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Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Oxygen Records

Version 1.0

2009-2021

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Acknowledgments

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Executive summary

The Southern Ocean Time Series (SOTS) Observatory located near 142°E and 47°S provides high temporal resolution observations in Subantarctic waters. It is focused on the Subantarctic Zone because waters formed at the surface in this region by deep wintertime convection slide under warmer subtropical and tropical waters, carrying CO_2 and heat into the deep ocean, where it is out of contact with the atmosphere. This process also supplies oxygen for deep ocean ecosystems, and exports nutrients that fuel ~70% of global ocean primary production. Local biological production also impacts carbon cycling and the SOTS moorings measure several variables important to these processes.

This report describes the quality control (QC) procedures applied to oxygen data collected from the SOTS moorings between 2009 and 2021. These measurements help to quantify net community production (and thus carbon export). The quality-controlled datasets are publicly available via the Australian Ocean Data Network (AODN) Portal: Open Access to Ocean Data (aodn.org.au). This report should be consulted when using the data.

The QC procedures apply automated tests following QARTOD recommendations for in-situ oxygen control (Bushnell & Worthington, 2020), with the test parameters tailored to reflect regional oceanography. QARTOD is an initiative of the US Integrated Ocean Observing System for Quality Assurance of Real Time Oceanographic Data: https://ioos.noaa.gov/project/qartod/. The procedures detailed in this document yield QC flags for each observation, as well as uncertainty estimates for the overall results. Gridded datasets are available from the AODN, and their production is described in Jansen et al. (2022b).

Document Versions

Version 1.0 of this report Initial Issue.

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1 Introduction

The Southern Ocean Time Series (SOTS) Observatory provides high temporal resolution observations in Subantarctic waters. Observations are broad and include measurements of physical, chemical and biogeochemical parameters from multiple deep-water moorings in the Subantarctic Zone southwest of Tasmania (Figure 1). The emphasis is on seasonal and inter-annual variations of lower atmosphere and upper ocean properties and their influence on exchange with the deep ocean. The continuous time-series information allows the study of ocean physics and chemistry, climate change, carbon cycling and biogeochemical controls on marine productivity. These moorings provide cost-effective observations and overcome the infrequent availability of ships in the region. The Southern Ocean Time Series is an Australian contribution to the international OceanSITES global network of time series observatories (www.OceanSITES.org) and is one of the few comprehensive Southern Ocean sites globally. More information on the SOTS Sub-Facility is available on-line at http://www.imos.org.au/facilities/deepwatermoorings/sots.

The Southern Ocean (south of 30°S) is responsible for ~40% of the total global ocean uptake of human-induced CO_2 emissions, and 75% of the additional heat that these emissions have trapped on Earth. The Southern Ocean Time Series site is focused on the Subantarctic Zone because waters formed at the surface in this region, the Subantarctic mode and Antarctic Intermediate waters, slide under warmer subtropical and tropical waters and carry this CO_2 and heat into the deep ocean, out of contact with the atmosphere. This process also supplies oxygen for deep ocean ecosystems, and exports nutrients that fuel ~70% of global ocean primary production. The Subantarctic Zone and these processes are expected to change with global warming, but the potential impacts of these changes are not yet known.

The Southern Ocean Time Series site southwest of Tasmania is comprised of a number of elements including a deep ocean sediment trap mooring (SAZ), a surface biogeochemistry mooring (Pulse) and an air-sea flux mooring (SOFS). Located in the Subantarctic Zone near 142°E, 47°S, the site is particularly vulnerable to the extreme weather events that typify the area including very large waves, strong currents and severe storms, presenting significant technical and engineering challenges.

The SOTS site (red star in Figure 1. Location of the SOTS observatory.) is in a low current region, north of the Subantarctic Front (SAF) that marks the northern edge of the Antarctic Circumpolar Current. It is in deep waters (>4500m) west of the Tasman Rise (the shallow region south of Tasmania; with waters less than 2000m deep, shown in blue). The SOTS site exhibits oceanographic properties representative of the Australian sector of the Subantarctic Zone (from ~90 to 145˚E; Trull et al., 2001). Waters flowing southward in the East Australian Current reach this region by transiting through channels in the Tasman Rise (Herraiz-Borreguero & Rintoul, 2011).

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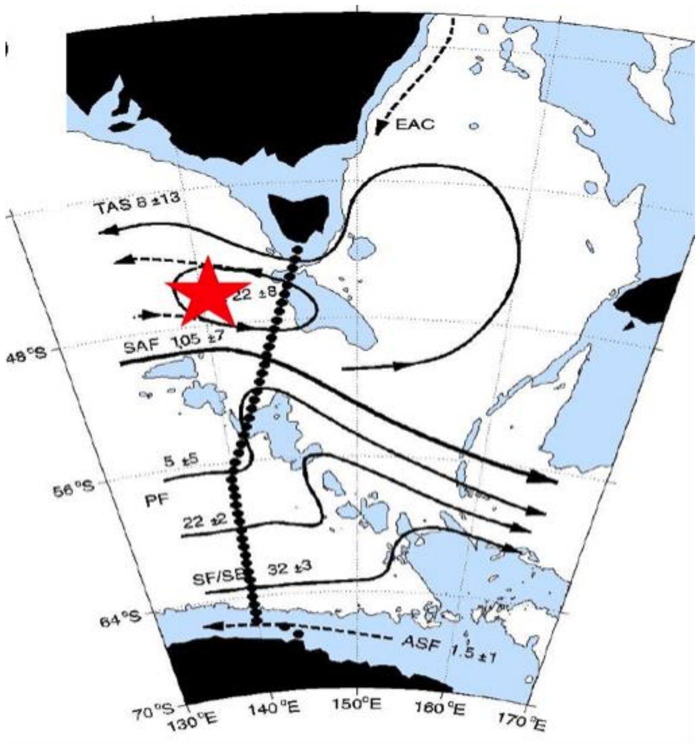

Figure 1. Location of the SOTS observatory.
EAC – East Australia Current, TAS – Tasman Sea Leakage, SAF-Subantarctic Front, PF-Polar Front, SF/SB – Slope Front/Southern Boundary, ASF, Antarctic Shelf Flow. Adapted from Herraiz-Borreguero et al., 2011

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2 Moorings Description

The Southern Ocean Time Series moorings are the Pulse biogeochemistry mooring, the Subantarctic Zone (SAZ) sediment trap mooring, and the Southern Ocean Flux Station (SOFS).

The Pulse biogeochemistry mooring is used to measure upper ocean carbon cycle and phytoplankton productivity processes. Measured parameters include temperature, salinity, dissolved oxygen, total dissolved gases, nitrate, chlorophyll fluorescence and optical particulate backscatter. This mooring also collects water samples for measurements of dissolved nutrients, and phytoplankton microscopic identification.

The SAZ sediment trap mooring collects sinking particles to quantify carbon fluxes and provides current meter measurements and a deep ocean CTD to measure heat contents below the depth of Argo profiling float measurements.

The SOFS meteorological tower mooring has dual sets of incoming solar radiometers, temperature and humidity sensors, precipitation gauges and sonic anemometers, and a pCO_2 sensor provided by NOAA. Surface photosynthetically active radiation (PAR) is also measured to help assess light available for phytoplankton production.

All three moorings are anchored to the ocean floor ~4.5 kilometres below the surface. The SOFS and Pulse moorings are S-tether designs that are longer than this, and correspondingly their surface floats move in large 'watch circles'. In contrast, the SAZ mooring is a stiff subsurface mooring with all components more than 700m below the surface. The moorings record hourly sensor observations until they are swapped with a duplicate mooring the following year.

In the 2016-17 year, the SOFS and Pulse capabilities were combined into a single prototype mooring known as FluxPulse-1. After this initial trial, the combined mooring nomenclature continued using the SOFS prefix.

Surface data collected from Pulse and SOFS are relayed back by satellite. The sub-surface data are stored and downloaded when the moorings are retrieved (approximately a year later). All data are available via the Australian Ocean Data Network (AODN) Portal.

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3 Summary of Instruments

All oxygen records from the SOTS moorings in the 2009-2021 period were based on oxygen measurements using Sea-Bird Electronics (2 different models) and Aanderra instruments (3 different models). All the sensors were paired with temperature and conductivity measurements. Sampling frequency was at least hourly. In general, the sensors were deployed on the Pulse and SOFS moorings, as individually logged instruments spaced from the surface to about 500m depth.

Data logging was internal to the instruments for the SBE37-SMP-ODO sensors. The SBE43 output voltage was logged by a SBE16plusV2 CTD. The Aanderra Optode sensors were either attached to a SBE16plusV2 CTD, or in the case of the SOFS surface float logged by a CR1000 data logger. In general data was only recovered when the moorings were recovered (except surface data telemetered from the SOFS moorings).

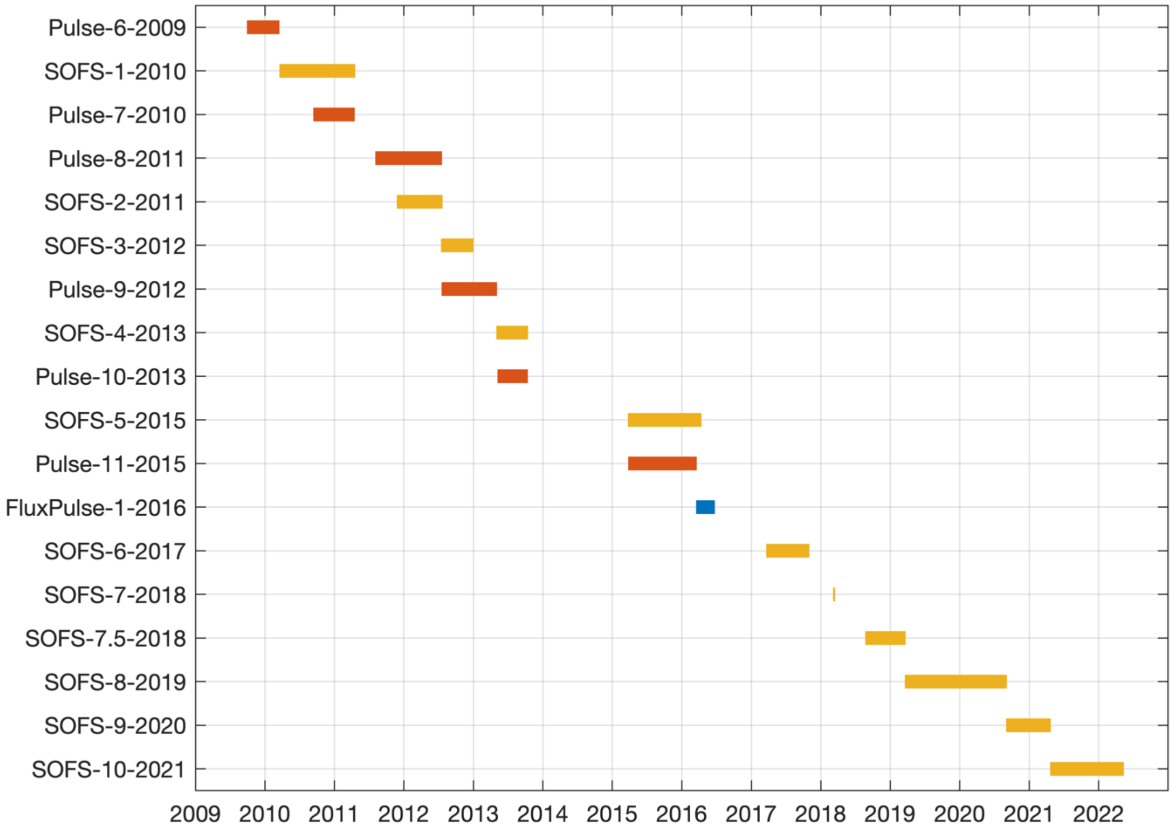

Figure 2. SOTS mooring deployments covered in this report.
Pulse in orange, and SOFS in yellow. Flux-Pulse in blue was a first (not fully successful) attempt to combine the SOFS and Pulse moorings.

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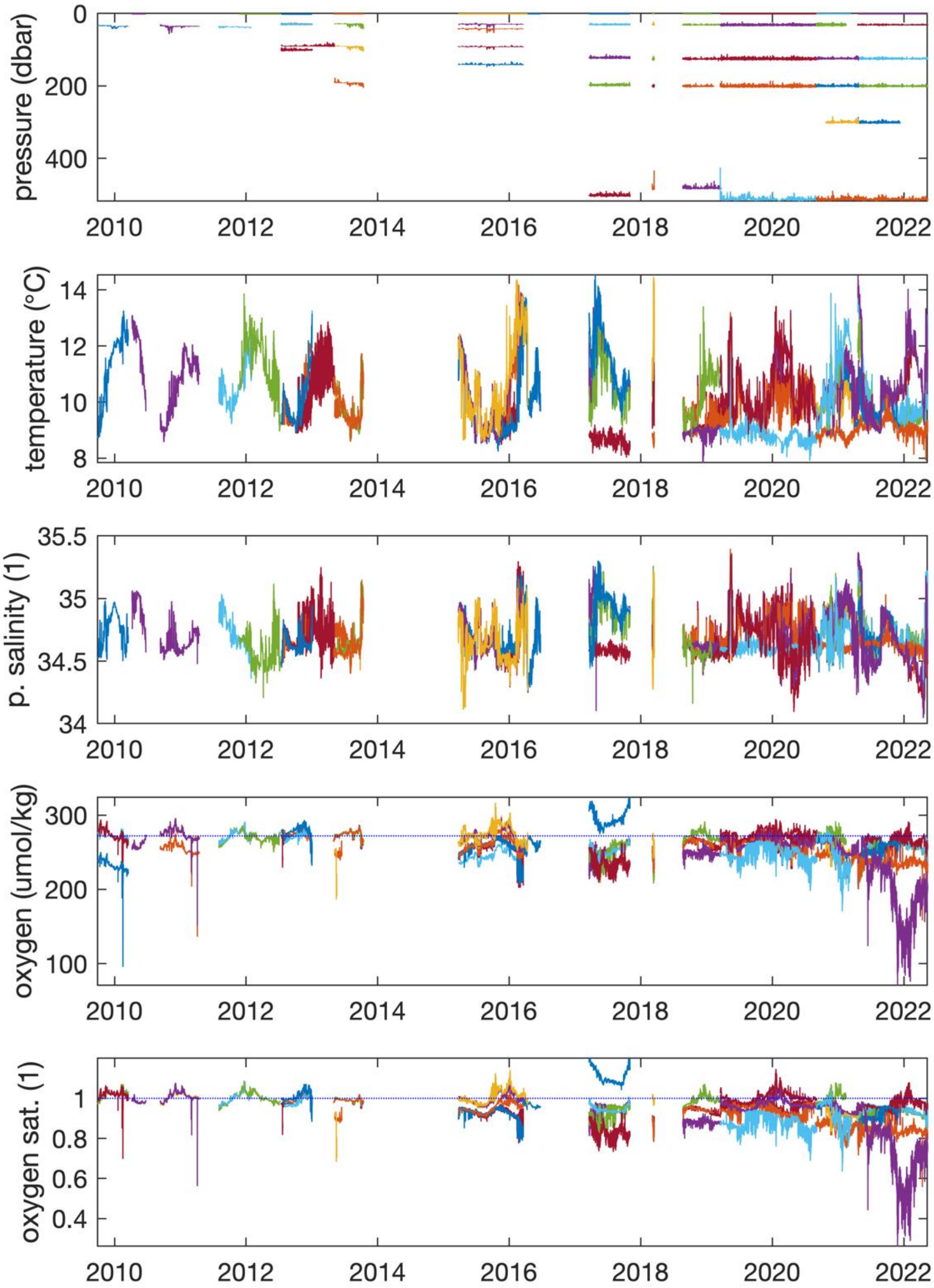

Figure 3. Overview of raw T, S, oxygen results prior to QC.

The colours correspond to the depth of the sensor, as shown in the top panel.

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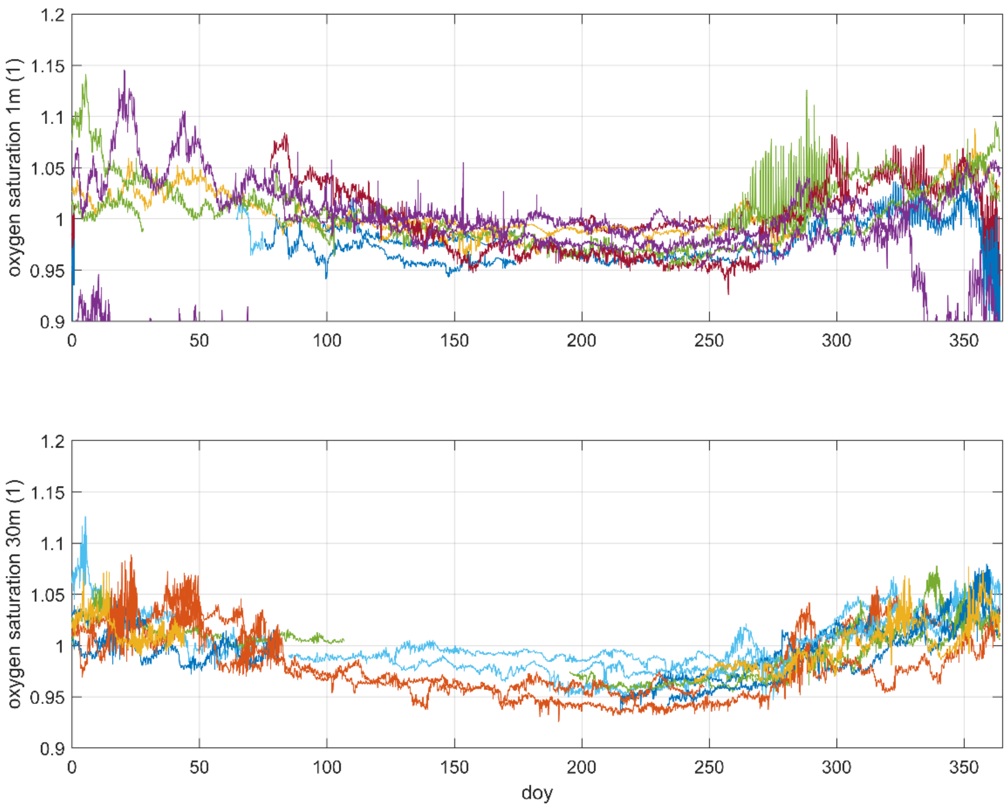

Figure 4. Oxygen at 1m and 30m by day of the year.

Different colours indicate different sensors.

