

Processing C-PROOF glider OXYGEN data

Version 0.2

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H. V. Dosser

Preamble: This document addresses oxygen data quality control (both real-time and delayed mode) for oxygen data collected by C-PROOF autonomous ocean gliders. The document describes steps taken toward that goal, including documentation of metadata, sensor storage, calibration, and tracking, and data processing protocols and procedures.

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Version summary:

Version number	Authors	Modifications
0.1	H. V. Dosser	First version of report
0.2	H. V. Dosser	Updated drift correction

1 Introduction and oxygen sensor overview

Gliders in the C-PROOF fleet are equipped with one of two types of sensors to measure dissolved oxygen (DO) in the ocean: 1) Aanderaa Optodes and 2) Rinko Optodes manufactured by JFE Advantech Co., Ltd. Both types of sensors use an optical method based on the principle of dynamic fluorescence quenching. Both optodes also measure temperature and calculate oxygen concentration internally. Neither sensor provides corrected DO in units of $\mu\text{mol/kg}$, our preferred unit for dissolved oxygen concentration (and the official Argo float unit for DO). For both sensors, additional processing steps must be applied to correct for temperature, salinity, and pressure effects, as well as for asymmetries between upcasts and downcasts and for sensor drift, before the final data is output.

1.1 Variable name conventions

The data transmitted by the oxygen sensor are given the following variable names:

- oxygen_concentration (equivalent to Argo's oxygen_concentration variable) from the Aanderaa optode 4831 output for DO concentration at zero pressure in either fresh water or at a reference salinity, or when the Rinko AROD_FT optode outputs DO concentration at zero pressure in fresh water (Unit = $\mu\text{mol/L}$)
- temperature_oxygen (equivalent to Argo's TEMP_DOXY variable) for the Aanderaa optode or Rinko optode output for temperature (Unit = deg C)
- TPHASE_DOXY for the Aanderaa optode 4831 output for TPhase (Unit = degree)
- C1PHASE_DOXY and C2PHASE_DOXY for the Aanderaa optode 4831 outputs for C1Phase and C2Phase (Unit = degree)

Note that we are not currently able to output phase directly from our oxygen sensors as doing so prevents outputting DO concentration and temperature.

The dissolved oxygen data in $\mu\text{mol/L}$ with automated real-time processing steps applied is stored in oxygen_concentration_adjusted in the real-time netCDF file. The fully post-processed dissolved oxygen value in $\mu\text{mol/L}$ with all corrections applied is stored in oxygen_concentration_adjusted in the delayed-mode netCDF file.

2 Oxygen related metadata

The information included in the oxygen related metadata is at a minimum:

- Manufacturer-provided sensor accuracy and resolution (if available)
- Sensor model and serial number
- Date of last sensor calibration

In future, it would also be desirable to include:

- Calibration documentation file name and/or calibration coefficients
- Reference salinity value, if applicable for that sensor

2.1 Aanderaa sensor specific metadata requirements

All metadata necessary to correct the oxygen data output by the Aanderaa sensors is available on the calibration sheet provided by the manufacturer.

2.2 Rinko sensor specific metadata requirements

To correct the oxygen data output by the Rinko sensors, the metadata on the calibration sheet provided by the manufacturer is combined with information from the Rinko manual, specifically that the reference salinity is set to zero for all Rinko sensors.

3 Aanderaa optode

Information provided herein is taken from the “TD 269 OPERATING MANUAL OXYGEN OPTODE 4330, 4831, 4835 (June 2017)” published by Aanderaa Data Instruments AS.

3.1 Measurements and data processing

3.1.1 Pressure and salinity compensation

Before any other correction is applied, corrections for pressure and salinity effects must be applied to the dissolved oxygen concentration in $\mu\text{mol/L}$ (oxygen_concentration).

The pressure compensation factor is estimated as:

$$p_factor = (|P| / 1000) \cdot \text{coeff_for_pressure_comp} + 1;$$

where P is the pressure from the CTD in dbars, and the coeff_for_pressure_comp = 0.032 for all Aanderaa sensors, following Uchida et al., 2008.

The salinity compensation factor is estimated as:

$$s_factor = \exp[(S - \text{sal_ref}) \cdot (B0 + B1 \cdot Ts + B2 \cdot Ts^2 + B3 \cdot Ts^3) + C0 \cdot (S^2 - \text{sal_ref}^2)];$$

where S is the salinity from the CTD in PSU, B0 to B3 and C0 are coefficients specified in the Aanderaa manual, Ts is the scaled temperature: $Ts = \ln[(298.15 - T) / (273.15 + T)]$; T is the temperature from the CTD in degrees Celsius, and sal_ref is a reference salinity.

