear functional fit including the cast or time-dependent SOCcn/dt was then fit to the group determining coefficients for *E*, *SOC1*, and *F* while holding *A, B, C,* and *Voff* constant. After iterative fitting and outliers removed, residuals were examined again as a function of pressure, temperature, oxygen concentration and cast number to ensure no linear dependence of residuals as a function of time. Outliers were determined as values more than three scaled median absolute deviations from the median.

For each cruise, CTD-derived measurements of salinity and oxygen solubility were calculated using the TEOS-10 Gibbs-SeaWater Oceanographic Toolbox (McDougall and Barker, 2011). Measurements from primary CTD sensors recorded in line with the SBE43 oxygen sensors were used to calculate oxygen concentrations unless collected data was poor. In these instances, measurements from the secondary CTD sensors were used. Bottle-calibrated CTD salinity measurements were used to produce oxygen concentrations when available (Years 5 - 9). The measurements of temperature, salinity, pressure and oxygen voltage (processed with SBE default hysteresis correction) used to produce oxygen concentration profiles are included in files for downcasts (indicated with ‘d’ appended) or upcasts (indicated with ‘u’ appended).

Throughout this documentation, oxygen profiles calibrated using a constant SOC value are indicated by SOCk while oxygen profiles calibrated using an SOC term that varies with time or cast (station) number are indicated by SOCdt and SOCcn, respectively. Lastly, oxygen sensor gain is determined as the Winkler-determined SOC value over the factory-determined SOC to assess changes in oxygen calibration slope since factory calibration. Note, the manufacturer recommends factory service inspection and calibration for a SBE43 DO sensor with a gain correction greater than 1.2 from the original factory value (Application Note 64-2).

Post-processing Aanderaa oxygen calibrations

Oxygen concentration was calculated from raw Aanderaa oxygen optode output in volts following the methods detailed in Bittig et al. (2018). Raw voltage outputs are converted to calphase, which is used to calculate oxygen concentration using the optode-specific calibration coefficients from factory calibration, the Stern

Volmer equation, and compensation equations to correct for salinity and pressure effects. The measurements of temperature, salinity (bottle-calibrated), pressure, and raw Aanderaa voltage used to produce oxygen concentration profiles are included in files for downcasts (indicated with ‘d’ appended) or upcasts (indicated with ‘u’ appended).

Aanderaa optodes are not routinely used for profiling applications on shipboard CTD casts, since oxygen optodes have a significantly slower response time than Clark electrodes such as the SBE43. This complicates or precludes the ability to resolve strong oxygen gradients at the speed at which CTD rosettes are routinely raised and lowered. Aanderaa optode data were used in place of SBE43 oxygen sensor on cruises where the SBE43 was malfunctioning (AR35-05; August 2019) or was unable to be calibrated with shipboard discrete oxygen measurements (AR46; August 2020). The time lag was quantified by empirically determining the optode’s temperature-dependent boundary layer thickness based on paired upwards and downwards profiles (Gordon et al. 2020) and corrected for following the methods of Bittig and Kortzinger (2017), using the optode-response-time code provided by Gordon et al.

Bottle dissolved oxygen samples were used to calculate a gain correction for the Aanderaa optode after all other corrections were applied. Because of the optode’s inability to resolve strong oxygen gradients at CTD profiling speeds, only Winkler samples collected in relatively stable sections of the water column (below 500 m) were used to determine the Aanderaa optode gain correction.

Irminger Sea 1 Deployment Cruise KN221-04

A complete cruise report and results of water sample analyses for KN221-04 are available on Alfresco. A total of nine CTD casts were performed on-board the R/V Knorr. Bottle-calibrated CTD salinity measurements are not available for this cruise; however, the shipboard measurements of salinity were used to validate the CTD-derived salinity measurements. The oxygen sensor was switched from SN 1646 to SN 1679 prior to Station 2. The hysteresis between upcast and downcast oxygen data due to sensor response time was removed by advancing the oxygen sensor data 4 seconds relative to the pressure sensor data. Data from the primary CTD sensor package was used to determine SBE oxygen concentrations.

Oxygen calibration Results

Calibration coefficients for SOC and E in Equation 1 were attempted using a non-linear least squares fit between CTD oxygen values and 44 Winkler samples from Casts 2-9. The model fit using all Winklers was poor with a RMSE of 9.95 µmol/kg, R2 value of -0.543 and no outliers determined. An inspection of residuals (Winkler - SOCk model) determined a negative correlation between residuals and CTD DO concentrations. Negative correlation between residuals and CTD DO concentrations in conjunction with the determined high oxygen sensor gain value of 1.368 suggests that fouling of the oxygen sensor membrane greatly impacted the oxygen data collected. In order to salvage interpretable oxygen data from this cruise, a non-linear functional fit of the calibration equation was performed using 4 Winkler samples collected at Station 4 (RMSE = 2.98 µmol/kg, R2 = 0.922, n = 4). The calibration coefficients determined from Station 6 were then applied to data collected at Stations 2-9.