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Table 1. SOTS Oxygen Sensors 2006-2021

Deployment	Model	Serial Number	Nominal Depth
Pulse-6-2009	Optode 3975	1161	37.5
Pulse-6-2009	SBE43	1634	37.5
SOFS-1-2010	Optode 3830	1157	1.2
Pulse-7-2010	SBE16plus	01606331	31.1
Pulse-7-2010	Optode 3975	1161	31.1
Pulse-7-2010	SBE43	1635	31.1
Pulse-8-2011	Optode 3975	1158	34
Pulse-8-2011	SBE43	1634	34
SOFS-2-2011	Optode 3830	1157	1.5
SOFS-3-2012	Optode 3830	1420	2
SOFS-3-2012	SBE37SMP-ODO-RS232	9513	30
SOFS-3-2012	SBE37SMP-ODO-RS232	9514	100
Pulse-9-2012	Optode 3975	1158	38.5
Pulse-9-2012	SBE43	1635	38.5
Pulse-9-2012	SBE37SMP-ODO-RS232	03709515	100
SOFS-4-2013	Optode 3830	1157	1.01
Pulse-10-2013	Optode 3975	1420	28
Pulse-10-2013	SBE43	1634	28
Pulse-10-2013	SBE37SMP-ODO-RS232	03709538	100
Pulse-10-2013	SBE37SMP-ODO-RS232	03709513	200
SOFS-5-2015	Optode 3830	1419	1
Pulse-11-2015	SBE16plus	01606330	28
Pulse-11-2015	Optode 3975	1420	28
Pulse-11-2015	SBE43	1634	28
Pulse-11-2015	SBE37SMP-ODO-RS232	03709538	50
Pulse-11-2015	SBE37SMP-ODO-RS232	03709513	100
Pulse-11-2015	SBE37SMP-ODO-RS232	03709514	150
FluxPulse-1-2016	Optode 3830	1157	1.01
SOFS-6-2017	Optode 3830	1158	1
SOFS-6-2017	SBE37SMP-ODO-RS232	03709538	30
SOFS-6-2017	SBE37SMP-ODO-RS232	03709513	125
SOFS-6-2017	SBE37SMP-ODO-RS232	03709514	200
SOFS-6-2017	SBE37SMP-ODO-RS232	03714700	500
SOFS-7-2018	Optode 3830	1420	1
SOFS-7-2018	SBE37SMP-ODO-RS232	03715969	30
SOFS-7-2018	SBE37SMP-ODO-RS232	03715970	125
SOFS-7-2018	SBE37SMP-ODO-RS232	03715971	200
SOFS-7-2018	SBE37SMP-ODO-RS232	03715972	480
SOFS-7.5-2018	Optode 3830	1420	1
SOFS-7.5-2018	SBE37SMP-ODO-RS232	03715969	30
SOFS-7.5-2018	SBE37SMP-ODO-RS232	03715970	125
SOFS-7.5-2018	SBE37SMP-ODO-RS232	03715971	200
SOFS-7.5-2018	SBE37SMP-ODO-RS232	03715972	480
SOFS-8-2019	Optode 3830	1419	1

Deployment	Model	Serial Number	Nominal Depth
SOFS-8-2019	SBE37SMP-ODO-RS232	03720126	30
SOFS-8-2019	SBE37SMP-ODO-RS232	03709513	125
SOFS-8-2019	SBE37SMP-ODO-RS232	03709514	200
SOFS-8-2019	SBE37SMP-ODO-RS232	03720127	510
SOFS-9-2020	Optode 3830	1420	1
SOFS-9-2020	SBE37SMP-ODO-RS232	03715969	30
SOFS-9-2020	SBE37SMP-ODO-RS232	03715970	125
SOFS-9-2020	SBE37SMP-ODO-RS232	03714700	200
SOFS-9-2020	SBE37SMP-ODO-RS232	03715971	300
SOFS-9-2020	SBE37SMP-ODO-RS232	03715972	510
SOFS-10-2021	Optode 4831	506	1
SOFS-10-2021	SeaPHOXv2	2016	30
SOFS-10-2021	SBE37SMP-ODO-RS232	03709513	125
SOFS-10-2021	SBE37SMP-ODO-RS232	03709514	200
SOFS-10-2021	SBE37SMP-ODO-RS232	3720126	300
SOFS-10-2021	SBE37SMP-ODO-RS232	3721154	510

Only recovered sensors with useful data are listed. **Depth in meters is nominal, as estimated from mooring designs and anchor positions. Sensor pressure measurements provide the best estimates of the actual time-varying sensor depths. These are detailed in the Annual SOTS Sensor Reports and provided in the NetCDF data files.*

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3.1 Oxygen Sensor Types

- Aanderra Optode 3830 (with 3975 adaptor) logged by SOFS data logger, with separate SBE37 to measure temperature and salinity, assumed depth of 1m, unpumped
- Aanderra Optode 4831 logged by SOFS data logger, with separate SBE37 to measure temperature and salinity, assumed depth of 1m, unpumped
- Aanderra Optode 3830 (with 3975 adaptor) using voltage output logged by SBE16plus along with pressure, temperature and salinity (on Pulse 30m package), pumped
- SBE43 voltage output, logged by SBE16plus along with pressure, temperature and salinity (on Pulse 30m package) pumped.
- SBE63 attached to SBE37-SMP used after 2012 on Pulse and SOFS moorings, pressure, temperature and salinity logged all measured by SBE37-SMP, pumped.

3.1.1 SBE43

Performance

Measurement Range	120% of surface saturation in all natural waters (fresh and salt)
Initial Accuracy	± 2% of saturation
Typical Stability	0.5% per 1000 hours of deployed time (clean membrane)
Response Time Tau*	2 to 5 sec for 0.5-mil membrane. 8 to 20 sec for 1.0-mil membrane *Time to reach 63% of final value for a step change in oxygen; dependent on ambient water temperature and flow rate (see Application Note 64 for discussion)

Comparison of SBE43 SN 1643 calibrations

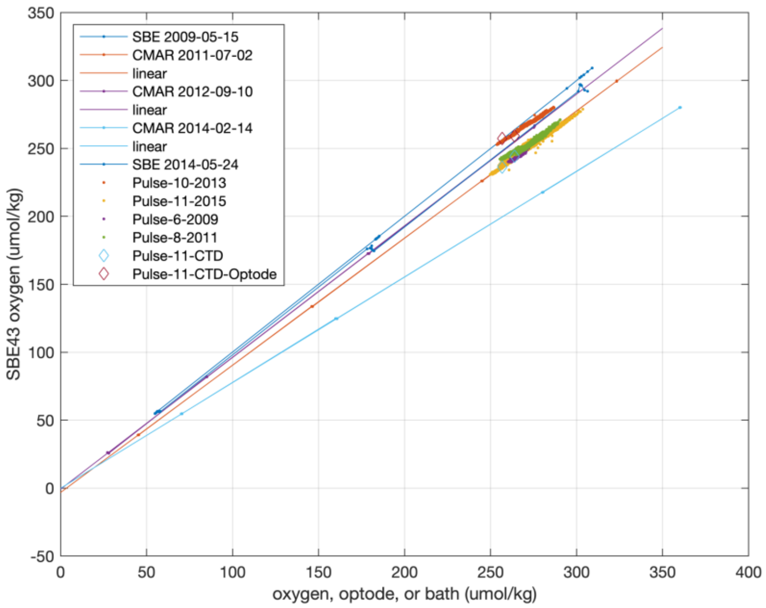

Figure 5. SBE43 SN 1634 plot of calibration, sensor oxygen vs bath and sensor oxygen vs optode oxygen for deployment data

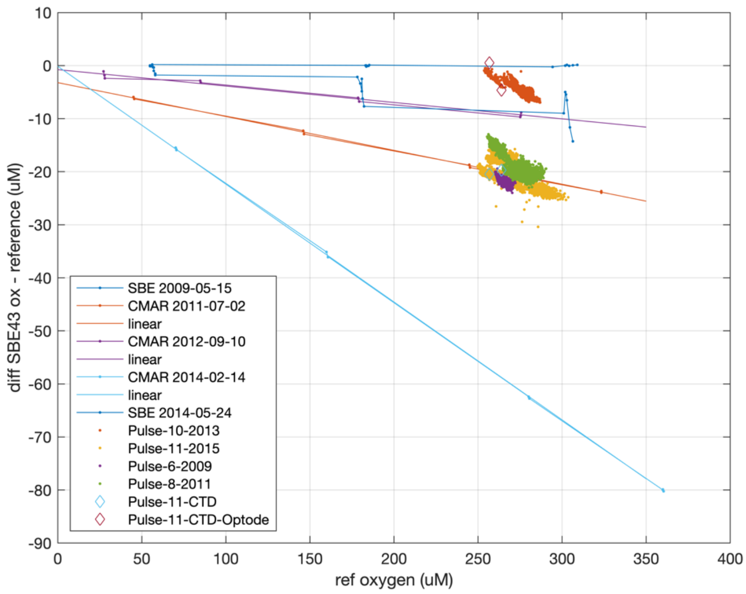

Figure 6 Sensor differences to reference (bath or Optode) oxygen.

Figure 5 and Figure 6show calibrations compared to initial calibration in 2009,

- deployed on Pulse-6 in 2009 then calibrated by CMAR in 2011,
- deployed on Pulse-8, calibrated by CMAR in 2012,
- deployed on Pulse-10 in 2013, calibrated by Sea Bird in 2014
- deployed on Pulse-11 in 2015.

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Between the Sea Bird calibrations in 2009 and 2015 the sensor only changed by 10 umol/kg (at 270 umol/kg); the Pulse-10 data compared to the Optode is between these two calibrations. The Sea Bird calibration in 2012 is similar to the CMAR calibration in 2012. This sensor is ~ 20 umol/kg low in the Pulse-6, Pulse-8 and Pulse-11 deployments, compared to the Optode data. In general, the changes were towards reduced sensitivity over time, consistent with sensor properties as observed by others (Bittig et al., 2018).

3.1.2 Optode Sensor

Technical Details

Oxygen:	O_2- Consentration	Air Saturation
Measurement Range:	0 – 1000 µM[1)]	0 - 300%
Calibration method:	40-point automatic calibration, 20-point verification, 3 fully Winkler calibrated optodes for referencing	
Foils:	Pre-burned PreSens Pst3 foils	
Calibration Range [2)]:	0 – 500 µM	0 - 150%
Resolution:	< 0.1 µM	0.05 %
Accuracy:	< 2 µM or 1.5%[3)]	<1.5 %[4)]
Response Time (63%):		
4831F	(with fast response foil)	<8 sec
4831	(with standard foil)	<25 sec
Typical field drift:	<0.5 % per year	

Figure 7. Optode specifications from Aandreaa Optode sensors

Optode sensors are paired with a SBE37 (or SBE16) temperature sensor to measure the sea water temperature (and salinity).

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3.1.3 SBE64 Optical DO sensor

Performance

Measurement Range	120% of surface saturation in all natural waters (fresh and salt)
Initial Accuracy	larger of ± 3 μmol/kg (equivalent to 0.07 ml/L or 0.1 mg/L) or ± 2%
Sample-Based Drift	< 1 μmol/kg/100,000 samples (20 °C)
Resolution	0.2 μmol/kg
Response Time	(τ, 63% response): < 6 sec (20 °C)
Sampling Speed	1 Hz (1 sample/sec)

3.2 Oxygen Calculation

Two oxygen parameters are calculated

DOX2 – cf standard_name moles_of_oxygen_per_unit_mass_in_sea_water with units of umol/kg

DOXS – cf standard_name fractional_saturation_of_oxygen_in_sea_water with units of 1, ie. dimensionless

the ratio: $\frac{\text{moles\_of\_oxygen\_per\_unit\_mass\_in\_sea\_water}}{\text{moles\_of\_oxygen\_per\_unit\_mass\_in\_sea\_water\_at\_saturation}}$

OXSOL – long_name moles_of_oxygen_per_unit_mass_in_sea_water_at_saturation with units of umol/kg is also included in the netCDF files.

3.2.1 SBE43

Data processing: From Sea Bird AN64 (Sea Bird 2013)

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$$Oxygen\ (ml/l) = \left\{ Soc * \left(V + Voffset + tau(T,P) * \frac{\partial V}{\partial t} \right) \right\} * Oxsol(T,S) * \left(1.0 + A*T + B*T^2 + C*T^3\right) * e^{\left(\frac{E*P}{K}\right)}$$

where.....

Description	Symbol	Definition
Computed	Oxygen	Dissolved oxygen concentration (ml/l)
Measured Parameters	T	CTD Temperature (ITS-90, °C)
	P	CTD Pressure (decibars)
	S	CTD Salinity (psu)
	V	SBE 43 temperature-compensated output oxygen signal (volts)
Calibration Coefficients	Soc	Oxygen signal slope
	Voffset	Voltage at zero oxygen signal
	A, B, C	Residual temperature correction factors
	E	Pressure correction factor
	tau20	Sensor time constant tau (T,P) at 20 °C, 1 atmosphere, 0 PSU; slope term in calculation of tau(T,P)
	D1, D2	Temperature and pressure correction factors in calculation of tau(T,P)
	H1, H2, H3	Hysteresis correction factors
Calculated Value	Oxsol(T,S)	Oxygen saturation value after Garcia and Gordon (1992); see *Appendix A*
	δV/δt	Time derivative of SBE 43 output oxygen signal (volts/second)
	tau(T,P)	Sensor time constant at temperature and pressure = tau20 * exp (D1 * P + D2 * [T – 20])
	K	Absolute temperature

Sea-Bird uses the following equations to convert oxygen calibrated in ml/l to umol/kg, in which the factor 44600 is the reciprocal of the specific molar volume for O_2 gas at standard temperature and pressure (22,391.6 mL mol^{-1}; (Garcia & Gordon, 1992):

$$\left[\frac{umol}{kg}\right] = \left[\frac{ml}{l}\right] * {}^{44600}\!/\!(sigma\ theta(P = 0, Theta, S) + 1000)$$

where

sigma_theta (potential density) is the density a parcel of water would have if it were raised adiabatically to the surface without change in salinity. sigma_theta is calculated with: pressure = 0;

Theta (potential temperature; temperature a parcel of water would have if it were raised adiabatically to the surface); and S (salinity)

3.2.2 Optode

By nature the relationship between the phase shift and oxygen concentration should follow Stern-Volmer relationship. Uchida et al., 2008 suggested a modified Stern-Volmer function:

$$[O_2]' = \frac{(\frac{P_0}{P_c} - 1)}{K_{SV}}$$

And:

$$Ksv = C0 + c1\ t + c2\ t\ 2$$

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$$P0 = c3 + c4\ t$$

$$Pc = c5 + c6\ P_r$$

Where t is temperature (^{0}C) and Pr is the raw phase shift reading.

3.2.3 Salinity Compensation of Data

The O_2 concentration sensed by the Optode is the partial pressure of dissolved oxygen in water.

Since the foil is only permeable to gas and not water, the Optode cannot sense the effect of salt dissolved in the water, hence the Optode always measures as if immersed in fresh water.

If the salinity property in the sensor is set to zero, then the compensated O_2 concentration, O2c in uM is calculated from the following equation

$$O2c = [O2]e^{S(B0+B1\ Ts+B2\ Ts2+B3\ Ts3)+C0\ S2}$$

Where:

O2 is the measured O_2 concentration

S = measured practical salinity

Ts = scaled temperature = $\ln(\frac{298.15-t}{273.15+t})$

T = temperature (^{0}C)

B0 = -6.24097 C0 = -3.11680e-7

B1 = -6.934498e-3

B2 = -6.90358e-3

B4 = -4.29155e-3

3.2.4 Depth Compensation of Data

The response of the sensing foil decreases to some extent with the ambient water pressure (3.2% lower response per 1000 m of water depth or dbar (Uchida et al., 2008).

The depth compensated O_2 concentration O2s is calculated from the following equation

$$O2s = O2\left(1 + \frac{0.032\ d}{1000}\right)$$

Where:

d is depth in dbar

O2 is the measured O2 concentration in uM.

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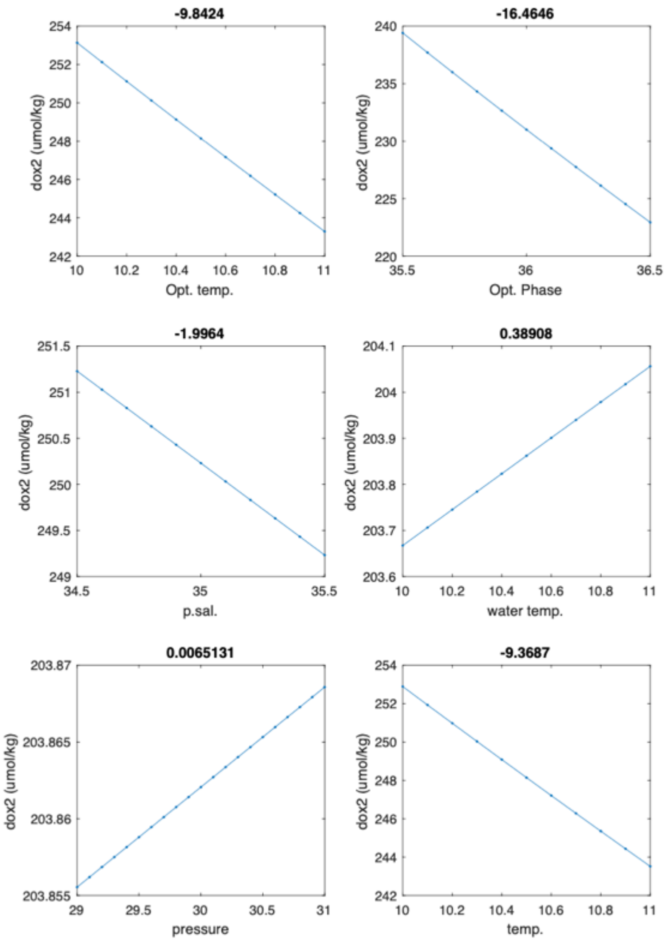

Figure 8. Optode Oxygen Calculation sensitivity to input parameters

Figure 8 shows the sensitivity of each input parameter in the calculation of oxygen, at nominal temperature of 10 (^{o}C), salinity of 35 (1) and pressure of 30 (dbar). The Optode temperature is the effect of temperature on the sensing foil, and the water temperature is the effect of temperature on the solubility of oxygen in water.

Resulting sensitivity equation:

$$dOx = -9.84 * dOptodeTemp - 16.46 * dOptodePhase - 1.99 * dPSal + 0.39 * dwaterTemp + 0.0065 * dPressure$$

Combining the OptodeTemp and waterTemp terms

$$dOx = -9.37 * dTemp - 16.46 * dOptodePhase - 1.99 * dPSal + 0.0065 * dPressure$$

dOx in umol/kg

dTemp, dwaterTemp, dOptodeTemp in degrees C,

dPSAL in practical salinity units (1)

dPressure in dBar

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Figure 9. Difference between optode temp and SBE temp.

Figure 9 shows that the ~0.05C difference between the two translates to a 0.5umol/kg oxygen difference or 0.2% saturation. This is consistent with previous work and principles from Bittig et al., 2018

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Comparison of Optode SN 1158 calibrations

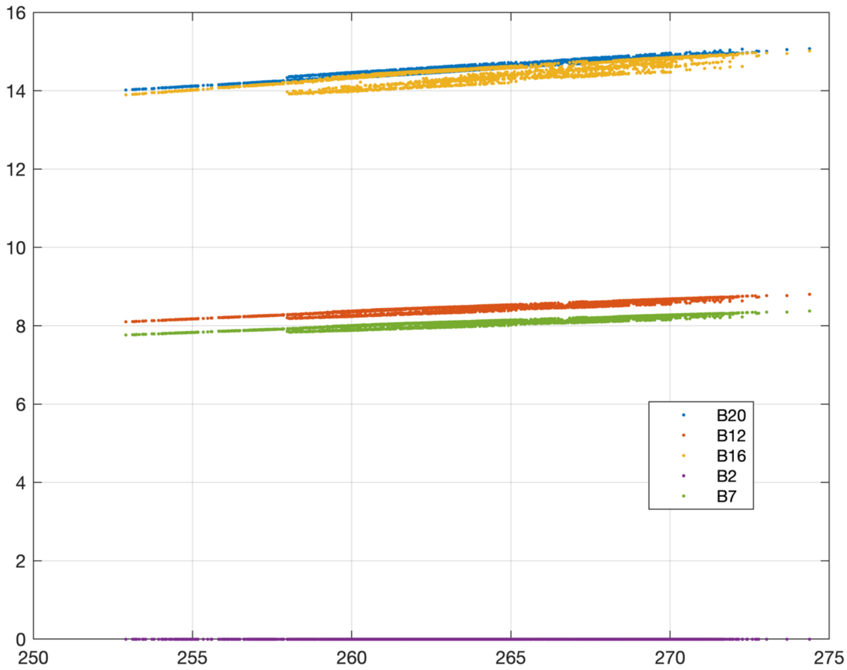

Figure 10. delta Oxygen vs oxygen for calibrations compared to 2010 calibration

Figure 10 shows the difference between calculated oxygen using batch B2 calibration coefficients and the subsequent calibrations B7, B12, B16 and B20 using data from Pulse-8 mooring data.