The sensor stores an internal salinity S_0 , which is supposed to be set to a default value of 0 when optodes are delivered from the factory, however ours were set to 35 PSU, so it is always necessary to check. Use $\text{sal_ref} = S_0$ if the sensor outputs oxygen_concentration, and use $\text{sal_ref} = 0$ if the sensor outputs CalPhase and no conversion from oxygen_concentration to CalPhase (as described in 3.1.1) is performed.

Then compensated oxygen concentration is calculated as:

$$\text{oxygen_comp} = \text{oxygen_uncomp} \cdot s_factor \cdot p_factor;$$

The units of oxygen_comp are $\mu\text{mol/L}$. For all corrections and conversions involving CTD data, the most accurate CTD data available should be used. For real-time processing, the real-time CTD data must be used although it will itself introduce some uncertainty, however for delayed mode processing, the fully corrected CTD data should be used.

3.1.2 Optode 4831 calculation of dissolved oxygen from phase

An uncalibrated phase measurement (TPhase) is the difference between the phase obtained when the foil is excited by blue (C1Phase) and red light (C2Phase), with a possible temperature, T, compensation:

$$\text{TPhase} = \text{A(T)} + (\text{C1Phase} - \text{C2Phase}) \cdot \text{B(T)}$$

where A(T) and B(T) are 3rd order temperature dependent polynomials. To determine if a temperature compensation is applied, check the coefficients for A and B in the sensor properties PTC0Coef and PTC1Coef. Normally, A(T) = 0 and B(T) = 1.

The calibrated phase (CalPhase) is then calculated using sensor coefficients ‘PhaseCoef’ as:

$$\text{CalPhase} = \text{PhaseCoef}_0 + \text{PhaseCoef}_1 \cdot \text{TPhase} + \text{PhaseCoef}_2 \cdot \text{TPhase}^2 + \text{PhaseCoef}_3 \cdot \text{TPhase}^3$$

The time response correction (5.1) is applied to the calibrated phase, provided no temperature compensation has been used. The calibrated phase is then converted to dissolved oxygen concentration in $\mu\text{mol/L}$ using the Stern-Volmer relationship proposed by Uchida et al., 2008:

$$\text{DO}[\mu\text{mol/L}] = \frac{\left(\frac{c3 + c4 \cdot T}{c5 + c6 \cdot \text{CalPhase}} - 1 \right)}{c0 + c1T + c2T^2}, \text{ where coefficients } c0 \text{ etc. are stored in the SVUFoilCoef sensor property.}$$

Our sensors are normally set to output dissolved oxygen concentration in $\mu\text{mol/L}$ (oxygen_concentration), which is then converted to calibrated phase (CalPhase) using the temperature measurement from the oxygen sensor, the time response correction is applied (5.1), and then the resulting field is converted to DO[$\mu\text{mol/L}$] using the corrected temperature measurement from the CTD. Check the manual for the names of additional variables that can be output by the sensor. Note that it is possible to output CalPhase instead of oxygen_concentration, but it does not appear possible to output both simultaneously.

4 Rinko optode

Information provided herein is taken from the “A-0133-05 User’s Manual for Fast optical DO sensor for integration RINKO FT (Model name: ARO-FT, AROD-FT)” published by JFE Advantech Co., Ltd.

4.1 Measurements and data processing

4.1.1 Pressure and salinity compensation

Before the time response correction (5.1) is applied, corrections must be applied for pressure and salinity effects to the dissolved oxygen concentration in $\mu\text{mol/L}$ (oxygen_concentration).

The pressure compensation factor is estimated as:

$$p_factor = (|P| / 100) \cdot C_p + 1;$$

where P is the pressure from the CTD in dbars, and C_p is the calibration coefficient for pressure correction, listed on the calibration certificate for each sensor.

The salinity compensation factor is estimated as:

$$s_factor = \exp[S \cdot (B_0 + B_1 \cdot T_s + B_2 \cdot T_s^2 + B_3 \cdot T_s^3) + C_0 \cdot S^2];$$

where S is the salinity from the CTD in PSU, B_0 to B_3 and C_0 are coefficients specified in the Rinko manual, T_s is the scaled temperature: $T_s = \ln[(298.15 - T) / (273.15 + T)]$; and T is the temperature from the CTD in degrees Celsius.