Irminger Sea 2 Deployment Cruise AT30-01

A complete cruise report and results of water sample analyses for AT30-01 are available on Alfresco. A total of 13 CTD casts were performed on-board the R/V Atlantis. Bottle-calibrated CTD salinity measurements are not available for this cruise; however, the shipboard measurements of salinity were used to validate the CTD-derived salinity measurements. The hysteresis between upcast and downcast oxygen data due to sensor response time was removed by advancing the oxygen sensor (SN 0712) data 8 seconds relative to the pressure sensor data. Data from the primary CTD sensor package was used to determine SBE oxygen concentrations.

Oxygen calibration Results

Calibration coefficients for SOC and E in Equation 1 were determined using a non-linear least squares fit between CTD oxygen values and 106 Winkler samples from Station 1-13. Residuals (Winkler - SOCk model) were found to be linearly dependent on station number. Application of the non-linear regression model using a station-dependent SOC term (Equation 2) was found to further minimize the residuals between Winkler oxygen and CTD oxygen. No relationship between residuals (Winkler- SOCcn model) and pressure, temperature, station or oxygen concentration remained. The SOCcn model (RMSE = 1.03 µmol/kg, R2 = 0.999, n = 106) flagged 1 Winkler sample (0.94%) as an outlier.See the supplemental data docs for the summary of the Winkler-optimized calibration coefficients and model results.

Irminger Sea 3 Deployment Cruise AR07-01

A complete cruise report and results of water sample analyses for AR07-01 are available on Alfresco. A total of 10 CTD casts were performed on-board the R/V Armstrong. Bottle-calibrated CTD salinity measurements are not available for this cruise; however, the shipboard measurements of salinity were used to validate the CTD-derived salinity measurements. The hysteresis between upcast and downcast oxygen data due to sensor response time was removed by advancing the oxygen sensor (SN 0338) data 4 seconds relative to the pressure sensor data. Data from the primary CTD sensor package was used to determine SBE oxygen concentrations.

Oxygen calibration Results

Calibration coefficients for SOC and E in Equation 1 were determined using a non-linear least squares fit between CTD oxygen values and 69 Winkler samples from Station 5-10. Residuals (Winkler - SOCk model) were minimized by creating two groups. Group 1 consisted of Stations 5 and 6 and Group 2 consisted of Stations 7-10. Residuals in both groups were found to be linearly dependent with cruise time. Application of the non-linear regression model using a time-dependent SOC term (Equation 2) was found to further minimize the residuals between Winkler oxygen and CTD oxygen. No relationship between residuals (Winkler- SOCdt model) and pressure, temperature, station or oxygen concentration remained with the SOCdt model fit. The SOCdt model for Group 1 (RMSE = 1.3 µmol/kg, R2 = 0.956, n = 23) flagged no outliers.The SOCdt model for Group 2 (RMSE = 0.806 µmol/kg, R2 = 0.994, n = 46) flagged 2 Winklers (4.3%) as outliers. See the supplemental data docs for the summary of the Winkler-optimized calibration coefficients and model results.

Irminger Sea 4 Deployment Cruise AR21

A complete cruise report and results of water sample analyses for AR21 are available on Alfresco. A total of 12 CTD casts were performed on-board the R/V Armstrong. Salinity and oxygen data at Stations 1-8 experienced issues consistent with clogging of the CTD pump. The primary CTD package pump was switched prior to Station 9. Bottle-calibrated CTD salinity measurements are not available for this cruise; however, the shipboard measurements of salinity were used to validate the CTD-derived salinity measurements. The hysteresis between upcast and downcast oxygen data due to sensor response time was minimized by not advancing the oxygen sensor (SN 0930) data relative to the pressure sensor data. Data from the primary CTD sensor package was used to determine SBE oxygen concentrations for Casts 9 –12.

Oxygen calibration Results

Calibration coefficients for SOC and E in Equation 1 were determined using a non-linear least square fit between CTD oxygen values and the 35 Winkler samples collected at Stations 10-12. Residuals (Winkler - SOCk model) determined using a constant SOC revealed no relationship between residuals and pressure, temperature, station or oxygen concentration. The SOCk model (RMSE = 0.968 µmol/kg, R2 = 0.988, n = 35) flagged 2 Winkler samples (5.7%) as outliers.See the supplemental data docs for the summary of the Winkler-optimized calibration coefficients and model results.

Irminger Sea 5 Deployment Cruise AR30-03

A complete cruise report and results of water sample analyses for AR30-03 are available on Alfresco. A total of 23 CTD casts were performed on-board the R/V Armstrong. CTD-derived salinity data were calibrated by Leah McRaven using discrete bottle samples, and results are summarized in the AR30-03 CTD Calibration Report. The secondary CTD package is recommended for calibration use on this cruise; therefore, the temperature, bottle-calibrated salinity and depth data from the secondary CTD package were used in the oxygen sensor calibration equation to calibrate SBE43 (SN 0113) oxygen sensor data. The hysteresis between upcast and downcast oxygen data due to sensor response time was removed by advancing the oxygen sensor data 6 seconds relative to the pressure sensor data.