B (batch)	date	file	slope	Offset (umol/kg)
2	2010-11	calcoef_3975_1158_Uch-CMAR_cal-B2svs.txt	1.000	0.00
7	2011-12	calcoef_3975_1158_Uch-CMAR_cal-B7wink.txt	0.973	-0.86
	2012-07	Deploy Pulse-9		
12	2013-05	calcoef_3975_1158_Uch-CMAR_cal-B12svs.txt	0.970	-0.17
16	2014-08	calcoef_3975_1158_Uch-CMAR_cal-B16svs.txt	0.953	-1.37
20	2016-05	CSV_calcoef_T-aux_3975_1158_CMAR_cal-B20svs.txt	0.952	-1.16

Figure 10 shows four characteristics of Optode sensors

- The drift during deployment is low, and less than 1 umol/kg,
- The drift when the Optode is out of the water (not deployed) was higher, around 6 umol kg-1 year-1, and this is consistent with previous observations (Bittig et al., 2018).
- The temperature compensation between calibrations is good and less than 0.5 umol/kg,
- The change in sensitivity (slope) dominates the difference over any offset change, again as observed previously (Bittig et al., 2018)

3.3 All SBE43 data compared to Optode data

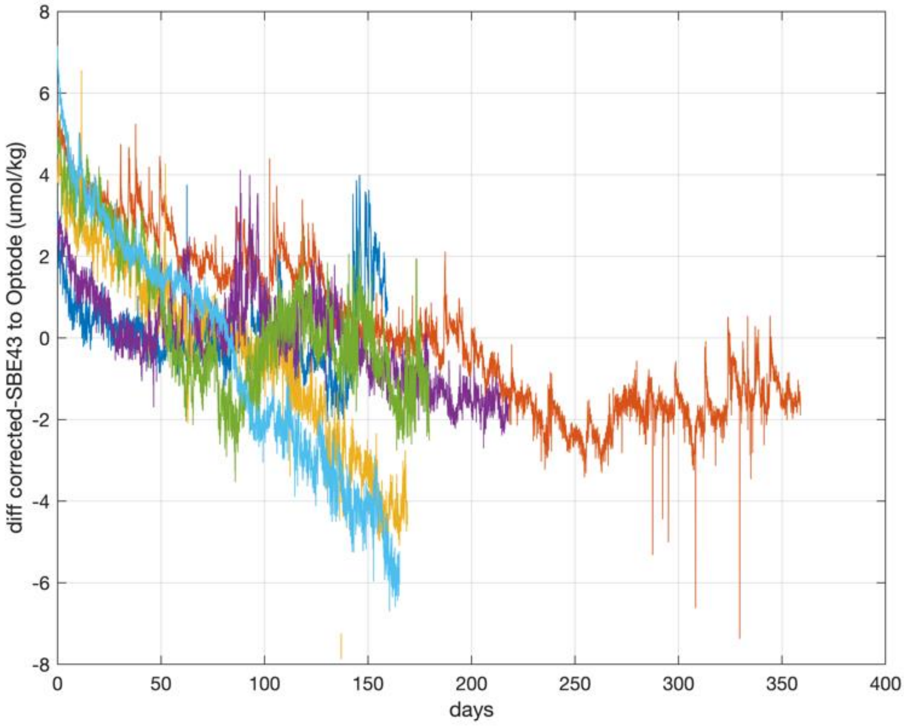

Figure 11 Differences between SBE43 and Optode data, deployed on Pulse mooring at 30m vs days deployed.
Overall the SBE43 can drift 12 umol/kg over a 6 month deployment

Conclusion: The SBE43 sensors drifted (towards lower sensitivity) faster than the Optode sensors. On the other hand, the SBE43 does not suffer from the need for pre-soaking that applies to the Optode sensors.

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4 Summary of Instrument Handling and Data Processing

Pre-deployment preparation

Instruments were prepared following manufacturer recommendations, including drying of pressure cases, greasing of seals, and insertion of new batteries. Instrument clocks were set to UTC via on-line synchronization. Instruments were mounted and measurement frequencies were scheduled as described for each instrument in the SOTS Annual Sensor reports. In general, mounting was via clamping to the mooring wires for SBE37-ODO instruments and inside in-line instrument cages for other models, with the instruments downward-facing. Measurement frequency was at least hourly, the details are shown in Table 1.

In some cases, batches of the instruments were operated either in a common water bath or on the CTD-Rosette at sea prior to deployment to provide an inter-comparison of their outputs. This data is sparse and is discussed in section 6.4.2 as part of the assessment of measurement uncertainty.

Post-deployment evaluations

After recovery, the instruments were connected to a UTC time-synchronized computer and any clock drift was noted.

Instrument Calibrations

Pre- and post-deployment calibrations were carried out either by the manufacturer or the CSIRO Hydrochemistry Facility.

Common time scale product

In this report, sensor data is examined at its full temporal resolution, which varied from 30 minutes to every two hours. No interpolation to a common grid is provided in the gridded product.

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5 QC Specifics

Our overall Quality Control philosophy is to remove no data, only to indicate probable data quality for each observation using a system of QC flags, as shown in Table 2. Flags 1 to 4 are standard in the US IOOS, QARTOD, and Argo programs (citations below). Flag 6 is added here to indicate data collected before or after mooring deployment, which has not been evaluated further.

Table 2. Flags used in salinity quality control

FLAG	DESCRIPTION
Pass, Good data = 1	Data have passed the highest level of quality control
Probably good = 2	Data were unable to be evaluated by at least one test, but were not flagged as suspect or fail by any other tests
Bad data that are potentially correctable = 3	Data have failed one or more tests indicating suspicious values, however it is possible that sensor failure has not occurred, and possibly correctable
Bad data = 4	Data have failed one or more tests indicating instrument or mooring failure
Sensor active but not deployed = 6	Data obtained when the sensor was out of water, or not at the assigned depth.

As the starting point for delayed mode quality control (DMQC) we adopted the hierarchy of tests, listed in Table 3 recommended by the Integrated Ocean Observing System (IOOS) for Quality Assurance of Real-Time Oceanographic Data (QARTOD; https://ioos.noaa.gov/project/QARTOD), using Version 2.1 of the Manual for Real-Time Quality Control of In-situ Temperature and Salinity Data (Bushnell & Worthington, 2020).

Each test was applied to all data points, including those that had been flagged as fail (flag=4) or suspect (flag=3) in previous tests. At the end of the sequence of tests, the highest flag produced by any test was assigned to each data point.

Importantly, salinity is a derived product obtained by combining temperature and conductivity observations. For this purpose, we used only those temperature and salinity measurements that received QC flags of 1 or 2 in our previous examination of these sensors (Jansen et al., 2022a; Jansen et al., 2020).

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Table 3. QC tests recommended by QARTOD

TEST GROUP	TEST NO.	TEST NAME	CONDUCTED
Group 1 *Required*	1	Timing/Gap Test	Yes, modified
	2	Syntax Test	Yes, modified
	3	Location Test	Yes
	4	Gross Range Test	Yes
	5	Climatology Test	Yes
Group 2 *Strongly Recommended*	6	Spike Test	No
	7	Rate of Change Test	No
	8	Flat Line Test	No
Group 3 *Suggested*	9	Multivariate Test	Yes
	10	Attenuated Signal Test	Via visualisation
	11	Neighbour Test	Via visualisation

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5.1 Applied tests

5.1.1 Data visualization and identification of common problems

In working through the QARTOD tests, visualisation of the measured oxygen records and the flagging results made it clear that some tests functioned better than others, and many tests required compromises. Put simply, defining thresholds for flagging the data represents an optimal compromise between identifying too many false positives (i.e. data is accepted, even though it is bad) versus too many false negatives (i.e. data is rejected, even though it is good). To some degree, this optimal compromise depends on the use of the data. For example, if quantifying the annual dissolved oxygen cycle is the target, then flagging occasional short-lived oxygen excursions (which might be either instrumental spikes or rare events related to the passage of sub-tropical water parcels) as bad eliminates noise in the seasonal cycle and represents little loss of fidelity. However, if identification of the occasional presence of small subtropical water parcels is the target, then it is better not to exclude these results.

Ideally, the sensor records would unambiguously separate rare but real events from episodic sensor faults, but this can be very hard to assess, especially if there is only one sensor in the region of interest and if the full nature of the oceanic variability in the region is not yet known. The second of these problems is particularly problematic in the Southern Ocean at very shallow depths, because rough conditions generally mean that CTD casts sample the top 5m of the sea poorly if at all, and the large footprints of satellite sea surface measurements mean that spatially restricted high intensity events would not be visible.

Visualisation is an essential tool to define the nature of sensor problems and thus the selection of appropriate thresholds for the tests.

The issues informed the selection of thresholds for the QARTOD tests to flag ‘bad’ (flag 4).

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5.2 Detailed specifications and applications of the QARTOD tests

Test 1) Timing/Gap Test (Required)

Check for arrival of data.		
Test determines that the most recent data point has been measured and received within the expected time window (TIM_INC) and has the correct time stamp (TIM_STMP). **Note:** For those systems that do not update at regular intervals, a large value for TIM_STMP can be assigned. The gap check is not a solution for all timing errors. Data could be measured or received earlier than expected. This test does not address all clock drift/jump issues.		
Flags	**Condition**	**Codable Instructions**
Fail=4	Data have not arrived as expected.	If NOW – TIM_STMP > TIM_INC, flag = 4
Suspect=3	N/A	N/A
Pass=1	Applies for test pass condition.	N/A
Test Exception: None.		
Test specifications to be established locally by the operator. **Example:** TIM_INC = 1 hour		

Implementation for SOTS delayed mode QC was as follows:

This test is designed for real time data, and its application to delayed mode is very limited.

For SOTS instruments we retain all time-stamped data, and do not do any flagging or filling if a time point is missing. In other words, we accept missing intervals and expect the user to recognize that the time series may not be evenly spaced. Thus, calculations should always estimate the time interval when integrating values across adjacent data points, e.g. when calculating rates of oxygen content changes.

For time stamps which are missing values of one or more variables (T, S, etc.), these are set to NaNs when the data is parsed from the instrument transmissions. These values are then flagged by Test 4) Gross Range Test (below).

Test 2) Syntax Test (Required)

Check to ensure that the message is structured properly		
Received data message (full message) contains the proper structure without any indicators of flawed transmission such as parity errors. Possible tests are: a) the expected number of characters (NCHAR) for fixed length messages equals the number of characters received (REC_CHAR), or b) passes a standard parity bit check, cyclic redundancy check (CRC), etc. Many such syntax tests exist, and the operator should select the best criteria for one or more syntax tests. Capabilities for dealing with flawed messages vary among operators; some may have the ability to parse messages to extract data within the flawed message sentence before the flaw. A syntax check is performed only at the message level and not within the message content. In cases where a data record requires multiple messages, this check can be performed at the message level but is not used to check message content.		
Flags	**Condition**	**Codable Instructions**
Fail=4	Data sentence cannot be parsed to provide a valid observation.	If REC_CHAR ≠ NCHAR, flag = 4
Suspect =3	N/A	N/A
Pass=1	Expected data sentence received; absence of parity errors.	
Test Exception: None.		
Test specifications to be established locally by the operator. **Example:** NCHAR = 128		

Implementation for SOTS delayed mode QC was as follows:

This test is designed for real time data, and its application to delayed mode is very limited.

If the message cannot be parsed, then the record will show a missing time stamp. No flagging is done.

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Test 3) Location Test (Required)

Check for reasonable geographic location.		
Test checks that the reported present physical location (latitude/longitude) is within operator-determined limits. The location test(s) can vary from a simple impossible location to a more complex check for displacement (DISP) exceeding a distance limit (RANGEMAX) based upon a previous location and platform speed. Operators may also check for erroneous locations based upon other criteria, such as reported positions over land, as appropriate.		
Flags	**Condition**	**Codable Instructions**
Fail=4	Impossible location.	|LAT | > 90 or |LONG | > 180
Suspect=3	Unlikely platform displacement.	DISP > RANGEMAX
Pass=1	Applies for test pass condition.	N/A
Test Exception: Test does not apply to fixed deployments when no location is transmitted.		
Test specifications to be established locally by the operator. **Example:** Displacement DISP calculated between sequential position reports, RANGEMAX = 20 km		

Implementation for SOTS delayed mode QC was as follows:
The locations of the sensors were designated as being the locations of the mooring anchor positions (as estimated from the anchor drop position and/or acoustic triangulation - details are in the SOTS Annual Overview Reports). This location information is provided as a single pair of latitude and longitude values in the NetCDF files.

In addition, for the SOFS and Pulse surface floats, which collect and transmit GPS positions, this information is provided as time series of latitudes and longitudes, with flagging of:
Flag 4, QARTOD conventions for impossible latitudes and longitudes
Flag 3, latitude outside 30-60°; longitude outside 130-150 °E.
Note that this wide range does NOT flag data outside the mooring 'watch circles', that has at times been collected after surface portions of the moorings have broken free and drifted. Note also that the locations of the annual re-deployments of the SOTS moorings have typically varied by ~10 miles, and at times by as much as 60 miles.
Users who wish to limit data to within a watch circle, to some other restricted area, or to examine variations with location should use these time series of latitudes and longitudes, rather than the nominal positions provided by the anchor locations.

We also extended this test to include flagging the pressure records of the sensors (as an indication of their depth location). This allows us to flag data collected before and after the mooring has reached its resting place on the sea floor. This data can be useful for testing changes in calibrations, examining pressure effects on sensors, etc. After visualizing the mooring pressure records, we set a single pair of date/time stamps for the beginning and end of the moored period for all sensors on each mooring, and all data before and after these times is assigned Flag 6 to indicate that it was not collected as part of the 'moored observations' period. Note that the pressures of individual sensors may still vary in this period, and this should be assessed using those records (just as the locations may vary and must be assessed using the latitude and longitude variables as described above).

Test 4) Gross Range Test (Required)

Data point exceeds sensor or operator-selected min/max. Applies to T, SP, C and P.		
All sensors have a limited output range, and this can form the most rudimentary gross range check. No values less than a minimum value or greater than the maximum value the sensor can output (T_SENSOR_MIN, T_SENSOR_MAX) are acceptable. Additionally, the operator can select a smaller span (T_USER_MIN, T_USER_MAX) based upon local knowledge or a desire to draw attention to extreme values. **NOTE:** Operators may choose to flag as suspect values that exceed the calibration span but not the hardware limits (e.g., a value that sensor is not capable of producing or negative conductivity).		
Flags	**Condition**	**Codable Instructions**
Fail=4	Reported value is outside of sensor span.	If T_n < T_SENSOR_MIN, or T_n > T_SENSOR_MAX, flag = 4
Suspect=3	Reported value is outside of operator-selected span.	If T_n < T_USER_MIN, or T_n > T_USER_MAX, flag = 3
Pass=1	Applies for test pass condition.	
Test Exception: None.		
Test specifications to be established locally by the operator. **Examples:** The following global range min/max are applied on some climate and forecast standard-names in the IMOS toolbox: depth: -5/12,000 m sea_water_pressure: -5/12,000 decibars (dbar) sea_water_pressure_due_to_sea_water: -15/12,000 dbar sea_water_salinity: 2/41 sea_water_temperature: -2.5/40 °C		

Limits are applied to DOX2 (oxygen concentration in umol/kg) and also Oxygen Saturation.

Implementation for SOTS delayed mode QC was as follows:

Flag 4: Value outside of the following limits:

DOX2_Sensor_Min = 150 DOX2_Sensor Max = 350

DOXS_Sensor_Min = 0.5 DOXS_Sensor Max = 1.2

Flag 3: no thresholds or flags assigned

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Test 5) Climatology Test (Required)

Test that data point falls within seasonal expectations. Applies to T and SP.		
This test is a variation on the gross range check, where the thresholds T_Season_MAX and T_Season_MIN are adjusted monthly, seasonally, or at some other operator-selected time period (TIM_TST). Expertise of the operator is required to determine reasonable seasonal averages. Longer time series permit more refined identification of appropriate thresholds. The ranges should also vary with water depth, if the measurements are taken at sites that cover significant vertical extent and if climatological ranges are meaningfully different at different depths (e.g., narrower ranges at greater depth).		
Flags	**Condition**	**Codable Instructions**
Fail=4	Because of the dynamic nature of T and S in some locations, no fail flag is identified for this test.	N/A
Suspect=3	Reported value is outside of operator-identified climatology window.	If T_n < T_Season_MIN or T_n > T_Season_MAX, flag = 3
Pass=1	Applies for test pass condition.	N/A
Test Exception: None.		
Test specifications to be established locally by operator: A seasonal matrix of T_{max} and T_{min} values at all TIM_TST intervals. **Examples:** T_SPRING_MIN = 12 °C, T_SPRING_MAX = 18.0 °C		

No depth gradient has been applied to oxygen as we have not deployed sensors below 500m at SOTS

Implementation for SOTS delayed mode QC was as follows:

Flag 4, none assigned

Flag 3, assigned as follows, based on CTD casts near SOTS (shown at Figure 14 And Figure 15),

DOX2_Sensor_Min = 180 DOX2_Sensor Max = 310

DOXS_Sensor_Min = 0.8 DOXS_Sensor Max = 1.15

Figure 12 and 13, all oxygen data plotted by depth, in oxygen concentration and oxygen saturation. Colours indicate different sensor deployments.

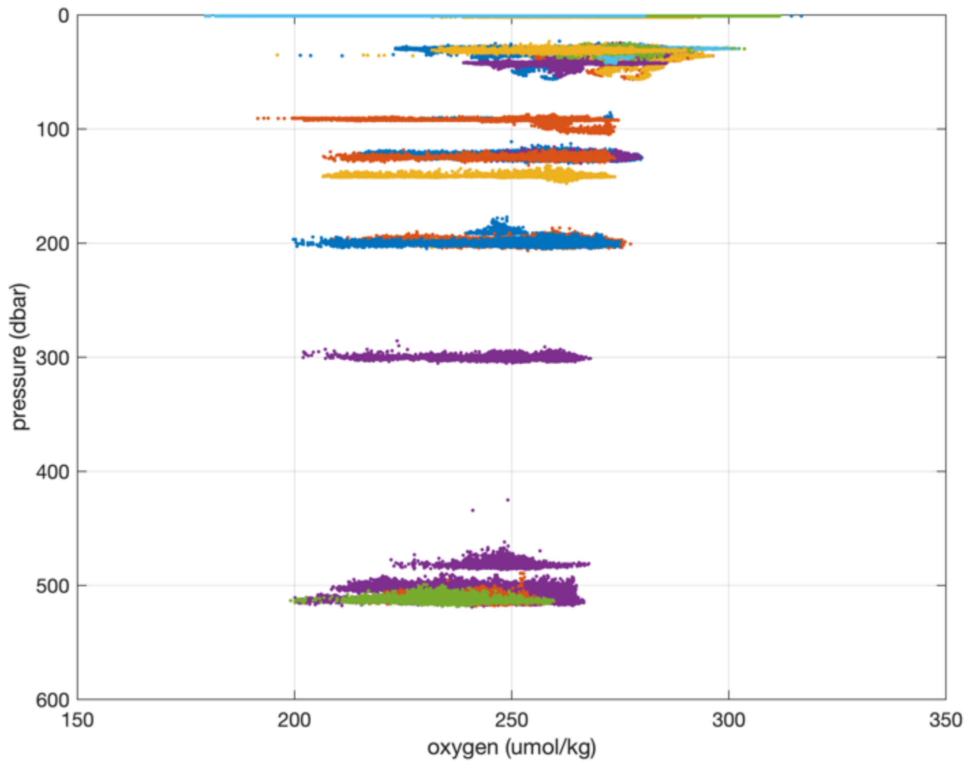

Figure 12 All data oxygen measurements vs depth

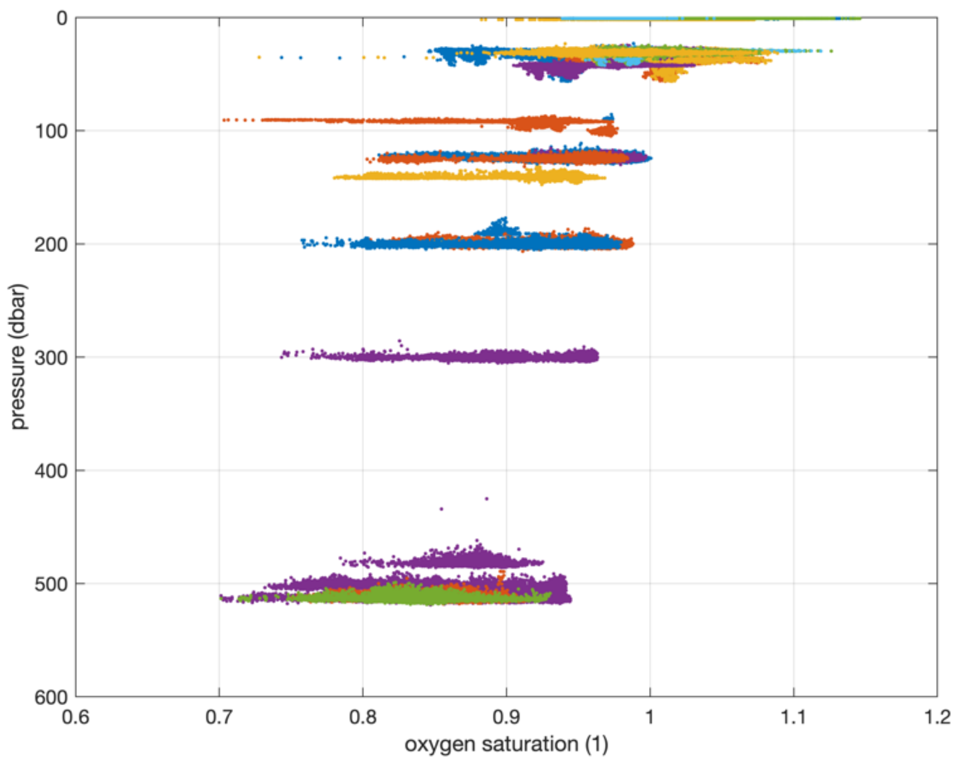

Figure 13 All data oxygen saturation vs depth

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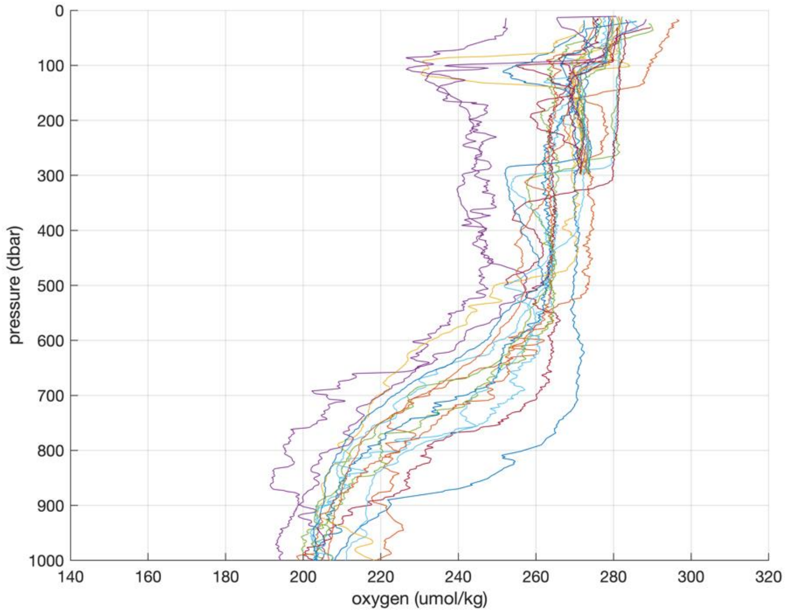