Unlike the Aanderaa sensors, the Rinko optodes apparently do not have an internal reference salinity. The manual states “Note that the physical value output of the instrument does not consider salinity and/or pressure.” This is equivalent to $sal_ref = 0$ for the purposes of the salinity compensation correction above.

Then compensated oxygen concentration is calculated:

$$oxygen_comp = oxygen_uncomp \cdot s_factor \cdot p_factor;$$

The units of oxygen_comp are $\mu\text{mol/L}$. For all corrections and conversions involving CTD data, the most accurate CTD data available should be used. For real-time processing, the real-time CTD data must be used although it will itself introduce some uncertainty, however for delayed mode processing, the fully corrected CTD data should be used.

4.1.2 Rinko AROD_FT-CE calculation of dissolved oxygen from phase

The uncalibrated phase (Phase) is the difference between the phase obtained when the foil is excited by Blue light and by Red light. These hexadecimal values are referred to as ‘AD values’, as opposed to calculated temperature and dissolved oxygen concentration, which are referred to as ‘Physical values’.

Unlike Aanderaa sensors, it is not possible to connect to and communicate with a Rinko sensor without a separate Calibration Kit. As such, all necessary coefficients are printed on the Calibration Certificate. Some of these coefficients are sensor-specific, as is the case for the Aanderaa sensors.

The time response correction (5.1) is applied to the AD value of dissolved oxygen (AD value of DO), which is functionally equivalent to the calibrated phase. Then the dissolved oxygen concentration in $\mu\text{mol/L}$ is calculated using the Stern-Volmer relationship proposed by Uchida et al., 2010:

$$DO[\mu\text{mol/L}] = \left\{ \left(\frac{1 + d_0 \cdot T}{d_1 + d_2 \cdot N + d_3 \cdot t + d_4 \cdot t \cdot N} \right)^{e_0} - 1 \right\} \cdot \frac{1}{c_0 + c_1 \cdot T + c_2 \cdot T^2},$$

where calibration coefficients c_0 , d_0 , e_0 etc. are printed on the calibration certificate for that sensor, T is temperature, and N is the AD value of DO/10000. Typically $e_0 = 1$ and $d_3 = d_4 = 0$, so that we do not require values of t , the LED accumulation time [s].

Our sensors are normally set to output dissolved oxygen concentration in $\mu\text{mol/L}$ (oxygen_concentration), which is then converted to calibrated phase (AD value of DO) using the temperature measurement from the oxygen sensor, the time response correction is applied, and then the resulting field is converted back to DO [$\mu\text{mol/L}$] using the temperature measurement from the CTD. Check the manual for the names of additional variables that can be output by the sensor. Note that it is possible to output the physical values (T and oxygen_concentration) or the AD values, but it does not appear possible to output both simultaneously.

5 Additional corrections for real-time and delayed mode data processing

Two additional corrections are applied during the data processing stream, with different specifications for real-time and delayed mode data processing. These corrections are the time response correction (5.1) and the sensor drift correction (5.2).

5.1 Time response correction

The time response correction is applied to the calibrated optode phase (CalPhase for Aanderaa sensors and AD value of DO for Rinko sensors) to account for the slow sensor response time relative to the diving rate of the glider. It is important that the data sample interval for the sensor be kept an order of magnitude (or more) shorter than the response time if this correction is to be applied. The response time can be affected by differences in the glider speed during dives and/or between upcasts and downcasts, and by differences in temperature. In our study areas in the Northeast Pacific Ocean, ocean temperature varies between roughly 4°C and 20°C, often within a single profile during the summer months. However, we choose to use a constant value of the ‘response time constant’ τ for each mission, as the potential improvements are small and outweighed by the need for transparency in the processing steps.

5.1.1 Time response correction for real-time data processing

Based on laboratory and field results reported in Bittig et al., 2014, a single value of the response time constant τ is reported for each type of sensor. This value of τ is to be stored in the metadata, and is used for real-time data processing of all missions associated with that type of sensor (Aanderaa or Rinko). For delayed mode data processing, a value of τ is determined for each individual mission.

For Aanderaa oxygen optodes, values of τ between 25 and 100 seconds have been reported, and we use a value of $\tau = 45$ seconds for the real-time data processing. For Rinko oxygen optodes, values of τ between 1 and 10 seconds have been reported, and we use a value of $\tau = 1.5$ seconds for the real-time data processing. The time response correction is then applied as described in 5.1.3 below.