Oxygen calibration Results

Calibration coefficients for SOC and E in Equation 1 were first attempted using a non-linear least squares fit between CTD oxygen values and all 271 Winkler samples. Examination of residuals (Winkler - SOCk model) revealed higher residuals associated with Casts 10 and 21, perhaps due to sensor fouling. Therefore, calibration coefficients for SOC and E in Equation 1 were determined for all casts but 10 and 21 using a non-linear least squares fit between CTD oxygen values and 179 Winkler samples while calibration coefficients for A, B, C, and Voff were held constant at their factory-determined values. The SOCk model (RMSE = 1.31 µmol/kg, R2 = 0.989, n = 172) flagged 7 Winkler samples (4.1%) as outliers.

Calibration coefficients for SOC were then determined for casts 10 and 21 (both < 1000 m) while using pressure-associated E values determined from Casts 1-9, 11-20, 22-23 (included samples greater than 1000 m). The SOCk model for Cast 10 (RMSE = 0.62 µmol/kg , $R2$ = 0.998, n =42) flagged 10 Winkler samples (19.2%) as outliers, while the SOCk model for Cast 21 (RMSE = 0.80 µmol/kg, $R2$ = 0.996 , n = 34) flagged 6 Winkler samples (15.0%) as outliers. After optimizing calibration coefficients, no relationship between residuals (Winkler- SOCk model) and pressure, temperature, station or oxygen concentration remained. See the supplemental data docs for the summary of the Winkler-optimized calibration coefficients and model results.

Irminger Sea 6 Deployment Cruise AR35-05

A complete cruise report and results of water sample analyses for AR35-05 are available on Alfresco. A number of issues affected the quality of CTD-measured hydrographic and oxygen data on this cruise. Briefly, major biofouling issues were observed for all primary CTD sensors (temperature, salinity, and oxygen) resulting in no usable CTD-DO oxygen measurements for AR35-05. Therefore, an Aanderaa optode (SN 502) was integrated into the CTD rosette prior to Station 3. Additionally, failure of the pylon on the CTD rosette resulted in no bottle samples fit for calibration purposes prior to Station 11. Salinity data collected by the secondary CTD package were bottle calibrated for Stations 11-13 by Leah McRaven and results are summarized in AR35-05 CTD Calibration Report. Temperature, salinity, and pressure data collected by the secondary CTD package were used to calculate Aanderaa optode oxygen concentrations on this cruise for Stations 3-12.

Oxygen calibration Results

Oxygen concentrations were calculated from raw Aanderaa oxygen optode output in volts following the methods detailed in Bittig et al. (2018). Raw voltage outputs were converted to oxygen concentration using the optode-specific calibration coefficients from factory calibration, the Stern Volmer equation, and compensation equations to correct for salinity and pressure effects. Using the approach of Gordon et al. (2020), paired downcasts and upcasts were used to determine and then correct an optode time lag of 13 sec at a reference temperature of 4°C. A total of 55 Winklers (sampled at greater than 500 m) were used to calculate a gain correction of 1.0023 for the Aanderaa optode (SN 502) integrated into the CTD rosette. After applying the gain correction, absolute bias between Winklers and Aanderaa DO was 1.1 ± 0.96 µmol/kg (n = 55). Residuals (Winkler - Aanderaa DO) showed no relationship with pressure, temperature, station or oxygen concentration.

Irminger Sea 7 Deployment Cruise AR46

A complete cruise report and results of water sample analyses for AR46 are available on Alfresco. A total of 19 CTD casts were performed on-board the R/V Armstrong. CTD-derived salinity data were calibrated by Leah McRaven using discrete bottle samples, and results are summarized in the AR46 CTD Calibration Report. Temperature, bottle-calibrated salinity and depth data from the primary CTD package were used to calculate oxygen concentrations at Stations 1-10 and 18-19 while bottle-calibrated data from the secondary CTD package were used to calculate oxygen concentrations at Stations 12-17 .

The COVID-19 pandemic presented a number of challenges for sea-going operations in 2020. Traditionally, Winkler measurements are made at sea by trained technicians; however, in 2020 discrete samples for oxygen were collected and stored until subsequent analysis back on land to minimize shipboard personnel. The storage of discrete oxygen samples according to methods described by Zhang et al. (2002) allowed for quality measurements from the previous cruise (AR45) but not from AR46. As a result, there are no discrete oxygen measurements for calibration purposes for AR46. Additionally, the SBE43 oxygen sensor was changed between AR45 and AR46 excluding the possibility of using the SBE43 oxygen calibration coefficients determined on AR45 on oxygen data collected on AR46. However, the same Aanderaa optode (SN 277) was integrated into the CTD rosette for both AR45 and AR46. Aanderaa optodes are relatively stable in their calibration, allowing the gain correction determined on AR45 to be applied to optode data collected during AR46.