Figure 14 CTD DOX2 from SOTS site

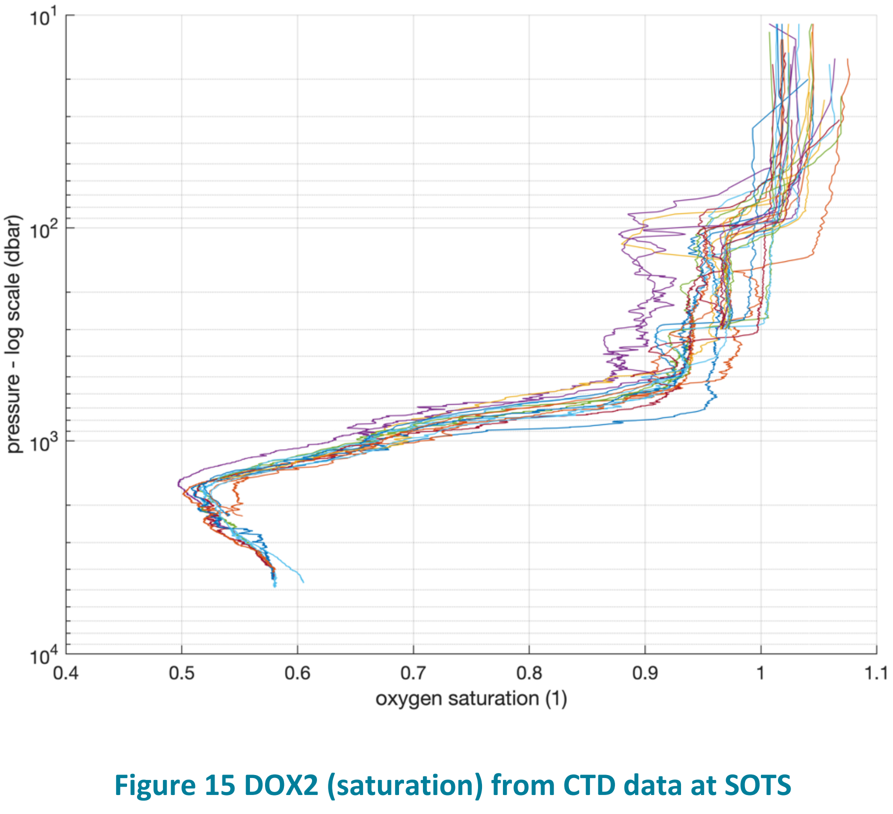

Figure 15 DOX2 (saturation) from CTD data at SOTS

Figure 14 and 15 show oxygen profiles taken at SOTS by CTD between 2009 and 2022, colours are different CTD casts.

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Test 6) Spike Test (Strongly Recommended)

Data point *n*-1 exceeds a selected threshold relative to adjacent data points. Applies to T, SP, C, and P.		
This check is for single value spikes, specifically the value at point *n*-1. Spikes consisting of more than one data point are difficult to capture, but their onset may be flagged by the rate of change test. The spike test consists of two operator-selected thresholds, THRSHLD_LOW and THRSHLD_HIGH. Adjacent data points (n_{-2} and n_0) are averaged to form a spike reference (SPK_REF). The absolute value of the spike is tested to capture positive and negative spikes. Large spikes are easier to identify as outliers and flag as failures. Smaller spikes may be real and are only flagged suspect. The thresholds may be fixed values or dynamically established (for example, a multiple of the standard deviation over an operator-selected period).		
Flags	**Condition**	**Codable Instructions**
Fail=4	High spike threshold exceeded.	If $\mid T_{n-1}$ - SPK_REF$\mid$ > THRSHLD_HIGH, flag = 4
Suspect=3	Low spike threshold exceeded.	If $\mid T_{n-1}$ - SPK_REF$\mid$ > THRSHLD_LOW and $\mid T_{n-1}$ - SPK_REF$\mid$ $\leq$ THRSHLD_HIGH, flag = 3
Pass=1	Applies for test pass condition.	N/A
Test Exception: None.		
Test specifications to be established locally by the operator. **Examples:** THRSHLD_LOW = 3 °C, THRSHLD_HIGH = 8 °C		

NOT Implemented for SOTS delayed mode QC of oxygen

The optical oxygen sensors (SBE63 and Optode) don’t seem to exhibit data spikes. For the SBE43 data some negative spikes are evident, as these sensors were deployed with Optode sensors spike tests were not seen as much advantage. Most ‘spikes’ in the data are coincident with salinity or temperature changes and as such are probably real or indistinguishable from real events.

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Test 7) Rate of Change Test (Strongly Recommended)

Excessive rise/fall test. Applies to T, SP, C, and P.

This test inspects the time series for a time rate of change that exceeds a threshold value identified by the operator. T, SP, C, P values can change substantially over short periods in some locations, hindering the value of this test. A balance must be found between a threshold set too low, which triggers too many false alarms, and one set too high, making the test ineffective. Determining the excessive rate of change is left to the local operator.

The following shows two different examples of ways to select the thresholds provided by QARTOD VI participants. Implementation of this test can be challenging. Upon failure, it is unknown which of the points is bad. Further, upon failing a data point, it remains to be determined how the next iteration can be handled.

Example 1

The rate of change between temperature T_{n-1} and T_n must be less than three standard deviations (3*SD). The SD of the T time series is computed over the previous 25-hour period (operator-selected value) to accommodate cyclical diurnal and tidal fluctuations. Both the number of SDs (N_DEV) and the period over which the SDs (TIM_DEV) are calculated and determined by the local operator.

Example 2

The rate of change between temperature T_{n-1} and T_n must be less than 2 °C +2SD.

$|T_{n-1} - T_{n-2}| + |T_{n-1} - T_n| <= 2*N\_DEV*SD$ (example provided by EuroGOOS).

Flags	Condition	Codable Instructions
Fail=4	No fail flag is identified for this test.	N/A
Suspect=3	The rate of change exceeds the selected threshold.	If $|T_n - T_{n-1}|>N\_DEV*SD$, flag = 3
Pass=1	Applies for test pass condition.	N/A

Test Exception: None.

Test specifications to be established locally by operator.
Example: N_DEV = 3, TIM_DEV = 25

NOT Implemented for SOTS delayed mode QC of oxygen for the same reasoning as the spike test 6.

Test 8) Flat Line Test (Strongly Recommended)

Invariant value. Applies to T, SP, C, and P.

When some sensors and/or data collection platforms fail, the result can be a continuously repeated observation of the same value. This test compares the present observation *n* to a number (REP_CNT_FAIL or REP_CNT_SUSPECT) of previous observations. Observation *n* is flagged if it has the same value as previous observations within a tolerance value, EPS, to allow for numerical round-off error. Note that historical flags are not changed.

Flags	**Condition**	**Codable Instructions**
Fail=4	When the five most recent observations are equal, T_n is flagged fail.	CNT = 0 For *I* = 1,REP_CNT_FAIL If $\lvert T_n - T_{n-i} \rvert$<EPS, CNT = CNT+1 If CNT = REP_CNT_FAIL, flag = 4
Suspect=3	It is possible but unlikely that the present observation and the two previous observations would be equal. When the three most recent observations are equal, T_n is flagged suspect.	CNT = 0 For *I* = 1,REP_CNT_SUSPECT If $\lvert T_n - T_{n-i} \rvert$<EPS, CNT = CNT+1 If CNT = REP_CNT_SUSPECT, flag = 3
Pass=1	Applies for test pass condition.	N/A

Test Exception: None.

Test specifications to be established locally by the operator.
Examples: REP_CNT_FAIL = 5, REP_CNT_SUSPECT= 3, EPS = 0.05°

NOT Implemented for SOTS delayed mode QC of oxygen

The choice of tolerance value for this test is very important, and testing with SOTS data found that for these sensors, which have high digital-analog resolution (SBE37, SBE16, etc.), five repeated values were not observed. Therefore, the test was not implemented. See also the discussion in Jansen et al., 2020 for low analog-digital resolution sensors where repeat values are common but do not indicate errors.

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Test 9) Multi-Variate Test (Suggested)

Comparison to other variables. Applies to T, SP, and P.		
This is an advanced family of tests, starting with the simpler test described here and anticipating growth towards full co-variance testing in the future. It is doubtful that anyone is conducting tests such as these in real time. As these tests are developed and implemented, they should be documented and standardized in later versions of this manual. This example pairs rate of change tests as described in test 7. The T (or SP or P) rate of change test is conducted with a more restrictive threshold (N_T_DEV). If this test fails, a second rate of change test operating on a second variable (salinity or conductivity would be the most probable) is conducted. The absolute value rate of change should be tested, since the relationship between T and variable two is indeterminate. If the rate of change test on the second variable fails to exceed a threshold (e.g., an anomalous step is found in T and is lacking in salinity), then the T_n value is flagged. Note that Test 12, TS Curve/Space Test is a well-known example of the multi-variate test.		
Flags	**Condition**	**Codable Instructions**
Fail=4	No fail flag is identified for this test.	N/A
Suspect=3	T_n fails the rate of change and the second variable does not exceed the rate of change.	If $\|T_n - T_{n-1}\|$>N_T_DEV*SD_T AND $\|SP_n - SP_{n-1}\|$<N_SP_DEV*SD_SP, flag = 3
Pass=1	N/A	N/A
Test Exception: None.		
Test specifications to be established locally by the operator. **Examples:** N_T_DEV = 2, N_TEMP_DEV = 2, TIM_DEV = 25 hours		

NOT Implemented for SOTS delayed mode QC of oxygen

Because oxygen saturation ratio depends on P, T and S, this aspect of the comparison to those variables is achieved implicitly.

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Test 10) Attenuated Signal Test (Suggested)

A test for inadequate variation of the time series. Applies to T, SP, C, and P.		
A common sensor failure mode can provide a data series that is nearly but not exactly a flat line (e.g., if the sensor head were to become wrapped in debris). This test inspects for an SD value or a range variation (MAX-MIN) value that fails to exceed threshold values (MIN_VAR_WARN, MIN_VAR_FAIL) over a selected time period (TST_TIM).		
Flags	**Condition**	**Codable Instructions**
Fail=4	Variation fails to meet the minimum threshold MIN_VAR_FAIL.	If During TST_TIM, SD <MIN_VAR_FAIL, or During TST_TIM, MAX-MIN <MIN_VAR_FAIL, flag = 4
Suspect=3	Variation fails to meet the minimum threshold MIN_VAR_WARN.	If During TST_TIM, SD <MIN_VAR_WARN, or During TST_TIM, MAX-MIN <MIN_VAR_WARN, flag = 3
Pass=1	Applies for test pass condition.	N/A
Test Exception: None.		
Test specifications to be established locally by the operator. **Examples:** TST_TIM = 12 hours MIN_VAR_WARN = 0.5 °C, MIN_VAR_FAIL = 0.1 °C		

Implementation for SOTS delayed mode QC was as follows:

The definition of the minimum variability thresholds (MIN_VAR_FAIL/WARN) requires precise understanding of the oceanographic expectation, and will vary strongly with depth. In this sense it has overlaps with Tests 6 and 7 for spikes and rates of change. Also, as noted in the introduction, such expectations of minimum variability are still under development for the Southern Ocean owing to the sparse history of temporally resolved observations. In practice, the best estimate of the expectation comes from sensors at SOTS that are considered to have functioned without attenuation, and thus are equivalent to an aspect of Neighbour tests. *For this reason, we did not perform Test 10 separately; rather its information was captured by our implementation of Test 11.* In future, as knowledge of minimum variability is obtained, separate implementation of Test 10 may become useful.

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Test 11) Neighbor Test (Suggested)

Comparison to nearby DO sensors		
The check has the potential to be the most useful test when a nearby second sensor is determined to have a similar response. In a perfect world, redundant DO sensors utilizing different technology would be co-located and alternately serviced at different intervals. This close neighbor would provide the ultimate QC check, but cost prohibits such a deployment in most cases. In the real world, there are very few instances where a second DO sensor is sufficiently proximate to provide a useful QC check. Just a few hundred meters in the horizontal and less than 10 meters vertical separation yield greatly different results. Nevertheless, the test should not be overlooked where it may have application. This test is the same as *9) Multi-variate Check – comparison to other variables* where the second variable is the second DO sensor. The selected thresholds depend entirely upon the relationship between the two sensors as determined by the local knowledge of the operator. In the instructions and examples below, data from one site (D01) are compared to a second site (D02). The standard deviation for each site (SD1, SD2) is calculated over the period (TIM_DEV) and multiplied as appropriate (N_DO1_DEV for site DO1) to calculate the rate of change threshold. Note that an operator could also choose to use the same threshold for each site since they are presumed to be similar.		
Flags	**Condition**	**Codable Instructions**
Fail=4	Because of the dynamic nature of DO, no red flag is identified for this test.	N/A
Suspect=3	DO_n fails the DO rate of change and the second DO sensor does not exceed the rate of change.	$\|DO1_n - DO1_{n-1}\|$>N_DO1_DEV*SD1 AND $\|DO2_n - DO2_{n-1}\|$<N_DO2_DEV*SD2
Fail=1		
Test Exception: Anoxic conditions introduce the possibility of repeated zero values, challenging the calculation of time-local thresholds. The neighbor check would only apply to co-located DO sensors in the presence of anoxic conditions.		
Test specifications to be established locally by operator **Examples:** N_DO1_DEV = 2, N_DO2_DEV=2, TIM_DEV = 25 hours		

Implementation for SOTS delayed mode QC was as follows:

In principle, this is a powerful test, particularly when sensors are mounted in pairs and thus either they reinforce the fidelity of the data when they are indistinguishable or emphasize that at least one of the sensors has failed when they differ. Obviously, examination of all neighbouring sensors provides the most powerful approach. Moreover, other aspects than the standard deviation need examination– for example two sensors may have the same standard deviation but may drift relative to each other. For these reasons, we did not codify paired tests, but instead used parallel visualization of all oxygen sensors on each mooring to search for problems. The sparse vertical distribution of sensors made this less useful than for temperature (which revealed offsets between some sensor types; Jansen et al., 2020). The visualization approach and results are detailed in the next section, after implementation of the remaining QARTOD tests is described. Manual Flagging via Neighbouring sensor visualizations

After extensive exploration, we settled on plots to visualize possible sensor problems (and provide these for all deployments below, with annotation of sensor errors that they revealed):

> Stacked time series for each deployment for all its oxygen sensors, showing sensor pressures, temperatures, conductivities, salinities, oxygen and oxygen solubility.

Using these plots, several problematic sensor records were identified and flagged as annotated on the plots shown in Appendix C and listed in Table 4.

These visualizations also reveal that the oxygen variations are fascinating in their diversity, rapidity, and origins. In particular: i. very rapid temporal variations occurred synchronously at all depths indicating very sharp and vertical boundaries between water parcels ii. Vertical movements (from both heave and mooring dynamics) cause mirror imaging of rapid oxygen (temperature and salinity) fluctuations for sensors above and below the seasonal pycnocline.