5.1.2 Time response correction for delayed mode data processing

Following Nicholson et al., 2008 and Howatt et al., 2018, a response time constant τ is determined by minimizing the error between all measured upcast values vs. all measured downcast values. A first-order lag correction is determined by calculating τ as in Fofonoff et al., 1974 based on the equation:

$Phase_{true} = Phase_{measured} + \tau \frac{d}{dt} Phase_{measured}$ where $Phase$ is the calibrated optode phase, ‘true’ is the true value and ‘measured’ is the measured value, and d/dt indicates a first derivative w.r.t. time during a given upcast or downcast. Derivatives are calculated using a centered finite difference scheme after successive upcasts and downcasts are interpolated onto the same depth grid. To avoid large derivatives caused by points at the start and end of individual profiles, any dt value greater than one standard deviation from the mean is excluded from the calculation. Then a least squares linear regression is performed on the following equation:

$$Phase_{measured}^{upcast} - Phase_{measured}^{downcast} = -\tau \left(\frac{d}{dt} Phase_{measured}^{upcast} - \frac{d}{dt} Phase_{measured}^{downcast} \right)$$

which assumes that successive upcasts and downcasts are identical ($Phase_{true}^{upcast} = Phase_{true}^{downcast}$). This assumption may not hold in regions where sharp spatial gradients exist or at times when the glider is passing through a front between different water masses. In such cases, data from the relevant segments of the mission trajectory should be excluded from the calculation of the response time constant.

It is expected that the calculated response time constant will be similar to that used for real-time data processing. A check is applied to ensure the calculated response time constant is within the expected ranges for each type of sensor based on Bittig et al., 2014. For our Aanderaa sensors, the calculated value of τ is accepted if it falls in the range 35 to 65 seconds. For our Rinko sensors, the calculated value of τ is accepted if it falls in the range 1 to 3 seconds.* If the calculated response time constant falls outside of these ranges, manual inspection of the mission data is required to determine the cause.

*Note: These ranges have been determined based on a combination of results reported in Bittig et al., 2014 and the performance of our existing sensors. The ranges may need to be expanded as new sensors are introduced into use by our glider fleet. It is best practice to compare each calculated value of τ to past values for that specific sensor, and investigate any major discrepancies.

5.1.3 Applying the time response correction

The optode measures a delayed, filtered version of the true upcast or downcast, and the goal of the correction is to reverse this process as much as possible. Our data processing applies the time response correction using the Bittig et al., 2014 correction with a boxcar filter. This approach and alternate options are discussed below:

Once τ is determined, multiple options exist to apply the correction. The simplest correction uses the equation: $Phase_{true} = Phase_{measured} + \tau \frac{d}{dt} Phase_{measured}$. This derivative-based approach is self-consistent with the least-squares regression method of determining τ , and provides a first-order linear correction.

Alternatively, a method described by Bittig et al., 2014 applies the correction using an inverse filtering algorithm based on Miloshevich et al., 2004. The procedure has two steps. First, the measurements are smoothed, then the correction is applied using an inverse bilinear transform to calculate the mean of the

‘true’ consecutive measurements: $\frac{Phase_{true}^{i+1} + Phase_{true}^i}{2} = \frac{1}{2b} \cdot \left(Phase_{measured}^{i+1} - a \cdot Phase_{measured}^i \right)$,

where $a = 1 - 2b$, $b = \left(1 + 2 \frac{\tau}{t_{i+1} - t_i} \right)^{-1}$ and t is the time. These mean values are then interpolated back to the original measurement times. This approach ensures the correct filter phase and is known to produce better gradient correction. We tested two smoothing filters: a moving-average boxcar filter with a span of τ and a Savitzky-Golay filter with a 3rd order polynomial and an odd-number frame size of $\frac{\tau}{2} \cdot 2 + 1$.

As shown in Figure 1, both filter options for the Bittig et al., 2014 approach produce similar results for the corrected field, while the derivative-based approach amplifies noise in the data. The Savitzky-Golay filter tends to produce some small-scale changes in the sign of the gradient with depth that are not present in the original measured phase.

We therefore elect to use the moving-average boxcar filter with the Bittig et al., 2014 inverse bilinear transform for all real-time and delayed mode time response corrections.