Oxygen calibration Results

Oxygen concentrations were calculated from raw Aanderaa oxygen optode output in volts following the methods detailed in Bittig et al. (2018). Raw voltage outputs were converted to oxygen concentration using the optode-specific calibration coefficients from factory calibration, the Stern Volmer equation, and compensation equations to correct for salinity and pressure effects. Using the approach of Gordon et al. (2020), paired downcasts and upcasts were used to determine and then correct an optode time lag of 13.1 sec at a reference temperature of 4°C

A total of 17 Winklers (sampled at greater than 500 m) from AR45 were used to calculate a gain correction for the Aanderaa optode (SN 277) integrated into the CTD rosette. Upon inspection, residuals (Winklers - Aanderaa DO) revealed a linear relationship between residuals and pressure using the standard pressure correction coefficient of 0.032 (Uchida et al. 2008). The pressure correction coefficient was then adjusted to 0.027 in order to remove the residual relationship with pressure, and resulted in a gain correction of 1.1386. After application of the gain correction, absolute bias between Winklers and Aanderaa DO was 0.74 ± 0.58 µmol/kg (n = 17) for AR45. The gain and adjusted pressure correction value D determined during AR45 were then applied to optode data collected during AR46.

Irminger Sea 8 Deployment Cruise AR60-01

A complete cruise report and results of water sample analyses for AR60-01 are available on Alfresco. A total of 12 CTD casts were performed on-board the R/V Armstrong. CTD-derived salinity data were calibrated by Leah McRaven using discrete bottle samples, and results are summarized in the AR60-01 CTD Calibration Report. This temperature, bottle-calibrated salinity and depth data from the primary CTD package were used in the oxygen sensor calibration equation to calibrate SBE43 (SN 0444) oxygen sensor data from this cruise. The hysteresis between upcast and downcast oxygen data due to sensor response time was removed by advancing the oxygen sensor data 8 seconds relative to the pressure sensor data.

Oxygen calibration Results

Calibration coefficients for SOC and E in Equation 1 were attempted using a non-linear least square fit between CTD oxygen values and the 134 Winkler samples collected (RMSE = 5.85 µmol/kg, R2 = 0.906, n = 79). Residuals were relatively large and more than half the Winklers were flagged as outliers. Examination of Winklers and CTD-measured oxygen values revealed issues with Winklers collected from casts 5 -12. Therefore, calibration coefficients for SOC and E in Equation 1 were determined using a non-linear least squares fit between CTD oxygen values and the 30 Winkler samples from casts 2 and 4. Residuals (Winkler - SOCk model) determined using a constant SOC revealed no relationship between residuals and pressure, temperature, station or oxygen concentration for the two stations used. The SOCk model (RMSE = 1.41 µmol/kg, R2 = 0.997, n = 23) flagged 7 Winkler samples (23.3%) as outliersSee the supplemental data docs for the summary of the Winkler-optimized calibration coefficients and model results. These calibration coefficients were applied to CTD oxygen data collected at Stations 1 through 12.

Irminger Sea 9 Deployment Cruise AR69-01

A complete cruise report and results of water sample analyses for AR69-01 are available on Alfresco. A total of 23 CTD casts were performed on-board the R/V Armstrong. The CTD experienced hardware issues that were sorted prior to Cast 6. CTD-derived salinity data were calibrated by Leah McRaven using discrete bottle samples, and results are summarized in the AR69-01 CTD Calibration Report (in prep). Bottle-calibrated salinity data from the primary CTD package were used in the oxygen sensor calibration equation to calibrate SBE43 (SN 1960) oxygen sensor data from this cruise. The hysteresis between upcast and downcast oxygen data due to sensor response time was removed by advancing the oxygen sensor data 6 seconds relative to the pressure sensor data.

Oxygen calibration Results

Calibration coefficients for SOC and E in Equation 1 were determined using a non-linear least squares fit between CTD oxygen values and 157 Winkler samples while calibration coefficients for A, B, C, and Voff were held constant at their factory-determined values (Appendix A). Residuals (Winkler - SOCk model) determined using a constant SOC were found to be linearly dependent on station number. Application of the non-linear regression model using a time-dependent SOC term (Equation 2) was found to further minimize the residuals between Winkler oxygen and CTD oxygen, and no relationship between residuals (Winkler- SOCdt model) and pressure, temperature, station or oxygen concentration remained. The SOCdt model (RMSE = 0.94 µmol/kg, R2 = 0.994) flagged 12 Winkler samples (7.6%) as outliers. See the supplemental data docs for the summary of the Winkler-optimized calibration coefficients and model results.