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Table 4. Manual flag assignments from Neighbour and Multi-variate test visualizations

Mooring	Feature identified	Flag assignment
SOFS-3-2012 SBE37 9513	Reading low compared to Surface Optode	4
Pulse-9-2012 SBE37 9515	Reading low, failed after 4 days	4
SOFS-3-2012 SBE37 9513	Reading low compared to Surface Optode	4
SOFS-3-2012 SBE37 9514	Reading low compared to Surface Optode	4
Pulse-10-2013 SBE37 9513	Reading low compared to 30m sensor, failed after June 16	4
Pulse-10-2013 SBE37 9538	Reading low compared to 30m sensor, failed after May16	4
Pulse-11-2015 SBE37 9513	Reading low	4
Pulse-11-2015 SBE37 9514	Reading low	4
Pulse-11-2015 SBE37 9538	Reading low	4
SOFS-6-2017 Optode 1158	Reading high compared to other sensors	4
SOFS-9-2020 Optode 1420	Bio fouled after November 24	4
SOFS-9-2020 SBE37 15971	Salinity faulty before October	4
SOFS-10-2021 Optode 506	Bio fouled after May 20, reading low	4

Table of data flagging. good - good data (1), p.good – probably good (2), p.bad - probably bad (3) , bad - bad data (4), ND - not deployed (6)

Flags

- loc – location test, out of location is flagged 6
- gr – global (and climate) range test 3 – climate range failed, 4 – global range failed
- in – input data to calculation, e.g. temperature or salinity measurement
- man – manual flagging

Table 5. Summary of flag statistics from the automated and manual QC efforts

Deployment code	Instrument model	Serial number	Nominal depth	# points		good	p.good	p.bad	bad	ND
Pulse-6-2009	Optode 3975	1161	37.5	4228						
					loc	4059	0	0	0	169
					gr	4059	169	0	0	0
					in	4056	0	3	0	169
					total	4056	0	3	0	169
Pulse-6-2009	SBE43	431634	37.5	4228						
					loc	4059	0	0	0	169
					gr	4051	177	0	0	0
					in	4048	0	8	3	169
					total	4048	0	3	8	169
SOFS-1-2010	Optode 3830	1157	1.2	2033						
					loc	1773	0	0	0	260
					gr	1773	260	0	0	0
					in	1773	0	0	0	260
					total	1773	0	0	0	260
Pulse-7-2010	SBE16plus	1606331	31.1	5918						
					loc	5228	0	0	0	690
					gr	5223	695	0	0	0
					in	5222	0	6	0	690
					total	5222	0	1	5	690
Pulse-7-2010	Optode 3975	1161	31.1	5918						
					loc	5228	0	0	0	690
					gr	5228	690	0	0	0
					in	5228	0	0	0	690
					total	5228	0	0	0	690
Pulse-7-2010	SBE43	431635	31.1	5918						
					loc	5228	0	0	0	690
					gr	5223	692	3	0	0

Deployment code	Instrument model	Serial number	Nominal depth	# points		good	p.good	p.bad	bad	ND
					in	5223	0	5	0	690
					total	5223	0	3	2	690
Pulse-8-2011	Optode 3975	1419	34	5435						
					loc	5296	0	0	0	139
					gr	5124	291	20	0	0
					in	4311	0	0	985	139
					total	4311	0	0	985	139
Pulse-8-2011	SBE43	431634	34	5435						
					loc	5296	0	0	0	139
					gr	5120	237	78	0	0
					in	4311	0	0	985	139
					total	4311	0	0	985	139
SOFS-2-2011	Optode 3830	1157	1.5	5799						
					loc	5414	0	0	0	385
					gr	5414	385	0	0	0
					in	5414	0	0	0	385
					total	5414	0	0	0	385
SOFS-3-2012	Optode 3830	1420	2	4770						
					loc	4098	0	0	0	672
					gr	4098	672	0	0	0
					in	4098	0	0	0	672
					total	4098	0	0	0	672
SOFS-3-2012	SBE37SMP-ODO-RS232	9513	30	9394						
					loc	8240	0	0	0	1154
					gr	8240	1154	0	0	0
					in	8240	0	0	0	1154
					total	8240	0	0	0	1154
SOFS-3-2012	SBE37SMP-ODO-RS232	9514	100	9397						
					loc	8240	0	0	0	1157
					gr	8240	1157	0	0	0
					in	8239	0	1	0	1157
					total	8239	0	1	0	1157
Pulse-9-2012	Optode 3975	1158	38.5	5429						
					loc	4653	0	0	0	776
					gr	4401	1021	7	0	0

Deployment code	Instrument model	Serial number	Nominal depth	# points		good	p.good	p.bad	bad	ND
					in	3966	0	0	687	776
					total	3966	0	0	687	776
Pulse-9-2012	SBE43	431635	38.5	5429						
					loc	4653	0	0	0	776
					gr	4101	1133	195	0	0
					in	3965	0	1	687	776
					total	3965	0	1	687	776
Pulse-9-2012	SBE37SMP-ODO-RS232	3709515	100	15004						
					loc	14005	0	0	0	999
					gr	242	14762	0	0	0
					man	0	0	13966	0	0
					in	14000	0	5	0	999
					total	153	0	89	13763	999
SOFS-4-2013	Optode 3830	1157	1.01	5269						
					loc	3991	0	0	0	1278
					gr	3991	1278	0	0	0
					in	3991	0	0	0	1278
					total	3991	0	0	0	1278
Pulse-10-2013	Optode 3975	1420	28	3856						
					loc	3828	0	0	0	28
					gr	3828	28	0	0	0
					in	3827	0	1	0	28
					total	3827	0	1	0	28
Pulse-10-2013	SBE43	431634	28	3856						
					loc	3828	0	0	0	28
					gr	3828	28	0	0	0
					in	3827	0	1	0	28
					totals	3827	0	1	0	28
Pulse-10-2013	SBE37SMP-ODO-RS232	3709538	100	8171						
					loc	7655	0	0	0	516
					gr	550	7621	0	0	0
					in	7580	0	3	72	516
					total	547	0	3	7105	516
Pulse-10-2013	SBE37SMP-ODO-RS232	3709513	200	8173						
					loc	7655	0	0	0	518

Deployment code	Instrument model	Serial number	Nominal depth	# points		good	p.good	p.bad	bad	ND
					gr	1927	6246	0	0	0
					in	7654	0	1	0	518
					total	1927	0	0	5728	518
SOFS-5-2015	Optode 3830	1419	1	9708						
					loc	9118	0	0	0	590
					gr	9115	590	3	0	0
					in	9118	0	0	0	590
					total	9115	0	3	0	590
Pulse-11-2015	SBE16plus	1606330	28	8856						
					loc	8614	0	0	0	242
					gr	8614	242	0	0	0
					in	8614	0	0	0	242
					total	8614	0	0	0	242
Pulse-11-2015	Optode 3975	1420	28	8856						
					loc	8614	0	0	0	242
					gr	8614	242	0	0	0
					in	8613	0	1	0	242
					totals	8613	0	1	0	242
Pulse-11-2015	SBE43	431634	28	8856						
					loc	8614	0	0	0	242
					gr	8614	242	0	0	0
					in	8613	0	1	0	242
					total	8613	0	1	0	242
Pulse-11-2015	SBE37SMP-ODO-RS232	3709538	50	18201						
					loc	17301	0	0	0	900
					gr	17301	900	0	0	0
					in	17299	0	2	0	900
					total	17299	0	2	0	900
Pulse-11-2015	SBE37SMP-ODO-RS232	3709513	100	18204						
					loc	17301	0	0	0	903
					gr	17301	903	0	0	0
					in	17301	0	0	0	903
					total	17301	0	0	0	903
Pulse-11-2015	SBE37SMP-ODO-RS232	3709514	150	18205						
					loc	17301	0	0	0	904
					gr	17300	905	0	0	0

Deployment code	Instrument model	Serial number	Nominal depth	# points		good	p.good	p.bad	bad	ND
					in	17301	0	0	0	904
					total	17300	0	0	1	904
FluxPulse-1-2016	Optode 3830	1157	1.01	2762						
					loc	2363	0	0	0	399
					gr	2363	399	0	0	0
					in	2363	0	0	0	399
					total	2363	0	0	0	399
SOFS-6-2017	Optode 3830	1158	1	6644						
					loc	5445	0	0	0	1199
					gr	4651	1199	794	0	0
					man	0	0	6644	0	0
					in	4393	0	921	131	1199
					total	0	0	5314	131	1199
SOFS-6-2017	SBE37SMP-ODO-RS232	3709538	30	11719						
					loc	10896	0	0	0	823
					gr	10896	823	0	0	0
					in	10894	0	2	0	823
					totals	10894	0	2	0	823
SOFS-6-2017	SBE37SMP-ODO-RS232	3709513	125	11719						
					loc	10896	0	0	0	823
					gr	10896	823	0	0	0
					in	10890	0	6	0	823
					totals	10890	0	6	0	823
SOFS-6-2017	SBE37SMP-ODO-RS232	3709514	200	11719						
					loc	10896	0	0	0	823
					gr	10896	823	0	0	0
					in	10896	0	0	0	823
					total	10896	0	0	0	823
SOFS-6-2017	SBE37SMP-ODO-RS232	3714700	500	11720						
					loc	10896	0	0	0	824
					gr	10896	824	0	0	0
					in	10895	0	1	0	824
					total	10895	0	1	0	824

Deployment code	Instrument model	Serial number	Nominal depth	# points		good	p.good	p.bad	bad	ND
SOFS-7-2018	Optode 3830	1420	1	618						
					loc	253	0	0	0	365
					gr	253	365	0	0	0
					in	253	0	0	0	365
					total	253	0	0	0	365
SOFS-7-2018	SBE37SMP-ODO-RS232	3715969	30	2844						
					loc	504	0	0	0	2340
					gr	504	2340	0	0	0
					in	504	0	0	0	2340
					total	504	0	0	0	2340
SOFS-7-2018	SBE37SMP-ODO-RS232	3715970	125	1485						
					loc	504	0	0	0	981
					gr	504	981	0	0	0
					in	504	0	0	0	981
					total	504	0	0	0	981
SOFS-7-2018	SBE37SMP-ODO-RS232	3715971	200	1487						
					loc	504	0	0	0	983
					gr	504	983	0	0	0
					in	504	0	0	0	983
					total	504	0	0	0	983
SOFS-7-2018	SBE37SMP-ODO-RS232	3715972	480	1487						
					loc	504	0	0	0	983
					gr	504	983	0	0	0
					in	504	0	0	0	983
					total	504	0	0	0	983
SOFS-7.5-2018	Optode 3830	1420	1	4482						
					loc	3826	0	0	0	656
					gr	3826	656	0	0	0
					in	3826	0	0	0	656
					total	3826	0	0	0	656
SOFS-7.5-2018	SBE37SMP-ODO-RS232	3715969	30	11459						
					loc	10193	0	0	0	1266
					gr	10193	1266	0	0	0

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Deployment code	Instrument model	Serial number	Nominal depth	# points		good	p.good	p.bad	bad	ND
					in	10193	0	0	0	1266
					total	10193	0	0	0	1266
SOFS-7.5-2018	SBE37SMP-ODO-RS232	3715970	125	11324						
					loc	10193	0	0	0	1131
					gr	10193	1131	0	0	0
					in	10193	0	0	0	1131
					total	10193	0	0	0	1131
SOFS-7.5-2018	SBE37SMP-ODO-RS232	3715971	200	11324						
					loc	10193	0	0	0	1131
					gr	10193	1131	0	0	0
					in	0	8181	0	2012	1131
					total	0	8181	0	2012	1131
SOFS-7.5-2018	SBE37SMP-ODO-RS232	3715972	480	11324						
					loc	10193	0	0	0	1131
					gr	10193	1131	0	0	0
					in	10191	0	2	0	1131
					total	10191	0	2	0	1131
SOFS-8-2019	Optode 3830	1419	1	13222						
					loc	12596	0	0	0	626
					gr	12596	626	0	0	0
					in	12596	0	0	0	626
					total	12596	0	0	0	626
SOFS-8-2019	SBE37SMP-ODO-RS232	3720126	30	27737						
					loc	25753	0	0	0	1984
					gr	25753	1984	0	0	0
					in	25752	0	1	0	1984
					total	25752	0	1	0	1984
SOFS-8-2019	SBE37SMP-ODO-RS232	3709513	125	27739						
					loc	25753	0	0	0	1986

Deployment code	Instrument model	Serial number	Nominal depth	# points		good	p.good	p.bad	bad	ND
					gr	25753	1986	0	0	0
					in	25748	0	5	0	1986
					total	25748	0	5	0	1986
SOFS-8-2019	SBE37SMP-ODO-RS232	3709514	200	27750						
					loc	25753	0	0	0	1997
					gr	25753	1997	0	0	0
					in	25752	0	1	0	1997
					total	25752	0	1	0	1997
SOFS-8-2019	SBE37SMP-ODO-RS232	3720127	510	24961						
					loc	22970	0	0	0	1991
					gr	22970	1991	0	0	0
					in	22942	0	28	0	1991
					total	22942	0	28	0	1991
SOFS-9-2020	Optode 3830	1420	1	4938						
					loc	4628	0	0	0	310
					gr	4618	310	10	0	0
					man	0	0	2616	0	0
					in	4592	0	36	0	310
					totals	2012	0	2616	0	310
SOFS-9-2020	SBE37SMP-ODO-RS232	3715969	30	95073						
					loc	94253	0	0	0	820
					gr	94253	820	0	0	0
					in	92804	0	1449	0	820
					totals	92804	0	1449	0	820
SOFS-9-2020	SBE37SMP-ODO-RS232	3715970	125	12868						
					loc	11272	0	0	0	1596
					gr	11272	1596	0	0	0
					in	11270	0	2	0	1596
					totals	11270	0	2	0	1596
SOFS-9-2020	SBE37SMP-ODO-RS232	3714700	200	16439						

Deployment code	Instrument model	Serial number	Nominal depth	# points		good	p.good	p.bad	bad	ND
					loc	11272	0	0	0	5167
					gr	11272	5167	0	0	0
					in	11272	0	0	0	5167
					total	11272	0	0	0	5167
SOFS-9-2020	SBE37SMP-ODO-RS232	3715971	300	15450						
					loc	11272	0	0	0	4178
					gr	11272	4178	0	0	0
					in	0	8687	1	2584	4178
					total	0	8687	1	2584	4178
SOFS-9-2020	SBE37SMP-ODO-RS232	3715972	510	16295						
					loc	11272	0	0	0	5023
					gr	11272	5023	0	0	0
					in	11272	0	0	0	5023
					total	11272	0	0	0	5023
SOFS-10-2021	Optode 4831	506	1	9857						
					loc	9300	0	0	0	557
					gr	6642	2061	1154	0	0
					man	0	0	8475	0	0
					in	6105	0	2293	902	557
					total	877	0	6919	1504	557
SOFS-10-2021	SeaPHOxV2	2016	30	18971						
					loc	18597	0	0	0	374
					gr	18597	374	0	0	0
					in	17843	0	754	0	374
					totals	17843	0	754	0	374
SOFS-10-2021	SBE37SMP-ODO-RS232	3709513	125	16898						
					loc	15664	0	0	0	1234
					gr	15664	1234	0	0	0
					in	15662	0	2	0	1234
					total	15662	0	2	0	1234
SOFS-10-2021	SBE37SMP-ODO-RS232	3709514	200	19721						

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Deployment code	Instrument model	Serial number	Nominal depth	# points		good	p.good	p.bad	bad	ND
					loc	18600	0	0	0	1121
					gr	18600	1121	0	0	0
					in	18599	0	1	0	1121
					total	18599	0	1	0	1121
SOFS-10-2021	SBE37SMP-ODO-RS232	3720126	300	12131						
					loc	11178	0	0	0	953
					gr	11178	953	0	0	0
					in	11177	0	1	0	953
					total	11177	0	1	0	953
SOFS-10-2021	SBE37SMP-ODO-RS232	3721154	510	19302						
					loc	18600	0	0	0	702
					gr	18596	705	1	0	0
					in	18592	0	5	3	702
					total	18592	0	5	3	702

6 **Discussion and recommendations**

6.1 QARTOD tests that were not performed

Some of the recommended QARTOD tests were deemed not applicable, specifically Tests 8 and 10. However, their intent, was captured by other approaches. See Section 5.2 for full details.

6.2 Main causes for data flagging

Data flagging generally fell into 3 categories:

- Bio fouling, causing sensor to read low,
- Sensor failure,
- Co-incident data difference.

6.3 Did the QC tests work and how good are the data?

Evaluating the success of the tests requires determining whether they correctly identified and flagged only and all *truly* bad data (flag 4) and possibly bad data (flag 3) and retained only and all *truly* good (flag 1) and *probably* good (flag 2) data. This requires some independent understanding of which data is good.

6.4 Sensor uncertainty estimates

Three measurements are used to check sensor accuracy and precision,

- Sea Bird pre and post deployment calibrations
- Sensor dips when attached to ships CTD before and after deployment, sensor readings are compared with winkler bottle samples,
- During deployment, when all sensors are within the mix-layer (temperature difference between sensors is < 0.3 degC) sensor values are compared between sensors on the mooring.

6.4.1 Sensor Post calibrations

Table 6 Oxygen Pre vs Post sensor calibrations in calibration lab

Mooring	*Depth*	*Logger Instrument*	*Oxygen Instrument*	*Post calibration cf pre calibration slope (From SeaBird calibration sheet)*
SOFS-9	30m	SeaPHOx 1001/SBE37-15969	SBE63-1526	1.0111
	125m	SBE37SMP-ODO-15970	SBE63-1680	1.0117
	200m	SBE37SMP-ODO-14700	SBE63-1378	1.0042
	300m	SBE37SMP-ODO-15971	SBE36-2007	1.0016
	510m	SBE37SMP-ODO-15972	SBE63-1682	1.0031
SOFS-10	30m	SeaPHOx 2016/SBE37-218008	SBE63-2496	0.9947
	125m	SBE37SMP-ODO-9513	SBE63-0144	0.9992
	200m	SBE37SMP-ODO-9514	SBE63-0603	0.9976
	300m	SBE37SMP-ODO-20126	SBE63-2007	1.0016
	510m	SBE37SMP-ODO-21154	SBE63-2331	sensor rebuilt

Sensor post calibrations show that SBE63 sensors change the order of 0.66% (sqrt-sum-of-squares) from the pre calibration to the post deployment comparison, to a lower sensitivity.

6.4.2 CTD bottle-Sensor comparison

For all deployments the sensor readings were compared to the nearest CTD bottle sample, values are considered coincident when the temperature difference was less than 0.1 ^{o}C and pressure within 20 dbar. This data is either when the sensor is deployed on the mooring or when the sensors were attached to the CTD frame pre or post deployment.

Jansen P, Wynn-Edwards CA, Shadwick EH and Trull TW (2023). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Oxygen Records Version 1.0. CSIRO, Australia. DOI: 10.26198/1te4-jq81

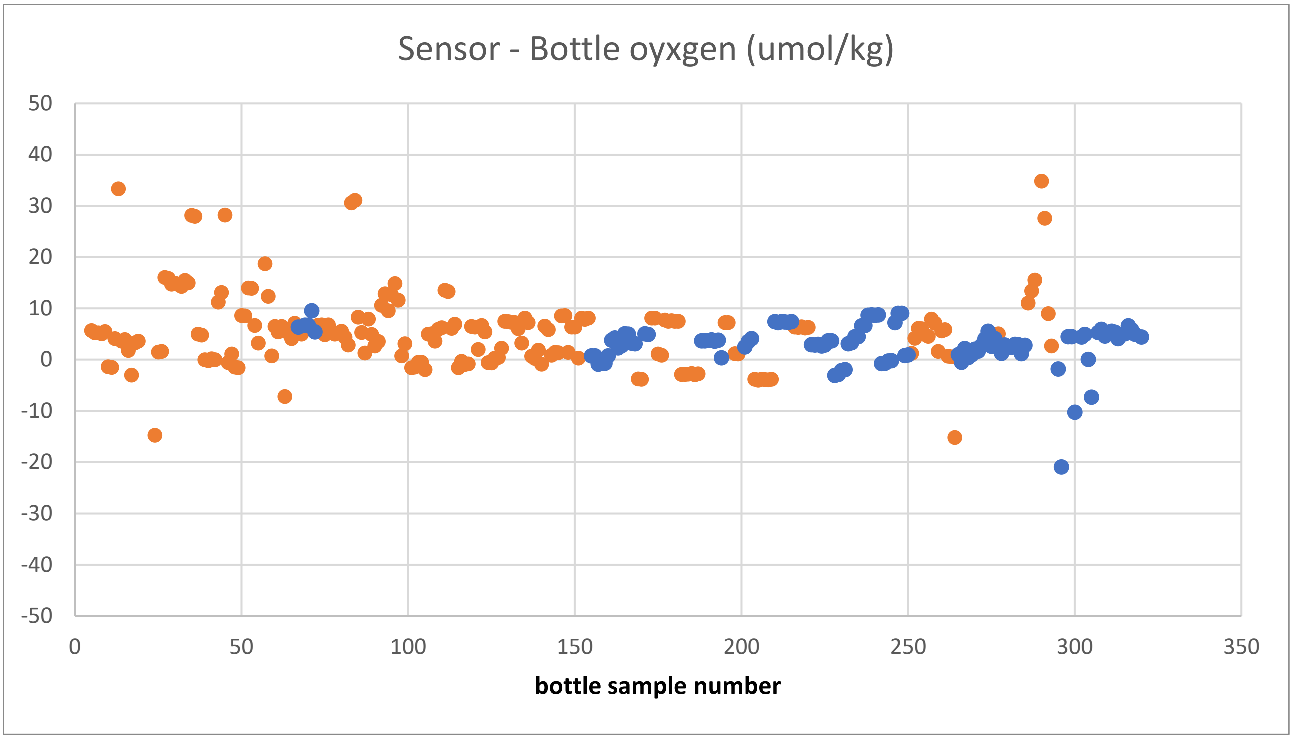

Figure 16 Sensor oxygen - bottle oxygen values for all sensors, sum-of-square difference of 8.3 umol/kg, or 3%, orange is in-situ comparison with CTD, blue is when sensor was mounted on CTD pre/post deployment.