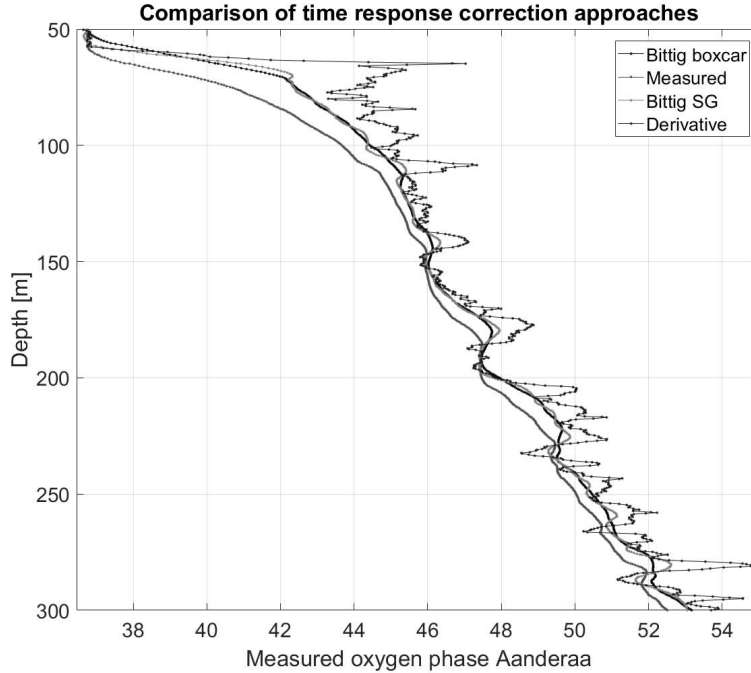


FIGURE 1: Comparison of the measured oxygen phase for a single profile calculated using output from an Aanderaa sensor (red line) with three different options for the time response correction: the Bittig et al., 2014 inverse bilinear transform correction using a boxcar smoothing filter (black line) or a Savitzky-Golay smoothing filter (gray line), and the derivative-based correction (blue line).

5.2 Sensor drift correction

The sensor drift correction is applied to the time-response corrected, compensated dissolved oxygen concentration data to account for the tendency of oxygen optodes to drift over time as the sensor ages. Although drift increases as a function of the number of samples collected, sensors tend to drift more quickly during storage than while in the field. To minimize the effects of drift, the following protocols are recommended by the manufacturers:

Aanderaa:

- Store sensors and spare foils in the dark, shielded from any ambient light. The black rubber protection cap can be used for this.
- Add a wet piece of natural sponge to the cap to keep the sensor foil wet during storage.
- Soak sensors in water at least 24 hours prior to calibration or deployment. For optimum accuracy, foils should be wet for 48 hours prior to use. Wet sponge in the cap can be used for this purpose.
- Annual recalibration is recommended by the factory, although a two-point calibration can be performed by the user (see Chapter 6 in the manual) and a linear correction can be automatically applied during the oxygen concentration calculation by the sensor.

Rinko:

- Do not leave the instrument under direct sunlight for a long time, as this will cause degradation of the oxygen detection film.
- When not in use, store with the protection cap on, and the power supply off.
- After every use, clean with fresh water and remove any moisture with a soft cloth before storage.
- Do not store at temperatures above 40°C or in locations with high humidity.
- A span/zero calibration can be performed by the user using the optional calibration kit (see Chapter 7 in the manual) and applied during the oxygen concentration calculation by the sensor.

The sensor drift correction attempts to correct for the drift that does occur by comparing the oxygen optode data to a trustworthy profile of dissolved oxygen concentration measurements collected nearby in space and time. Ideally, this comparison would be with Winkler titrated bottle samples collected at the same time and location as one of the glider's dives. In practice, a hierarchy of 'trustworthy' data sources is used, within some chosen tolerance for distance and time from the glider's sampling locations.

The drift correction itself is a linear adjustment applied to $DO[\mu\text{mol/kg}]$ with slope $p1$ and intercept $p2$:
 $\text{oxygen_concentration_adjusted} [\mu\text{mol/kg}] = p1 \cdot DO[\mu\text{mol/kg}] + p2$

Following Bittig et al., 2018, the drift is characterized by a reduced sensor response plus a small offset in the opposite direction. The slope should be positive, and within about 10% of unity. The intercept should be within a few $\mu\text{mol/kg}$ of zero and negative. In practice, the correction is determined both allowing for an intercept and setting the intercept to zero a priori, and the results are evaluated. We have found that an intercept of zero typically produces better agreement.