Problems/Issues

Quality flags applied to this dataset follow the recommendations of Jiang et al. 2022:

- 1 = not evaluated/quality unknown
- 2 = acceptable
- 3 = questionable
- 4 = known bad
- 6 = median of replicates

9 = Missing value

Year 1 KN221-04: Use of CTD oxygen data data from KN221-04 is generally poor due to suspected fouling and should be approached with caution. An oxygen sensor gain of 1.3675 was determined for this cruise; SBE recommends sensor maintenance for oxygen sensor gains greater than 1.2. All oxygen data has been flagged as questionable with the high gain correction likely resulting in oxygen concentrations that are biased low. For discrete water samples, there are discrepancies between bottle numbers (Niskin bottles) created by the SBE data processing software and bottle numbers (Niskin bottles) associated with shipboard Winkler analysis in OOI Alfresco datasheets.

Year 2 AT30-01: None

Year 3 AR07-01: Oxygen data collected at Stations 1-4 were not calibrated since casts at Stations 1-4 measured a very different water mass in the Western Labrador Sea, and these casts were not associated with any discrete oxygen samples. Surface oxygen measurements in the upper ~50 m of the downcast profile at Station 10 have been flagged as questionable.

Year 4 AR21: Oxygen and salinity sensors experienced issues consistent with clogging of the pump at Stations 1-8 and data was not salvageable. The pump was changed prior to Station 9. An oxygen sensor gain of 1.2218 was determined for this cruise and applied to Stations 9 -12, which is slightly over the recommended sensor maintenance gain value of 1.2.

Year 5 AR30-03: CTD data collected at Stations 7-12 experienced issues associated with biofouling. Portions of Casts from stations 7-8 and 11-12 have been flagged as questionable as they exhibit behavior indicative of biofouling.

Year 6 AR35-05: Oxygen profiles were collected using an Aanderaa optode because of issues with the SBE43-DO sensor. All data has been flagged as questionable because of the inability for Aanderaa optodes to resolve strong oxygen gradients at CTD rosette profiling speeds. A broken pylon resulted in no discrete water samples for calibration prior to Station 11.

Year 7 AR46: COVID-affected cruise. No discrete oxygen measurements for AR46. Oxygen profiles from AR46 were collected using an Aanderaa optode that was calibrated during the previous cruise (AR45) using water samples that were stored and not measured onboard. All data has been flagged as questionable because of these issues and also because of the inability for Aanderaa optodes to resolve strong oxygen gradients at CTD rosette profiling speeds.

Year 8 AR60-01: Examination of Winklers and CTD-measured oxygen values revealed issues with Winklers collected from casts 5 -12. Residuals from casts 5-12 were relatively large and more than half of the Winklers were flagged as outliers. Also, oxygen data collected on the upcast from Cast 10 between ~750 - 920 db is consistent with pump clogging and has been flagged as questionable.
Year 9 AR69-01: None

BCO-DMO Processing Description

* Merged all files into 1 data file
* Added lat/lon/time of ctd casts

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Data Files

File
904721_v1_palevsky_ctdcasts.csv (Comma Separated Values (.csv), 31.87 MB) MD5:34f0c97b40d5a43ac46004db868c3a3b Primary data file for dataset 904721.

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Supplemental Files

File
Appendix A filename: AppendixA.docx (Microsoft Word document, 19.74 KB) MD5:41a9b4b5b6aa4f47d8b920c33a700abf SBE-provided calibration coefficients for oxygen sensors
AR07-01.zip (ZIP Archive (ZIP), 102.26 KB) MD5:f078f25542e299ee6652327d71682762 Individual oxygen profile files for cruise AR07-01. Supplemental data for dataset 904721
AR21.zip (ZIP Archive (ZIP), 68.59 KB) MD5:a45e35a94fbf855d58ad32c1472175a2 Individual oxygen profile files for cruise AR21. Supplemental data for dataset 904721
AR30-03.zip (ZIP Archive (ZIP), 677.26 KB) MD5:bc71cc1b173496bd18434013fa933be2 Individual oxygen profile files for cruise AR30-03. Supplemental data for dataset 904721
AR35-05.zip (ZIP Archive (ZIP), 417.55 KB) MD5:1f47898e2b47dfc55a4c6151419450b3 Individual oxygen profile files for cruise AR35-05. Supplemental data for dataset 904721
AR46.zip (ZIP Archive (ZIP), 314.83 KB) MD5:ad9b347320a614713626f2e3f6695de3 Individual oxygen profile files for cruise AR46. Supplemental data for dataset 904721
AR60-01.zip (ZIP Archive (ZIP), 239.09 KB) MD5:5bc286d04dbab3351ef77756eef2b1df Individual oxygen profile files for cruise AR60-01. Supplemental data for dataset 904721
AR69-01.zip (ZIP Archive (ZIP), 374.02 KB) MD5:9f1ecc4e5a0b4c654314bad4dda4591d Individual oxygen profile files for cruise AR69-01. Supplemental data for dataset 904721
AT30-01.zip (ZIP Archive (ZIP), 265.79 KB) MD5:eca18788808aa7695f789e5bd2a109a0 Individual oxygen profile files for cruise AR30-01. Supplemental data for dataset 904721
Cast Processing Figures filename: Cast_Processing_Figures.docx (Microsoft Word document, 2.14 MB) MD5:6ae93cc6290e6cd1f48b8b1c9b06ea79 Figures for bottle-calibrated DO profiles for the OOI Irminger Sea Array dataset
KN221-04.zip (ZIP Archive (ZIP), 122.71 KB) MD5:2b007e058567a62a6555665c83cbc83e Individual oxygen profile files for cruise KN221-04. Supplemental data for dataset 904721
Winkler-determined calibration coefficients.xlsx (Microsoft Excel, 11.00 KB) MD5:200a4280dc637021c0dae5a6a6845e2e Winkler-determined calibration coefficients