Table 7 CTD bottle to Sensor comparison results for each sensor deployment

file	*mean sensor-bottle oxygen (umol/kg)*	*std*
Pulse-9-2012-Optode-3975-1158-38m	3.638748169	2.605622025
Pulse-9-2012-SBE37SMP-ODO-RS232-03709515-100m	5.277770996	0
Pulse-9-2012-SBE43-431635-38m	-2.164810181	1.181352562
Pulse-11-2015-Optode-3975-1420-28m	3.091888428	3.128333909
Pulse-11-2015-SBE16plus-01606330-28m		
Pulse-11-2015-SBE37SMP-ODO-RS232-03709513-100m	14.50642395	0.294361682
Pulse-11-2015-SBE37SMP-ODO-RS232-03709514-150m	13.71121216	1.919289076
Pulse-11-2015-SBE37SMP-ODO-RS232-03709538-50m	13.14636739	3.554688947
Pulse-11-2015-SBE43-431634-28m	0.335561117	0.696183146
SOFS-3-2012-Optode-3830-1420-2m	-1.483612061	0
SOFS-3-2012-SBE37SMP-ODO-RS232-9513-30m	5.346120199	1.086797884
SOFS-3-2012-SBE37SMP-ODO-RS232-9514-100m	5.041530064	0.948174394
SOFS-4-2013-Optode-3830-1157-1m	-2.590443929	10.52652185
SOFS-5-2015-Optode-3830-1419-1m	3.54442215	6.546378746
SOFS-6-2017-Optode-3830-1158-1m		
SOFS-6-2017-SBE37SMP-ODO-RS232-03709538-30m	4.110168457	10.1302954
SOFS-6-2017-SBE37SMP-ODO-RS232-03709513-125m	10.23888652	7.381432631
SOFS-6-2017-SBE37SMP-ODO-RS232-03709514-200m	4.448735555	2.210913794
SOFS-7.5-2018-Optode-3830-1420-1m	5.022155762	0
SOFS-7.5-2018-SBE37SMP-ODO-RS232-03715969-30m	6.923900604	3.365431691
SOFS-7.5-2018-SBE37SMP-ODO-RS232-03715970-125m	8.194107056	1.907276393
SOFS-7.5-2018-SBE37SMP-ODO-RS232-03715971-200m	3.633321126	1.792801019
SOFS-7.5-2018-SBE37SMP-ODO-RS232-03715972-480m	6.409057617	0
SOFS-8-2019-Optode-3830-1419-1m	-0.490937104	3.024858731
SOFS-8-2019-SBE37SMP-ODO-RS232-03720126-30m	6.77186684	3.027366965
SOFS-8-2019-SBE37SMP-ODO-RS232-03709513-125m	0.721388681	1.529283633
SOFS-8-2019-SBE37SMP-ODO-RS232-03709514-200m	-0.609028408	1.791269557
SOFS-8-2019-SBE37SMP-ODO-RS232-03720127-510m	7.065465927	2.037895195
SOFS-8-2019-SBE37SMP-ODO-RS232-03720127-510m	7.065465927	2.037895195
SOFS-9-2020-Optode-3830-1420-1m	5.483564104	1.760728574
SOFS-9-2020-SBE37SMP-ODO-RS232-03715969-30m	2.896728516	0.112691547
SOFS-9-2020-SBE37SMP-ODO-RS232-03715970-125m	3.024042765	2.240169098
SOFS-9-2020-SBE37SMP-ODO-RS232-03714700-200m	3.370296224	2.00475598
SOFS-9-2020-SBE37SMP-ODO-RS232-03715971-300m	2.929462978	1.018020546
SOFS-9-2020-SBE37SMP-ODO-RS232-03715972-510m	2.028468831	2.327490731
SOFS-10-2021-Optode-4831-506-1m	0.626777649	0.092412866
SOFS-10-2021-SeaPHOxV2-02016-30m	5.996269226	4.574114962
SOFS-10-2021-SBE37SMP-ODO-RS232-03709513-125m	4.33605957	1.579895468
SOFS-10-2021-SBE37SMP-ODO-RS232-03709514-200m	-0.487857056	7.654918965
SOFS-10-2021-SBE37SMP-ODO-RS232-03720126-300m	1.43758138	8.154133744
SOFS-10-2021-SBE37SMP-ODO-RS232-03721154-510m	15.54544067	0

Given the standard deviation of bottle samples vs sensors is around 2.7 umol/kg (~1 %), this is about the limit of the accuracy of the sensor – CTD bottle comparison.

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6.4.3 In situ comparison when well mixed

Where two sensors are in the mixed layer (as defined by the temperature difference being < 0.3 ^{o}C) pressure, and the sensor temperature – 30m sensor temperature is < 0.1 ^{o}C then data is compared between the sensor and the 30m sensor.

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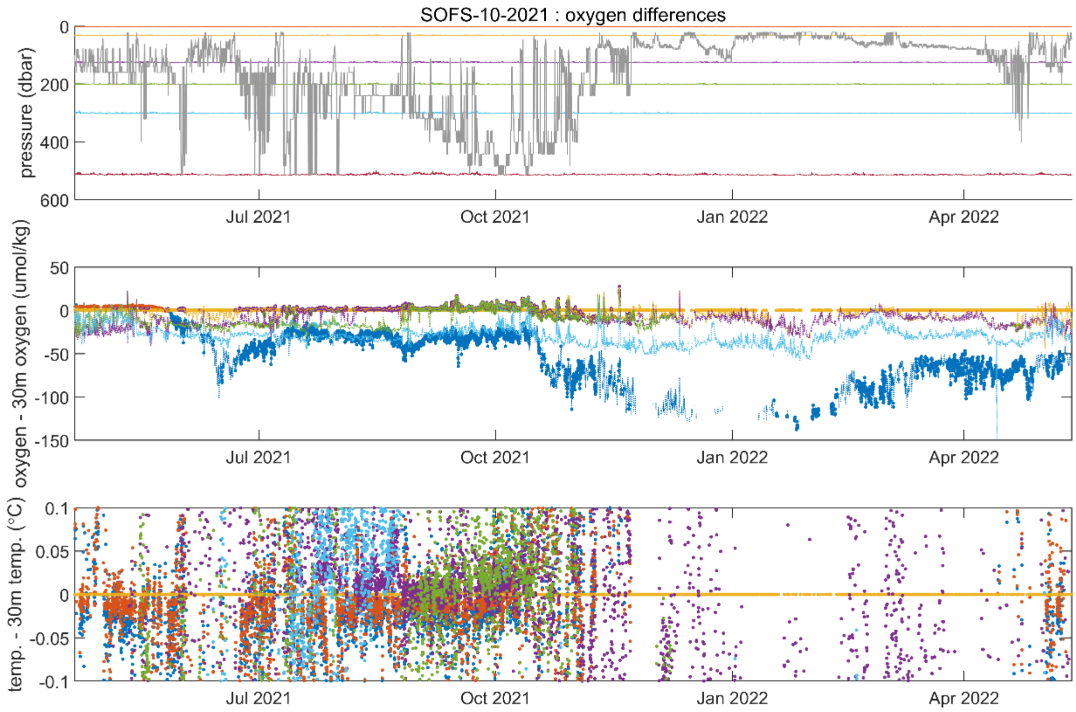

Figure 17 SOFS-10 plot of pressure, mixed layer depth and differences to oxygen compared to the 30m sensor

Figure 18 Initial comparison, Optode 2% high compared to 30m sensor, 125m sensor is ~1%

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Figure 19 zoom of September where mix layer is > 400m, 30m sensor can read low even when the temperature are the same and sensors are within the mix layer depth.

Table 8 Comparison between sensor and 30m oxygen sensor during deployment when well mixed

Mooring	*Depth*	*Logger Instrument*	*Oxygen Instrument*	*Difference to 30m sensor (umol/kg)*
SOFS-9	1m		Optode 3830 SN 1420	-7.46
	30m	SeaPHOx 1001/SBE37-15969	SBE63-1526	(reference)
	125m	SBE37SMP-ODO-15970	SBE63-1680	-1.30
	200m	SBE37SMP-ODO-14700	SBE63-1378	-3.61
	300m	SBE37SMP-ODO-15971	SBE63-2007	-15.5 (excluded, sensor issue)
	510m	SBE37SMP-ODO-15972	SBE63-1682	No Points
SOFS-10	1m		Optode 4831 SN 506	4.16
	30m	SeaPHOx 2016/SBE37-21808	SBE63-2496	(reference)
	125m	SBE37SMP-ODO-9513	SBE63-0144	1.95
	200m	SBE37SMP-ODO-9514	SBE63-0603	0.16
	300m	SBE37SMP-ODO-20126	SBE63-2007	Too Few samples
	510m	SBE37SMP-ODO-21154	SBE63-2331	No points

This comparison indicates that the sensors are within about 2% of each other when co-located in the mixed layer, 0.2 deg C temperature difference).

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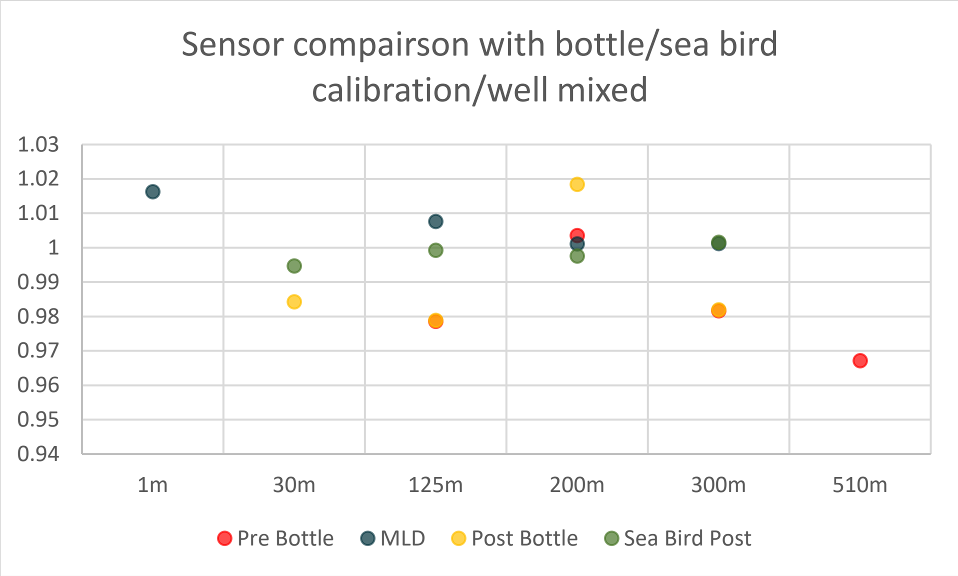
6.4.4 Summary

Plot of all comparisons for each sensor on the SOFS-10 mooring



Conclusion from comparisons

- The Sea Bird calibrations post deployment for this set of sensors is better than 1%.
- The pre and post sensor dips compared to Winkler bottle samples are within 2% (although the 500m sensor is 3%, this sensor failed and was rebuilt on return to Sea Bird).
- The mix layer depth (MLD) comparison of sensors is within 1% of the 30m sensor, although the Aanderra optode reads 1.6% higher, this maybe oceanographic or differences in sensor calibrations.

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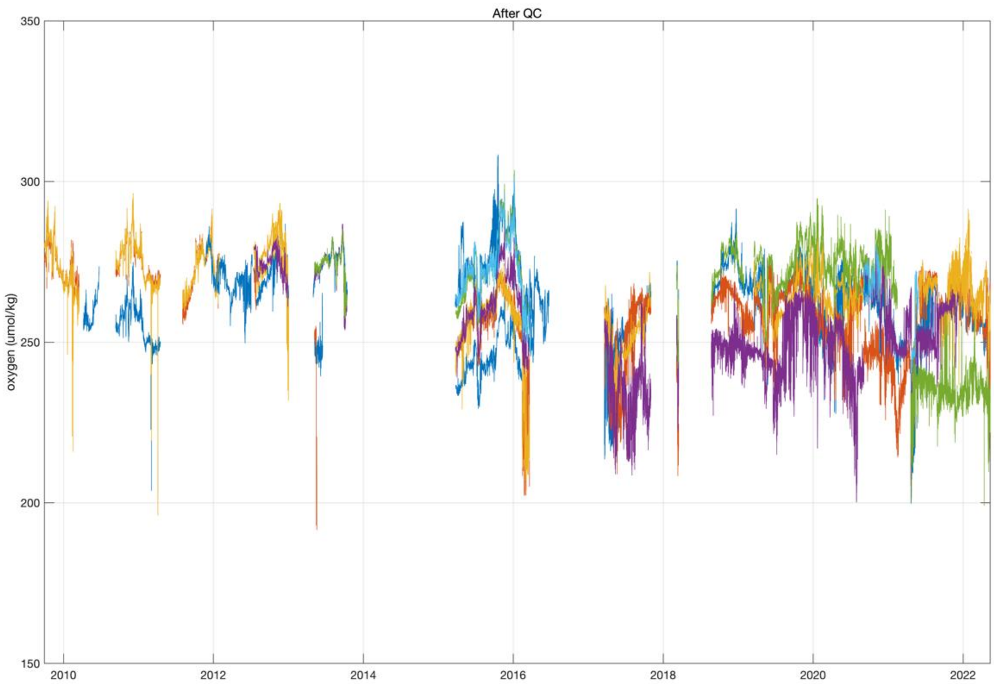

Figure 20 All data after QC

6.5 Could the QC tests be improved? What are the implications for QA?

In future years, it may be possible for an improved climatology based in part on the SOTS observations to improve the QARTOD test thresholds, and/or to implement more sophisticated filters.

A few overall recommendations for Quality Assurance have emerged from the QC:

1. Check all sensor calibrations against the growing record of calibrations to verify that none are unusual and thus potentially suspect.
2. Pair sensors whenever possible, and favour deploying pairs of sensors at a few depths over single sensors at more depths.
3. Compare all sensors against each other before and after deployment, either in the laboratory or via a common deployment on the CTD or both.

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6.6 Which data should you use, and what are their uncertainties?

We recommend use of all data with flag values of 2 or less. None of this data has failed a QC test (the only reason that a flag value of 2 has been assigned is that one or more of the tests could not be performed). Users interested in rapid surface events should also consider use of Flag 3 data.

Our selection of thresholds optimizes retention of data unless it can clearly be flagged as bad (Flag 4) or suspect (Flag 3), and thus will allow some bad data to pass these filters (as discussed in the Introduction). Using a running median filter to emphasize the typical rather than rare behaviour is a useful approach to obtain a low uncertainty time series, but as described in the Introduction, the oceanographic feature(s) of interest must determine the appropriate smoothing and this is thus left to data users to select to fit their purposes.

For the SBE43 sensors, where directly comparable to Optode sensors, the uncertainties could be in the +/- 6 umol/kg range once the initial slope correction is applied.

For Optode sensors, the suggested accuracy is 0.5 % (Bittig 2018), the stated accuracy from Aanderaa is 2% (or about 6 umol/kg).

For SBE63 sensors, CTD pre and post comparisons with CTD bottle samples show accuracy of +2/-9 umol/kg.

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7 Accessing the Data

Data are provided on-line from the Australian Ocean Data Network in CF compliant netCDF format files, with one file per deployment. We recommend using all data with flags of 1 or 2.

The URL for data access is:

https://portal.aodn.org.au/

Data file structure

```
netcdf IMOS_DWM-SOTS_COPST_20120627_SOFS_FV01_Pulse-9-2012-SBE37SMP-ODO-RS232-03709515-100m_END-20130507_C-20210811 {
dimensions:
	TIME = 15004 ;
variables:
	double TIME(TIME) ;
		TIME:long_name = "time" ;
		TIME:units = "days since 1950-01-01 00:00:00 UTC" ;
		TIME:calendar = "gregorian" ;
		TIME:axis = "T" ;
		TIME:standard_name = "time" ;
		TIME:valid_max = 90000. ;
		TIME:valid_min = 0. ;
	float TEMP(TIME) ;
		TEMP:_FillValue = NaNf ;
		TEMP:comment = "Temperature [ITS-90, deg C]" ;
		TEMP:units = "degrees_Celsius" ;
		TEMP:calibration_SerialNumber = "9515" ;
		TEMP:calibration_CalibrationDate = "10-May-12" ;
		TEMP:calibration_A0 = -7.638603e-05 ;
		TEMP:calibration_A1 = 0.0002987087 ;
		TEMP:calibration_A2 = -3.73475e-06 ;
		TEMP:calibration_A3 = 1.818577e-07 ;
		TEMP:calibration_Slope = 1. ;
		TEMP:calibration_Offset = 0. ;
		TEMP:coordinates = "TIME LATITUDE LONGITUDE NOMINAL_DEPTH" ;
		TEMP:long_name = "sea_water_temperature" ;
		TEMP:standard_name = "sea_water_temperature" ;
		TEMP:valid_max = 40.f ;
		TEMP:valid_min = -2.5f ;
		TEMP:ancillary_variables = "TEMP_quality_control TEMP_quality_control_loc TEMP_quality_control_gr TEMP_quality_control_spk TEMP_quality_control_roc" ;
	float CNDC(TIME) ;
		CNDC:_FillValue = NaNf ;
		CNDC:comment = "Conductivity [S/m]" ;
		CNDC:units = "S/m" ;
		CNDC:calibration_SerialNumber = "9515" ;
		CNDC:calibration_CalibrationDate = "10-May-12" ;
		CNDC:calibration_UseG_J = 1. ;
		CNDC:calibration_G = -0.9923906 ;
		CNDC:calibration_H = 0.1248248 ;
		CNDC:calibration_I = -0.000376197 ;
		CNDC:calibration_J = 4.100898e-05 ;
		CNDC:calibration_CPcor = -9.57e-08 ;
		CNDC:calibration_CTcor = 3.25e-06 ;
		CNDC:calibration_WBOTC = 3.241293e-07 ;
		CNDC:calibration_Slope = 1. ;
		CNDC:calibration_Offset = 0. ;
		CNDC:coordinates = "TIME LATITUDE LONGITUDE NOMINAL_DEPTH" ;
		CNDC:long_name = "sea_water_electrical_conductivity" ;
		CNDC:standard_name = "sea_water_electrical_conductivity" ;
		CNDC:valid_max = 50000.f ;
		CNDC:valid_min = 0.f ;
		CNDC:ancillary_variables = "CNDC_quality_control CNDC_quality_control_loc" ;
	float PSAL(TIME) ;
		PSAL:_FillValue = NaNf ;
```


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```
                PSAL:comment = "Salinity, Practical [PSU]" ;
                PSAL:units = "1" ;
                PSAL:coordinates = "TIME LATITUDE LONGITUDE NOMINAL_DEPTH" ;
                PSAL:long_name = "sea_water_practical_salinity" ;
                PSAL:standard_name = "sea_water_practical_salinity" ;
                PSAL:valid_max = 41.f ;
                PSAL:valid_min = 2.f ;
                PSAL:ancillary_variables = "PSAL_quality_control PSAL_quality_control_loc
PSAL_quality_control_gr PSAL_quality_control_spk PSAL_quality_control_roc" ;
        float PRES(TIME) ;
                PRES:_FillValue = NaNf ;
                PRES:comment = "Pressure, Strain Gauge [db]" ;
                PRES:units = "dbar" ;
                PRES:calibration_SerialNumber = "3537453" ;
                PRES:calibration_CalibrationDate = "07-May-12" ;
                PRES:calibration_PA0 = 0.09658488 ;
                PRES:calibration_PA1 = 0.001611054 ;
                PRES:calibration_PA2 = 3.322273e-12 ;
                PRES:calibration_PTEMPA0 = -61.83441 ;
                PRES:calibration_PTEMPA1 = 0.05481579 ;
                PRES:calibration_PTEMPA2 = -7.526737e-07 ;
                PRES:calibration_PTCA0 = 525385. ;
                PRES:calibration_PTCA1 = 4.731493 ;
                PRES:calibration_PTCA2 = -0.09109347 ;
                PRES:calibration_PTCB0 = 25.06012 ;
                PRES:calibration_PTCB1 = -0.000175 ;
                PRES:calibration_PTCB2 = 0. ;
                PRES:calibration_Offset = 0. ;
                PRES:applied_offset = -10.1353f ;
                PRES:coordinates = "TIME LATITUDE LONGITUDE NOMINAL_DEPTH" ;
                PRES:long_name = "sea_water_pressure_due_to_sea_water" ;
                PRES:standard_name = "sea_water_pressure_due_to_sea_water" ;
                PRES:valid_max = 12000.f ;
                PRES:valid_min = -15.f ;
                PRES:ancillary_variables = "PRES_quality_control PRES_quality_control_loc" ;
        float DENSITY(TIME) ;
                DENSITY:_FillValue = NaNf ;
                DENSITY:comment = "calculated using gsw-python https://teos-10.github.io/GSW-
Python/index.html" ;
                DENSITY:units = "kg/m^3" ;
                DENSITY:long_name = "sea_water_density" ;
                DENSITY:standard_name = "sea_water_density" ;
                DENSITY:valid_max = 1100.f ;
                DENSITY:valid_min = 1000.f ;
                DENSITY:ancillary_variables = "DENSITY_quality_control DENSITY_quality_control_loc"
;
        float DOX2(TIME) ;
                DOX2:_FillValue = NaNf ;
                DOX2:comment = "Oxygen, SBE 63 [umol/kg]" ;
                DOX2:units = "umol/kg" ;
                DOX2:calibration_SerialNumber = "0146" ;
                DOX2:calibration_CalibrationDate = "16-May-12" ;
                DOX2:calibration_A0 = 1.0513 ;
                DOX2:calibration_A1 = -0.0015 ;
                DOX2:calibration_A2 = 0.3902 ;
                DOX2:calibration_B0 = -0.24434 ;
                DOX2:calibration_B1 = 1.6217 ;
                DOX2:calibration_C0 = 0.1066 ;
                DOX2:calibration_C1 = 0.004597001 ;
                DOX2:calibration_C2 = 6.332e-05 ;
                DOX2:calibration_TA0 = 0.000667473 ;
                DOX2:calibration_TA1 = 0.0002487965 ;
                DOX2:calibration_TA2 = 7.2637e-07 ;
                DOX2:calibration_TA3 = 9.623948e-08 ;
                DOX2:calibration_pcor = 0.011 ;
                DOX2:calibration_Slope = 1. ;
                DOX2:calibration_Offset = 0. ;
                DOX2:ancillary_variables = "DOX2_quality_control DOX2_quality_control_loc" ;
        float OXSOL(TIME) ;
                OXSOL:_FillValue = NaNf ;
                OXSOL:comment = "Oxygen Saturation, Garcia & Gordon [umol/kg]" ;
                OXSOL:units = "umol/kg" ;
                OXSOL:ancillary_variables = "OXSOL_quality_control OXSOL_quality_control_loc" ;
        float DOX_TEMP(TIME) ;
                DOX_TEMP:_FillValue = NaNf ;
                DOX_TEMP:comment = "Oxygen Temperature, SBE 63 [ITS-90, deg C]" ;
```