If the slope is larger than 1.01, a flag will be raised and the comparison may be rejected. It is expected that the drift for an individual sensor will increase with time (though not linearly). If this is not the case,

or if a sudden large increase in drift is detected, the comparison should be re-evaluated and/or the sensor should be examined.

5.2.1 Drift correction for real-time data processing

For real-time data processing, the drift correction that was derived for the previous mission using that specific sensor is applied, provided that the sensor has not since been calibrated and that the previous mission was no more than 3 months prior. This correction is ideally stored in the metadata, and is specific to the individual sensor. Entering the correct sensor serial number and calibration date in the metadata is critical. If the sensor has been calibrated since its previous mission, no drift correction is applied during the real-time data processing.

5.2.2 Drift correction for delayed mode data processing

For delayed mode data processing, the following options are considered for comparison with the optode measurements, in order of preference:

1. Winkler titrated bottle samples collected in close spatiotemporal proximity to a glider dive.
2. Oxygen sensor profile collected in close spatiotemporal proximity to a glider dive, where the sensor is calibrated frequently using Winkler titrated bottle samples.
3. Winkler titrated bottle samples collected within 7 days and 10 km of a glider dive, provided the dive is not in a highly dynamic location and extends to 1000 m depth.
4. Oxygen sensor profile collected in close spatiotemporal proximity to a glider dive, where the oxygen sensor is calibrated within several months of the glider mission.
5. Any other available comparison within a month and 20 km of a glider dive if the dive is not in a dynamic region and extends to over 500 m depth.

Note that any oxygen sensor or bottle profile with only a few samples or with all samples near the surface (upper ~100m) is not suitable for use as the sole comparison with the glider data. Ideally, comparison profiles are collected off the continental shelf in the open ocean, though this is not required and shelf comparisons can be very good (but should be examined more critically for comparability, particularly in dynamic regions).

To determine the drift correction, a least-squares fit is performed in potential density space between all suitable comparison profiles and the associated glider optode measurements that are closest to the comparison profile in space and time. If a sharp pycnocline is present, the portion of the profiles that is within the pycnocline is excluded from the comparison by visually identifying a depth at the base of the pycnocline and retaining data below it and data in the very near surface that are close to the saturation value. Typical depths for the base of the pycnocline are from 150-200 m in the regions sampled by our gliders. The glider profiles to be used are bin-averaged to the potential densities associated with the oxygen measurements from the comparison profile, with a bin size of $\pm 0.1 \text{ kg/m}^3$. Note that potential density rather than in-situ density is used. The binning combines data from up to 10 glider profiles, the number of which are chosen by verifying that they are taken from the same water mass as the comparison profile (and not, say, while passing into an eddy or across a front). If the comparison is in a dynamic region, only the closest full-depth glider profile will be used.

Next, each possible comparison profile is evaluated individually against the glider profiles selected for comparison. A linear, least-squares fit is applied to the binned data from the glider vs. the data from the comparison profile. The associated correlation coefficient for the fit is expected to be above $r^2 = 0.95$, and in practice is often above $r^2 = 0.99$.

Once each comparison profile has been evaluated, the comparison profile that provides the best comparison with the glider data is selected and used to estimate the drift correction. This final least-squares fit produces our best estimate of the slope used to correct the sensor drift.

The goodness of fit is evaluated by examining the agreement between the full-depth unbinned drift-corrected glider profile(s) and the comparison profile. The shallowest drift-corrected glider oxygen values are compared with those from the comparison profile relative to the saturation value of oxygen at the comparison profile location to provide context for the expected near-surface oxygen concentration values. The deepest (1000 m) drift-corrected glider oxygen profiles are evaluated to ensure the correction causes a change of no more than 5 $\mu\text{mol/kg}$ change, and that the change increases the oxygen values, since sensor drift tends to cause sensors to read lower.

Finally, the linear sensor drift correction is applied to the DO [$\mu\text{mol/kg}$] measurements (not to the data binned by density) and converted back to $\mu\text{mol/L}$ to produce oxygen_concentration_adjusted [$\mu\text{mol/L}$].

To convert to $\mu\text{mol/kg}$, when that unit is preferred, the corrected dissolved oxygen (oxygen_concentration_adjusted) can be multiplied by a factor of 1000 and divided by the potential density in kg/m^3 estimated from the CTD temperature T, salinity S, and pressure P.

6 References

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