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Related Publications

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situ drift for oxygen optodes on profiling platforms. Ocean Science, 13(1), 1–11. https://doi.org/10.5194/os-13-1-2017
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Gordon, C., Fennel, K., Richards, C., Shay, L. K., & Brewster, J. K. (2020). Can ocean community production and respiration be determined by measuring high-frequency oxygen profiles from autonomous floats? Biogeosciences, 17(15), 4119–4134. https://doi.org/10.5194/bg-17-4119-2020
Software

Jiang, L.-Q., Pierrot, D., Wanninkhof, R., Feely, R. A., Tilbrook, B., Alin, S., Barbero, L., Byrne, R. H., Carter, B. R., Dickson, A. G., Gattuso, J.-P., Greeley, D., Hoppema, M., Humphreys, M. P., Karstensen, J., Lange, N., Lauvset, S. K., Lewis, E. R., Olsen, A., … Xue, L. (2022). Best Practice Data Standards for Discrete Chemical Oceanographic Observations. Frontiers in Marine Science, 8. https://doi.org/10.3389/fmars.2021.705638
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Palevsky, H., Clayton, S., Atamanchuk, D., Battisti, R., Batryn, J., Bourbonnais, A., Briggs, E. M., Carvalho, F., Chase, A. P., Eveleth, R., Fatland, R., Fogaren, K. E., Fram, J. P., Hartman, S. E., Le Bras, I., Manning, C. C. M., Needoba, J. A., Neely, M. B., Oliver, H., … Wingard, C. (2023). *OOI Biogeochemical Sensor Data Best Practices and User Guide. Version 1.1.1. [GOOS ENDORSED PRACTICE]*. Ocean Observatories Initiative, Biogeochemical Sensor Data Working Group. https://doi.org/10.25607/OBP-1865.2
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Methods

Uchida, H. Johnson, G.,C. and McTaggart, G,. C. (2010) CTD Oxygen Sensor Calibration Procedures. In, The GO-SHIP Repeat Hydrography Manual: A Collection of Expert Reports and Guidelines. Version 1, (eds Hood, E.M., C.L. Sabine, and B.M. Sloyan), 17pp. (IOCCP Report Number 14; ICPO Publication Series Number 134). DOI: https://doi.org/10.25607/OBP-1344
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Uchida, H., Kawano, T., Kaneko, I., & Fukasawa, M. (2008). In Situ Calibration of Optode-Based Oxygen Sensors. Journal of Atmospheric and Oceanic Technology, 25(12), 2271–2281. https://doi.org/10.1175/2008jtecho549.1 https://doi.org/10.1175/2008JTECHO549.1
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Zhang, J.-Z., Berberian, G., & Wanninkhof, R. (2002). Long-term storage of natural water samples for

dissolved oxygen determination. Water Research, 36(16), 4165–4168. https://doi.org/10.1016/s0043-1354(02)00093-3 https://doi.org/10.1016/S0043-1354(02)00093-3
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Related Datasets

IsRelatedTo

McRaven, L. (2022). *Water temperature, salinity, and others taken by CTD and Niskin bottles from the research vessel Neil Armstrong in the North Atlantic Ocean during 2020 Ocean Observations Initiative (OOI) Irminger Sea 7 and Overturning in the Subpolar North Atlantic Program – Greenland Deep Western Boundary Current, ONSAP-GDWBC, cruise AR46 from 2020-08-08 to 2020-08-26. (NCEI Accession 0252117)* [Data set]. NOAA National Centers for Environmental Information. https://doi.org/10.25921/51B4-AC30 https://doi.org/10.25921/51b4-ac30

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McRaven, L. (2022). *Water temperature, salinity, and others taken by CTD and Niskin bottles from the research vessel Neil Armstrong, cruise AR35-05, in the North Atlantic from 08-02-2019 to 08-25-2019 (NCEI Accession 0251721)* [Data set]. NOAA National Centers for Environmental Information. https://doi.org/10.25921/61KN-QV10 https://doi.org/10.25921/61kn-qv10