```
                DOX_TEMP:units = "degrees_Celsius" ;
                DOX_TEMP:ancillary_variables = "DOX_TEMP_quality_control
DOX_TEMP_quality_control_loc" ;
        double LATITUDE ;
                LATITUDE:axis = "Y" ;
                LATITUDE:long_name = "latitude" ;
                LATITUDE:reference_datum = "WGS84 geographic coordinate system" ;
                LATITUDE:standard_name = "latitude" ;
                LATITUDE:units = "degrees_north" ;
                LATITUDE:valid_max = 90. ;
                LATITUDE:valid_min = -90. ;
        double LONGITUDE ;
                LONGITUDE:axis = "X" ;
                LONGITUDE:long_name = "longitude" ;
                LONGITUDE:reference_datum = "WGS84 geographic coordinate system" ;
                LONGITUDE:standard_name = "longitude" ;
                LONGITUDE:units = "degrees_east" ;
                LONGITUDE:valid_max = 180. ;
                LONGITUDE:valid_min = -180. ;
        double NOMINAL_DEPTH ;
                NOMINAL_DEPTH:axis = "Z" ;
                NOMINAL_DEPTH:long_name = "nominal depth" ;
                NOMINAL_DEPTH:positive = "down" ;
                NOMINAL_DEPTH:reference_datum = "sea surface" ;
                NOMINAL_DEPTH:standard_name = "depth" ;
                NOMINAL_DEPTH:units = "m" ;
                NOMINAL_DEPTH:valid_max = 12000. ;
                NOMINAL_DEPTH:valid_min = -5. ;
        float SIGMA_T0(TIME) ;
                SIGMA_T0:_FillValue = NaNf ;
                SIGMA_T0:units = "kg/m^3" ;
                SIGMA_T0:long_name = "sea_water_sigma_theta" ;
                SIGMA_T0:standard_name = "sea_water_sigma_theta" ;
                SIGMA_T0:reference_pressure = "0 dbar" ;
                SIGMA_T0:valid_max = 100.f ;
                SIGMA_T0:valid_min = 0.f ;
                SIGMA_T0:comment = "calculated using gsw-python https://teos-10.github.io/GSW-
Python/index.html" ;
                SIGMA_T0:ancillary_variables = "SIGMA_T0_quality_control
SIGMA_T0_quality_control_loc" ;
        byte TEMP_quality_control(TIME) ;
                TEMP_quality_control:_FillValue = 99b ;
                TEMP_quality_control:long_name = "quality flag for sea_water_temperature" ;
                TEMP_quality_control:standard_name = "sea_water_temperature status_flag" ;
                TEMP_quality_control:quality_control_conventions = "IMOS standard flags" ;
                TEMP_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
                TEMP_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
                TEMP_quality_control:comment = "maximum of all flags" ;
        byte CNDC_quality_control(TIME) ;
                CNDC_quality_control:_FillValue = 99b ;
                CNDC_quality_control:long_name = "quality flag for
sea_water_electrical_conductivity" ;
                CNDC_quality_control:standard_name = "sea_water_electrical_conductivity status_flag"
;
                CNDC_quality_control:quality_control_conventions = "IMOS standard flags" ;
                CNDC_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
                CNDC_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
                CNDC_quality_control:comment = "maximum of all flags" ;
        byte PSAL_quality_control(TIME) ;
                PSAL_quality_control:_FillValue = 99b ;
                PSAL_quality_control:long_name = "quality flag for sea_water_practical_salinity" ;
                PSAL_quality_control:standard_name = "sea_water_practical_salinity status_flag" ;
                PSAL_quality_control:quality_control_conventions = "IMOS standard flags" ;
                PSAL_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
                PSAL_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
                PSAL_quality_control:comment = "maximum of all flags" ;
        byte PRES_quality_control(TIME) ;
                PRES_quality_control:_FillValue = 99b ;
                PRES_quality_control:long_name = "quality flag for
sea_water_pressure_due_to_sea_water" ;
                PRES_quality_control:standard_name = "sea_water_pressure_due_to_sea_water
status_flag" ;
                PRES_quality_control:quality_control_conventions = "IMOS standard flags" ;
```

```
                PRES_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
                PRES_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
                PRES_quality_control:comment = "maximum of all flags" ;
        byte DENSITY_quality_control(TIME) ;
                DENSITY_quality_control:_FillValue = 99b ;
                DENSITY_quality_control:long_name = "quality flag for sea_water_density" ;
                DENSITY_quality_control:standard_name = "sea_water_density status_flag" ;
                DENSITY_quality_control:quality_control_conventions = "IMOS standard flags" ;
                DENSITY_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
                DENSITY_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
                DENSITY_quality_control:comment = "maximum of all flags" ;
        byte DOX2_quality_control(TIME) ;
                DOX2_quality_control:_FillValue = 99b ;
                DOX2_quality_control:quality_control_conventions = "IMOS standard flags" ;
                DOX2_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
                DOX2_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
                DOX2_quality_control:comment = "maximum of all flags" ;
        byte OXSOL_quality_control(TIME) ;
                OXSOL_quality_control:_FillValue = 99b ;
                OXSOL_quality_control:quality_control_conventions = "IMOS standard flags" ;
                OXSOL_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
                OXSOL_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
                OXSOL_quality_control:comment = "maximum of all flags" ;
        byte DOX_TEMP_quality_control(TIME) ;
                DOX_TEMP_quality_control:_FillValue = 99b ;
                DOX_TEMP_quality_control:quality_control_conventions = "IMOS standard flags" ;
                DOX_TEMP_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
                DOX_TEMP_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
                DOX_TEMP_quality_control:comment = "maximum of all flags" ;
        byte SIGMA_T0_quality_control(TIME) ;
                SIGMA_T0_quality_control:_FillValue = 99b ;
                SIGMA_T0_quality_control:long_name = "quality flag for sea_water_sigma_theta" ;
                SIGMA_T0_quality_control:standard_name = "sea_water_sigma_theta status_flag" ;
                SIGMA_T0_quality_control:quality_control_conventions = "IMOS standard flags" ;
                SIGMA_T0_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
                SIGMA_T0_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
                SIGMA_T0_quality_control:comment = "maximum of all flags" ;
        byte TEMP_quality_control_loc(TIME) ;
                TEMP_quality_control_loc:_FillValue = 99b ;
                TEMP_quality_control_loc:long_name = "in/out of water flag for
sea_water_temperature" ;
                TEMP_quality_control_loc:units = "1" ;
                TEMP_quality_control_loc:comment = "data flagged not deployed (6) when out of water"
;
        byte CNDC_quality_control_loc(TIME) ;
                CNDC_quality_control_loc:_FillValue = 99b ;
                CNDC_quality_control_loc:long_name = "in/out of water flag for
sea_water_electrical_conductivity" ;
                CNDC_quality_control_loc:units = "1" ;
                CNDC_quality_control_loc:comment = "data flagged not deployed (6) when out of water"
;
        byte PSAL_quality_control_loc(TIME) ;
                PSAL_quality_control_loc:_FillValue = 99b ;
                PSAL_quality_control_loc:long_name = "in/out of water flag for
sea_water_practical_salinity" ;
                PSAL_quality_control_loc:units = "1" ;
                PSAL_quality_control_loc:comment = "data flagged not deployed (6) when out of water"
;
        byte PRES_quality_control_loc(TIME) ;
                PRES_quality_control_loc:_FillValue = 99b ;
                PRES_quality_control_loc:long_name = "in/out of water flag for
sea_water_pressure_due_to_sea_water" ;
                PRES_quality_control_loc:units = "1" ;
                PRES_quality_control_loc:comment = "data flagged not deployed (6) when out of water"
;
        byte DENSITY_quality_control_loc(TIME) ;
                DENSITY_quality_control_loc:_FillValue = 99b ;
                DENSITY_quality_control_loc:long_name = "in/out of water flag for sea_water_density"
;
                DENSITY_quality_control_loc:units = "1" ;
```

```
                DENSITY_quality_control_loc:comment = "data flagged not deployed (6) when out of
water" ;
        byte DOX2_quality_control_loc(TIME) ;
                DOX2_quality_control_loc:_FillValue = 99b ;
                DOX2_quality_control_loc:units = "1" ;
                DOX2_quality_control_loc:comment = "data flagged not deployed (6) when out of water"
;
        byte OXSOL_quality_control_loc(TIME) ;
                OXSOL_quality_control_loc:_FillValue = 99b ;
                OXSOL_quality_control_loc:units = "1" ;
                OXSOL_quality_control_loc:comment = "data flagged not deployed (6) when out of
water" ;
        byte DOX_TEMP_quality_control_loc(TIME) ;
                DOX_TEMP_quality_control_loc:_FillValue = 99b ;
                DOX_TEMP_quality_control_loc:units = "1" ;
                DOX_TEMP_quality_control_loc:comment = "data flagged not deployed (6) when out of
water" ;
        byte SIGMA_T0_quality_control_loc(TIME) ;
                SIGMA_T0_quality_control_loc:_FillValue = 99b ;
                SIGMA_T0_quality_control_loc:long_name = "in/out of water flag for
sea_water_sigma_theta" ;
                SIGMA_T0_quality_control_loc:units = "1" ;
                SIGMA_T0_quality_control_loc:comment = "data flagged not deployed (6) when out of
water" ;
        byte TEMP_quality_control_gr(TIME) ;
                TEMP_quality_control_gr:_FillValue = 99b ;
                TEMP_quality_control_gr:long_name = "global_range flag for sea_water_temperature" ;
                TEMP_quality_control_gr:units = "1" ;
                TEMP_quality_control_gr:comment = "Test 4. gross range test" ;
        byte TEMP_quality_control_spk(TIME) ;
                TEMP_quality_control_spk:_FillValue = 99b ;
                TEMP_quality_control_spk:long_name = "spike flag for sea_water_temperature" ;
                TEMP_quality_control_spk:units = "1" ;
                TEMP_quality_control_spk:comment = "Test 6. spike test" ;
        byte TEMP_quality_control_roc(TIME) ;
                TEMP_quality_control_roc:_FillValue = 99b ;
                TEMP_quality_control_roc:long_name = "rate_of_change flag for sea_water_temperature"
;
                TEMP_quality_control_roc:units = "1" ;
                TEMP_quality_control_roc:comment = "Test 7. rate of change test" ;
        byte PSAL_quality_control_gr(TIME) ;
                PSAL_quality_control_gr:_FillValue = 99b ;
                PSAL_quality_control_gr:long_name = "global_range flag for
sea_water_practical_salinity" ;
                PSAL_quality_control_gr:units = "1" ;
                PSAL_quality_control_gr:comment = "Test 4. gross range test" ;
        byte PSAL_quality_control_spk(TIME) ;
                PSAL_quality_control_spk:_FillValue = 99b ;
                PSAL_quality_control_spk:long_name = "spike flag for sea_water_practical_salinity" ;
                PSAL_quality_control_spk:units = "1" ;
                PSAL_quality_control_spk:comment = "Test 6. spike test" ;
        byte PSAL_quality_control_roc(TIME) ;
                PSAL_quality_control_roc:_FillValue = 99b ;
                PSAL_quality_control_roc:long_name = "rate_of_change flag for
sea_water_practical_salinity" ;
                PSAL_quality_control_roc:units = "1" ;
                PSAL_quality_control_roc:comment = "Test 7. rate of change test" ;

// global attributes:
                :abstract = "Oceanographic and meteorological data from the Southern Ocean Time
Series observatory in the Southern Ocean southwest of Tasmania" ;
                :acknowledgement = "Any users of IMOS data are required to clearly acknowledge the
source of the material derived from IMOS in the format: \"Data was sourced from the Integrated
Marine Observing System (IMOS) - IMOS is a national collaborative research infrastructure, supported
by the Australian Government.\" If relevant, also credit other organisations involved in collection
of this particular datastream (as listed in \'credit\' in the metadata record)." ;
                :author = "Jansen, Peter" ;
                :author_email = "peter.jansen@csiro.au" ;
                :citation = "The citation in a list of references is: \'IMOS [year-of-data-
download], [Title], [data-access-URL], accessed [date-of-access]\'." ;
                :comment = "Geospatial vertical min/max information has been filled using the
NOMINAL_DEPTH." ;
                :Conventions = "CF-1.6,IMOS-1.4" ;
                :data_centre = "Australian Ocean Data Network (AODN)" ;
                :data_centre_email = "info@aodn.org.au" ;
                :date_created = "2021-08-11T07:24:55Z" ;
```