McRaven, L. (2022). *Water temperature, salinity, and others taken by CTD and Niskin bottles from the research vessel Neil Armstrong, cruise AR60-01, in the North Atlantic from 08-03-2021 to 08-17-2021 (NCEI Accession 0247461)* [Data set]. NOAA National Centers for Environmental Information. https://doi.org/10.25921/P8QE-ME08 https://doi.org/10.25921/p8qe-me08

McRaven, Leah (in prep). Water temperature, salinity, and others taken by CTD and Niskin bottles from the research vessel Neil Armstrong, cruise AR69-01, in the North Atlantic from 06-20-2022 to 07-17-2022

Palevsky, H. I., Fogaren, K. E., Nicholson, D. P., Yoder, M. (2023) **Supplementary discrete sample measurements of dissolved oxygen, dissolved inorganic carbon, and total alkalinity from Ocean Observatories Initiative (OOI) cruises to the Irminger Sea Array 2018-2019.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2023-07-19 doi:10.26008/1912/bco-dmo.904722.1 [view at BCO-DMO]
Relationship Description: Supplementary measurements alongside salinity- and oxygen- calibrated Conductivity Temperature Depth (CTD) and oxygen sensor data from the depths where Niskin bottles were closed for sample collection and additional discrete oxygen measurements.

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Parameters

Parameter	Description	Units
Cruise	Cruise ID	unitless
Cast	CTD cast number	unitless
Direction	CTD direction: up or down	unitless
Lat	Sampling location latitude, south is negative	decimal degrees
Lon	Sampling location longitude, west is negative	decimal degrees
Date_UTC	Sampling date in UTC format (yyyy-mm-ddThh:mmZ)	unitless
CTDPRES	Hydrostatic pressure recorded from CTD at the depth where the sample was taken	dbar
CTDTEMP_ITS90	In situ temperature recorded from CTD on the ITS-90 scale	degrees C
CTDTEMP_flag	Quality control flag; all data processed by McRaven (2022) marked as 2	unitless
CTDSAL_PSS78	Calibrated salinity (Practical Salinity Scale of 1978) calculated from conductivity recorded with CTD	unitless
CTDSAL_flag	Quality control flag; all data processed by McRaven (2022) marked as 2	unitless
CTDOXYCUR	Oxygen current from the SeaBird SBE43 oxygen sensor on the CTD package processed with the SBE default hysteresis correction	volts
CTDOXYCUR_flag	Quality control flag; see data documentation with Fogaren and Palevsky, 2023 and Palevsky et al. 2023 datasets.	unitless
CTDOXY	Calibrated dissolved oxygen content from oxygen sensor mounted on the CTD	umol/kg
CTDOXY_flag	Quality control flag; see data documentation with Fogaren and Palevsky, 2023 and Palevsky et al. 2023 datasets.	unitless
AAOXYCUR	Raw oxygen current from the Aanderaa oxygen optode added to the CTD package	volts
AAOXYCUR_flag	Quality control flag; see data documentation with Fogaren and Palevsky, 2023 and Palevsky et al. 2023 datasets.	unitless
AAOXY	Calibrated dissolved oxygen content from oxygen optode added to the CTD package	umol/kg
AAOXY_flag	Quality control flag; see data documentation with Fogaren and Palevsky, 2023 and Palevsky et al. 2023 datasets.	unitless
file_name	Original file name	unitless

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Instruments

Dataset-specific Instrument Name	Aanderaa Oxygen Optode 4831
Generic Instrument Name	Aanderaa Oxygen Optodes
Generic Instrument Description	Aanderaa Oxygen Optodes are instrument for monitoring oxygen in the environment. For instrument information see the Aanderaa Oxygen Optodes Product Brochure.

Dataset-specific Instrument Name	SeaBird 911plus CTD
Generic Instrument Name	CTD Sea-Bird SBE 911plus
Dataset-specific Description	CTD casts were performed using a ship-provided SeaBird 911plus CTD and deck unit (http://www.seabird.com//sbe911plus-ctd) configured to measure pressure, temperature, conductivity, oxygen current, and other variables.
Generic Instrument Description	The Sea-Bird SBE 911 plus is a type of CTD instrument package for continuous measurement of conductivity, temperature and pressure. The SBE 911 plus includes the SBE 9plus Underwater Unit and the SBE 11plus Deck Unit (for real-time readout using conductive wire) for deployment from a vessel. The combination of the SBE 9 plus and SBE 11 plus is called a SBE 911 plus. The SBE 9 plus uses Sea-Bird's standard modular temperature and conductivity sensors (SBE 3 plus and SBE 4). The SBE 9 plus CTD can be configured with up to eight auxiliary sensors to measure other parameters including dissolved oxygen, pH, turbidity, fluorescence, light (PAR), light transmission, etc.). more information from Sea-Bird Electronics

Dataset-specific Instrument Name	SeaBird SBE43 oxygen sensor
Generic Instrument Name	Sea-Bird SBE 43 Dissolved Oxygen Sensor
Generic Instrument Description	The Sea-Bird SBE 43 dissolved oxygen sensor is a redesign of the Clark polarographic membrane type of dissolved oxygen sensors. more information from Sea-Bird Electronics

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Deployments

KN221-04

Website	https://www.bco-dmo.org/deployment/904856
Platform	R/V Knorr
Start Date	2014-09-07
End Date	2014-09-28

AT30-01

Website	https://www.bco-dmo.org/deployment/904859
Platform	R/V Atlantis
Start Date	2015-08-05
End Date	2015-09-01

AR07-01

Website	https://www.bco-dmo.org/deployment/904862
Platform	R/V Neil Armstrong
Start Date	2016-06-30
End Date	2016-07-28

AR21

Website	https://www.bco-dmo.org/deployment/904866
Platform	R/V Neil Armstrong
Start Date	2017-07-28
End Date	2017-08-30

AR30-03

Website	https://www.bco-dmo.org/deployment/904745
Platform	R/V Neil Armstrong
Start Date	2018-06-05
End Date	2018-06-24

AR35-05

Website	https://www.bco-dmo.org/deployment/904747
Platform	R/V Neil Armstrong
Start Date	2019-08-02
End Date	2019-08-24

AR46

Website	https://www.bco-dmo.org/deployment/904871
Platform	R/V Neil Armstrong
Start Date	2020-08-07
End Date	2020-09-07

AR60-01

Website	https://www.bco-dmo.org/deployment/904875
Platform	R/V Neil Armstrong
Start Date	2021-08-03
End Date	2021-08-26

AR69-01

Website	https://www.bco-dmo.org/deployment/904879
Platform	R/V Neil Armstrong
Start Date	2022-06-20
End Date	2022-07-19

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Project Information

Collaborative Research: The Annual Cycle of the Biological Carbon Pump in the Subpolar North Atlantic (OOI Irminger BCP)

Coverage: Irminger Sea

NSF abstract:
Ocean biology plays an important role in the Earth's carbon cycle. While most of the organic material produced by phytoplankton in the sunlit surface waters of the oceans is eaten and recycled in the surface waters, a small amount sinks to the deep ocean in what is called the "biological carbon pump." The biological pump is particularly hard to study in high latitude regions, which can be difficult to get to and challenging to work in. It is also particularly important to understand the biological pump in these parts of the ocean, where much of the world's deep ocean waters are formed. The export of carbon to deep waters can be estimated by carefully measuring the amount of excess oxygen left behind in surface waters. Oxygen in seawater can be measured very precisely using sensors deployed on moorings, floats, and gliders. These sensors can be deployed for years at a time, but their measurements must be carefully calibrated. In this project, investigators would use carefully calibrated oxygen sensors on gliders to, in turn, calibrate the oxygen sensors on a set of moorings in the high latitude North Atlantic Ocean, to study the biological carbon pump over a period of two years. The project would train several undergraduate students and a graduate student, and result in the development of educational laboratory materials that incorporate glider and mooring data from the project.

The goal of this proposal is to observationally constrain the annual magnitude and seasonal timing of the biological carbon pump (determined as annual net community production; ANCP) and its influence on air-sea carbon dioxide flux by using biogeochemical sensor measurements from the Ocean Observatories Initiative (OOI) Irminger Sea Array. However, existing OOI oxygen sensor calibration suffers from both pre- and post-deployment drift, currently precluding the ability to calculate ANCP by oxygen mass balance. The investigators therefore propose to improve the accuracy and utility of OOI Irminger Sea oxygen measurements by deploying two gliders configured for air calibration of their oxygen sensors when surfacing between profiles. These air-calibrated gliders will be used to intercalibrate all 12 existing oxygen sensors on the Irminger Sea Array and produce a calibrated oxygen product incorporating data from all sensors, which will ensure sufficient accuracy to calculate ANCP. Both the annual magnitude and seasonal timing of ANCP, including upper ocean biological productivity and thermocline respiration, will be determined using an oxygen mass balance approach within a data- constrained 1D physical model. A suite of 1D model simulations including the inorganic carbon system, gas exchange, and ANCP determined from oxygen mass balance will be used, together with OOI carbon dioxide measurements, to diagnose influences of physical and biological drivers of air-sea carbon dioxide flux, improving both quantitative and mechanistic understanding of how the biological pump influences the carbon cycle.

This award reflects NSF's statutory mission and has been deemed worthy of support through evaluation using the Foundation's intellectual merit and broader impacts review criteria.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1946072
NSF Division of Ocean Sciences (NSF OCE)	OCE-1756613
NSF Division of Ocean Sciences (NSF OCE)	OCE-1755574

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