```
                :deployment_code = "Pulse-9-2012" ;
                :disclaimer = "Data, products and services from IMOS are provided \"as is\" without
any warranty as to fitness for a particular purpose." ;
                :featureType = "timeSeries" ;
                :file_version_quality_control = "Raw data is defined as unprocessed data and data
products that have not undergone quality control. The data may be in engineering physical units,
time and location details can be in relative units and values can be pre-calibration measurements."
;
                :geospatial_lat_max = -46.84932 ;
                :geospatial_lat_min = -46.84932 ;
                :geospatial_lat_units = "degrees_north" ;
                :geospatial_lon_max = 142.39855 ;
                :geospatial_lon_min = 142.39855 ;
                :geospatial_lon_units = "degrees_east" ;
                :geospatial_vertical_max = 100. ;
                :geospatial_vertical_min = 100. ;
                :geospatial_vertical_positive = "down" ;
                :institution = "DWM-SOTS" ;
                :institution_references = "http://www.imos.org.au/aodn.html" ;
                :instrument = "Sea-Bird Electronics ; SBE37SMP-ODO-RS232" ;
                :instrument_model = "SBE37SMP-ODO-RS232" ;
                :instrument_nominal_depth = 100. ;
                :instrument_serial_number = "03709515" ;
                :keywords_vocabulary = "IMOS parameter names. See https://github.com/aodn/imos-
toolbox/blob/master/IMOS/imosParameters.txt" ;
                :license = "http://creativecommons.org/licenses/by/4.0/" ;
                :naming_authority = "IMOS" ;
                :platform_code = "SOFS" ;
                :principal_investigator = "Trull, Tom" ;
                :principal_investigator_email = "tom.trull@csiro.au" ;
                :project = "Integrated Marine Observing System (IMOS)" ;
                :site_code = "SOTS" ;
                :site_nominal_depth = 4300. ;
                :standard_name_vocabulary = "NetCDF Climate and Forecast (CF) Metadata Convention
Standard Name Table 67" ;
                :time_coverage_end = "2013-05-07T22:30:24Z" ;
                :time_coverage_start = "2012-06-27T05:28:40Z" ;
                :time_deployment_end = "2013-05-05T01:15:00Z" ;
                :time_deployment_start = "2012-07-17T07:00:00Z" ;
                :title = "Oceanographic mooring data deployment of SOFS at latitude -46.8 longitude
142.4 depth 100 (m) instrument Sea-Bird Electronics ; SBE37SMP-ODO-RS232 serial 03709515" ;
                :voyage_deployment =
"http://www.cmar.csiro.au/data/trawler/survey_details.cfm?survey=SS2012_V03" ;
                :voyage_recovery =
"http://www.cmar.csiro.au/data/trawler/survey_details.cfm?survey=SS2013_V03" ;
                :file_version = "Level 1 - Quality Controlled Data" ;
                :history = "2020-07-15 created from file SBE37SMP-ODO-
RS232_03709515_2013_05_07.cnv\n2020-07-15 : attributes added from file(s) [metadata/pulse-saz-sofs-
flux.metadata.csv, metadata/imos.metadata.csv, metadata/sots.metadata.csv,
metadata/sofs.metadata.csv, metadata/variable.metadata.csv]\n2021-07-30 : added DENSITY and SIGMA-
THETA0 from TEMP, PSAL, PRES, LAT, LON\n2021-08-11 : quality_control variables added.\n2021-08-11 :
in/out marked 999\n2021-08-11 TEMP global range min = -2 max = 30 marked 0.0\n2021-08-11 TEMP global
range min = 5 max = 16 marked 0.0\n2021-08-11 TEMP spike height = 2 marked 3\n2021-08-11 TEMP max
rate = 80 marked 0\n2021-08-11 PSAL global range min = 2 max = 41 marked 0.0\n2021-08-11 PSAL global
range min = 34 max = 35.5 marked 0.0\n2021-08-11 PSAL spike height = 0.4 marked 3\n2021-08-11 PSAL
max rate = 30 marked 0" ;
                :references = "http://www.imos.org.au; Jansen P, Weeding B, Shadwick EH and Trull TW
(2020). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Temperature Records
Version 1.0. CSIRO, Australia. DOI: 10.26198/gfgr-fq47 (https://doi.org/10.26198/gfgr-fq47)" ;
```

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Appendix A Python files used for processing

Please refer to the following link for access to the Python files involved in performing the QC tests described in this report:

https://github.com/petejan/imos-tools

Appendix B Sensor Calibrations

Calibration sheets for all DOX sensors deployed at the SOTS site are available at:

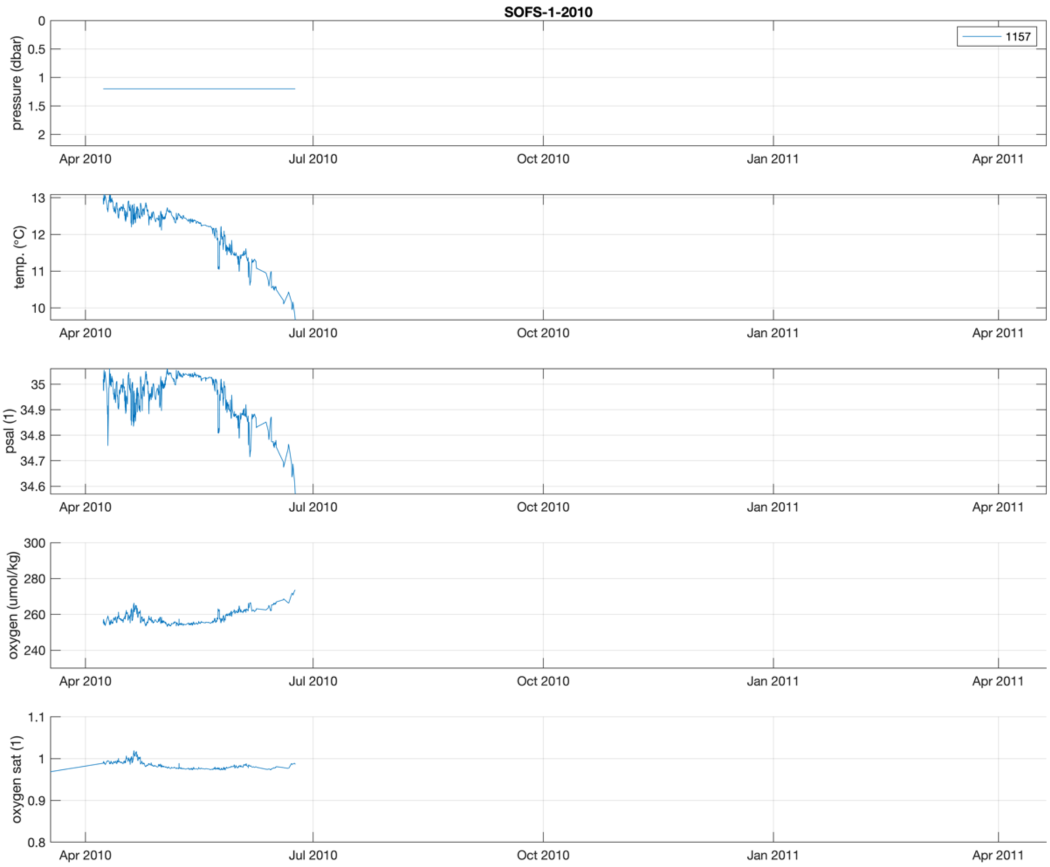
http://imos-data.s3-website-ap-southeast-2.amazonaws.com/?prefix=IMOS/DWM/SOTS/calibration/

Jansen P, Wynn-Edwards CA, Shadwick EH and Trull TW (2023). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Oxygen Records Version 1.0. CSIRO, Australia. DOI: 10.26198/1te4-jq81

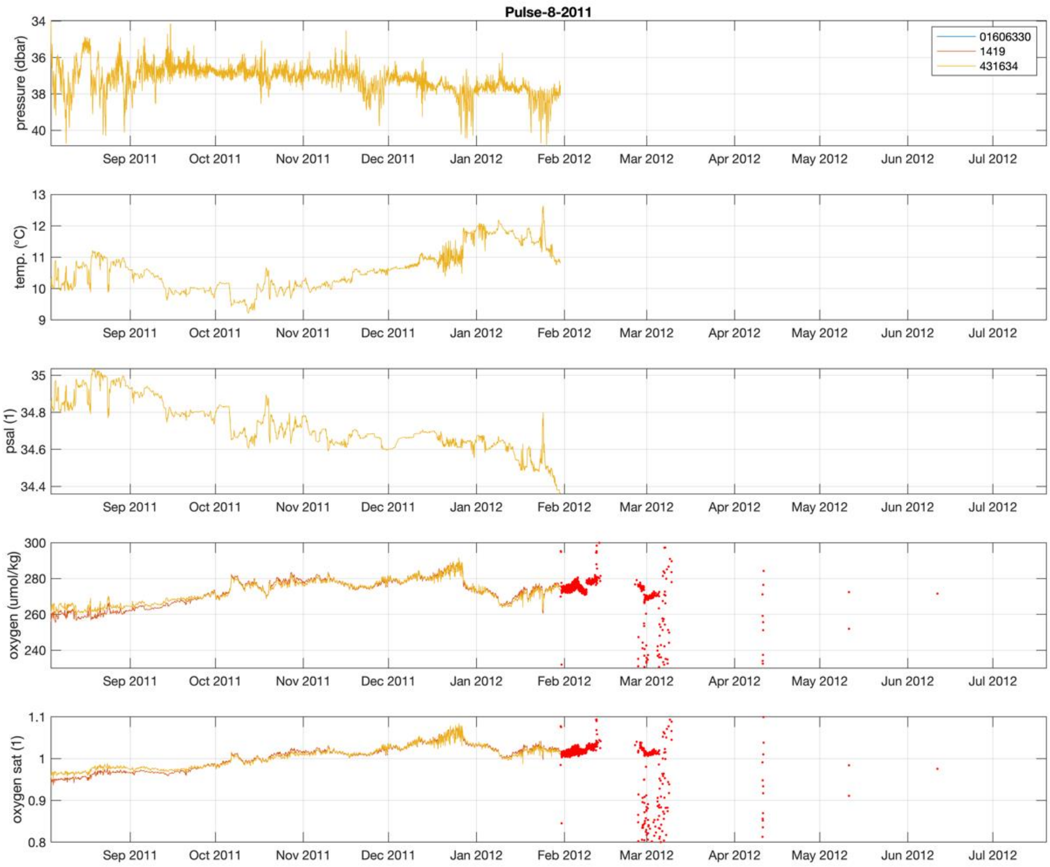
Appendix C Annotated QC plots for all deployments

Jansen P, Wynn-Edwards CA, Shadwick EH and Trull TW (2023). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Oxygen Records Version 1.0. CSIRO, Australia. DOI: 10.26198/1te4-jq81

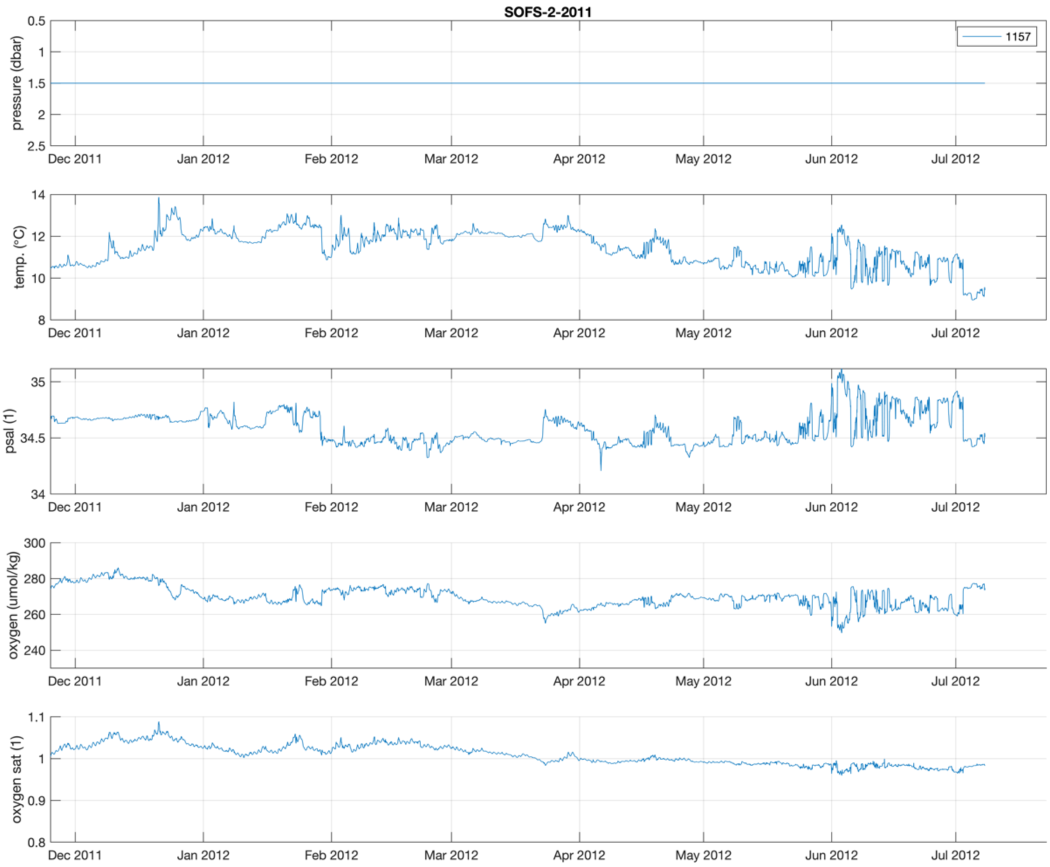
Jansen P, Wynn-Edwards CA, Shadwick EH and Trull TW (2023). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Oxygen Records Version 1.0. CSIRO, Australia. DOI: 10.26198/1te4-jq81


SOFS-1-2010
1157
pressure (dbar)
temp. (°C)
psal (1)
oxygen (umol/kg)
oxygen sat (1)
Apr 2010
Jul 2010
Oct 2010
Jan 2011
Apr 2011

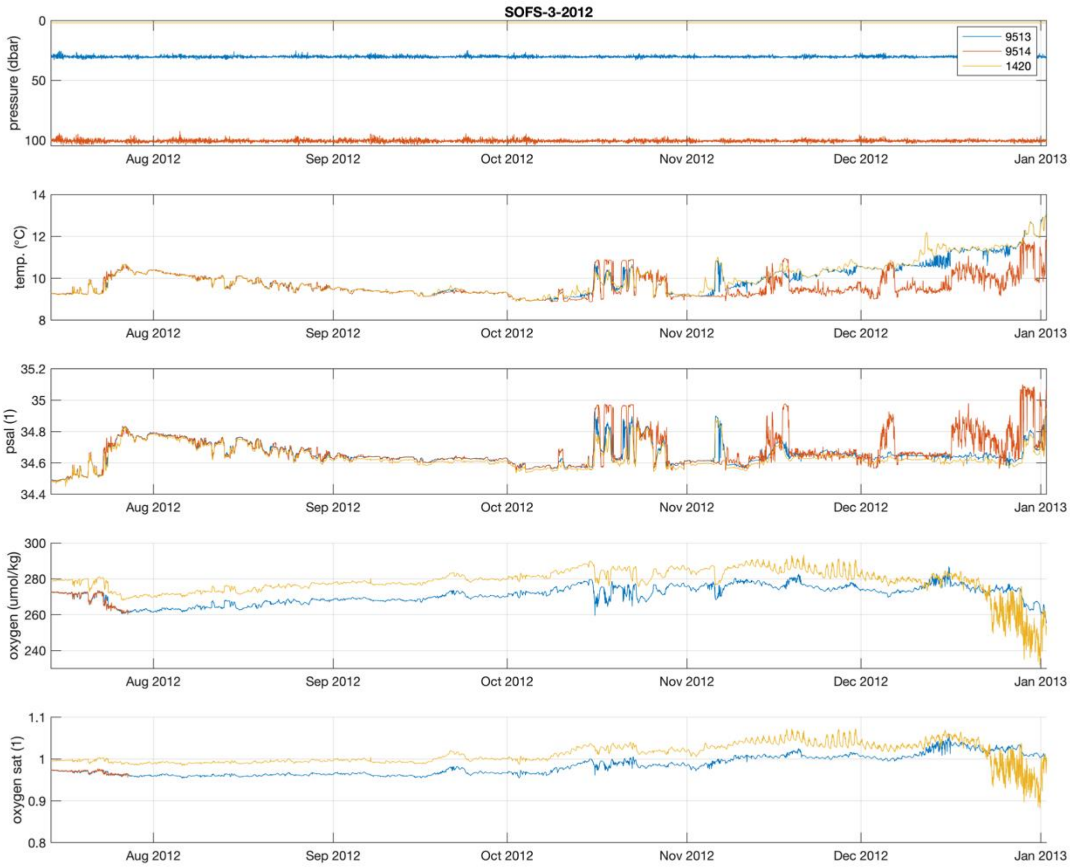
Pulse-7- blue line is SBE43 oxygen before scaled to Optode value.



The Optode O_2 estimate rises to meet the SBE43 values over the first month –this represents hydration.

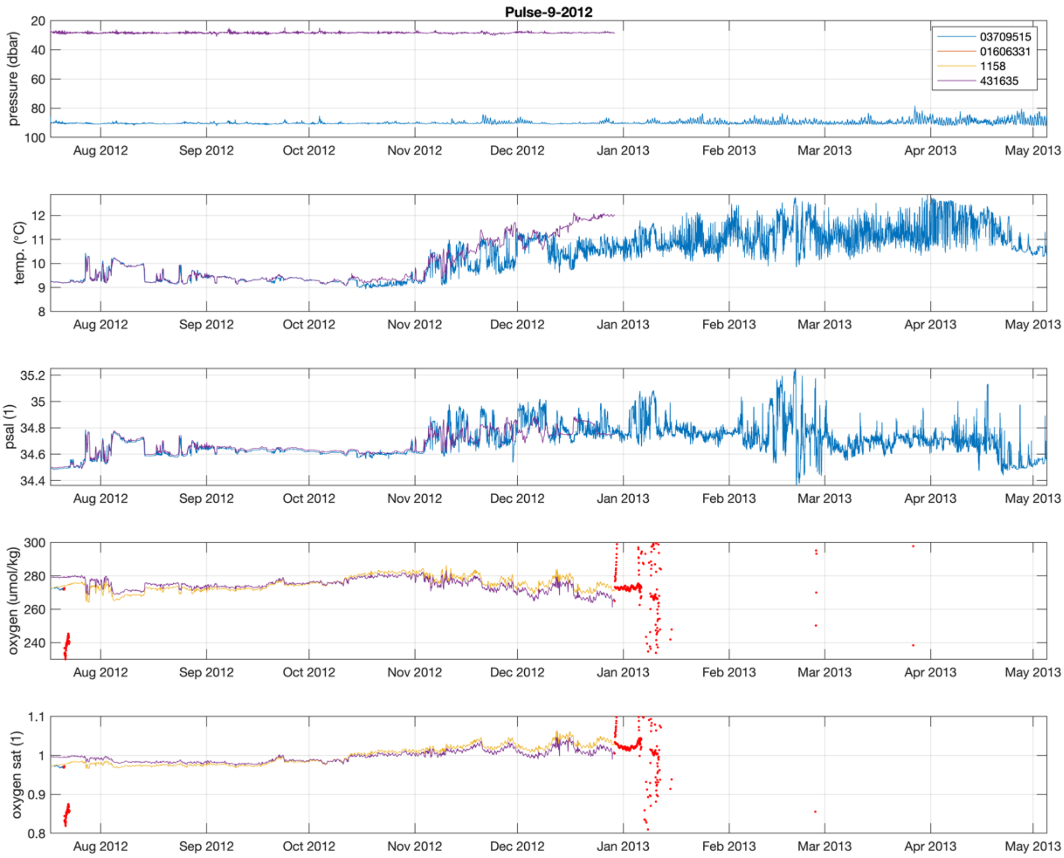


Jansen P, Wynn-Edwards CA, Shadwick EH and Trull TW (2023). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Oxygen Records Version 1.0. CSIRO, Australia. DOI: 10.26198/1te4-jq81



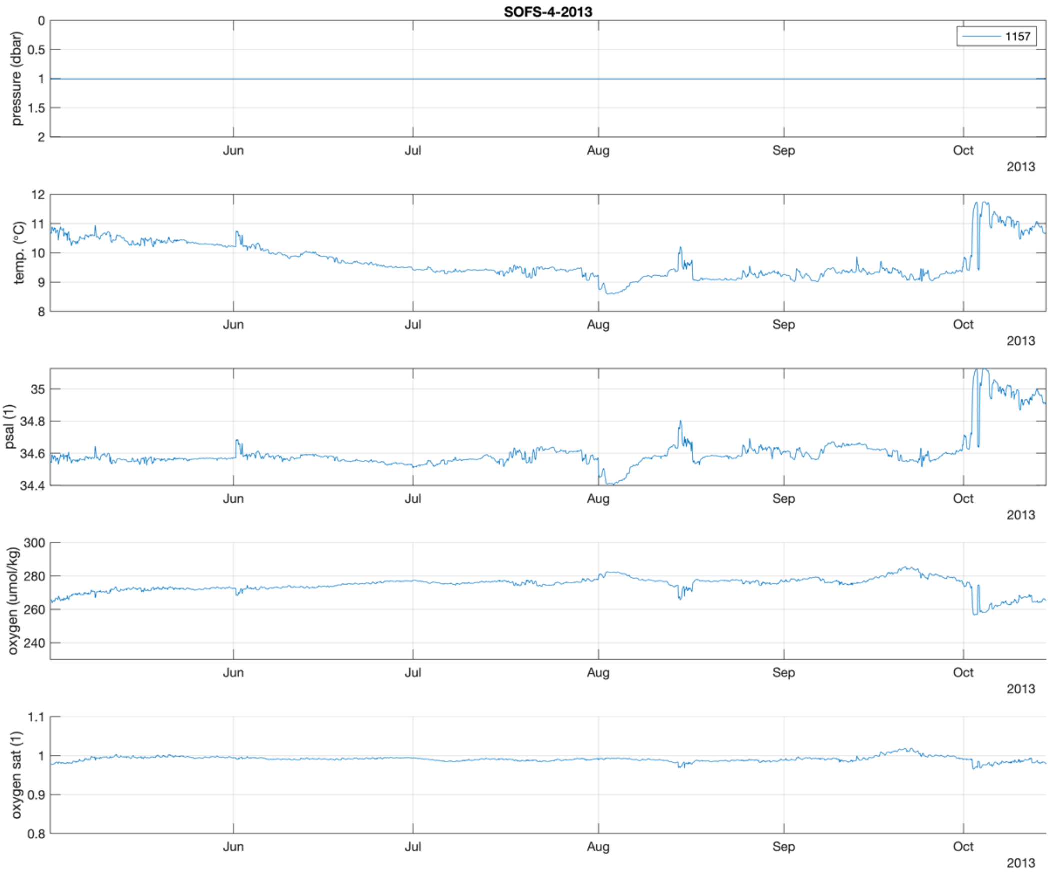
SOFS-3-2012, SBE37SMP-ODO 9514 failed in July.

Jansen P, Wynn-Edwards CA, Shadwick EH and Trull TW (2023). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Oxygen Records Version 1.0. CSIRO, Australia. DOI: 10.26198/1te4-jq81

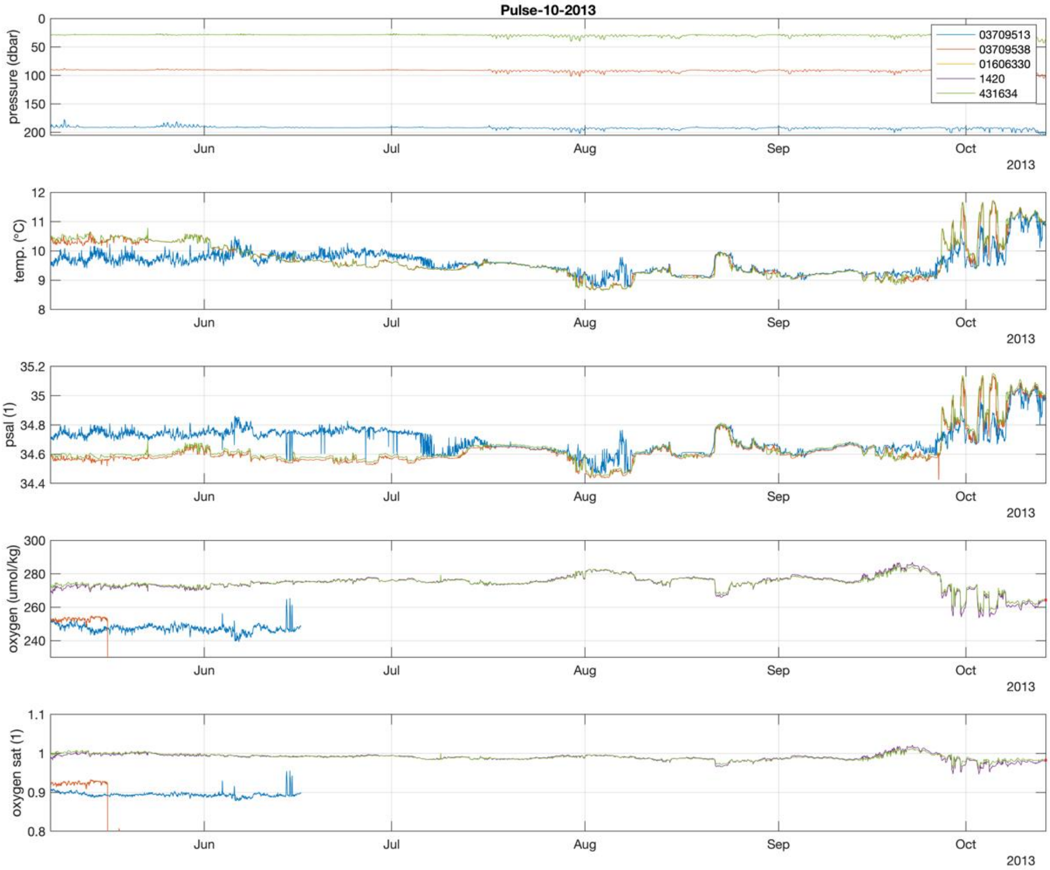


Pulse-9-2012 SBE37SMP-ODO 9515, failed in July 2012.

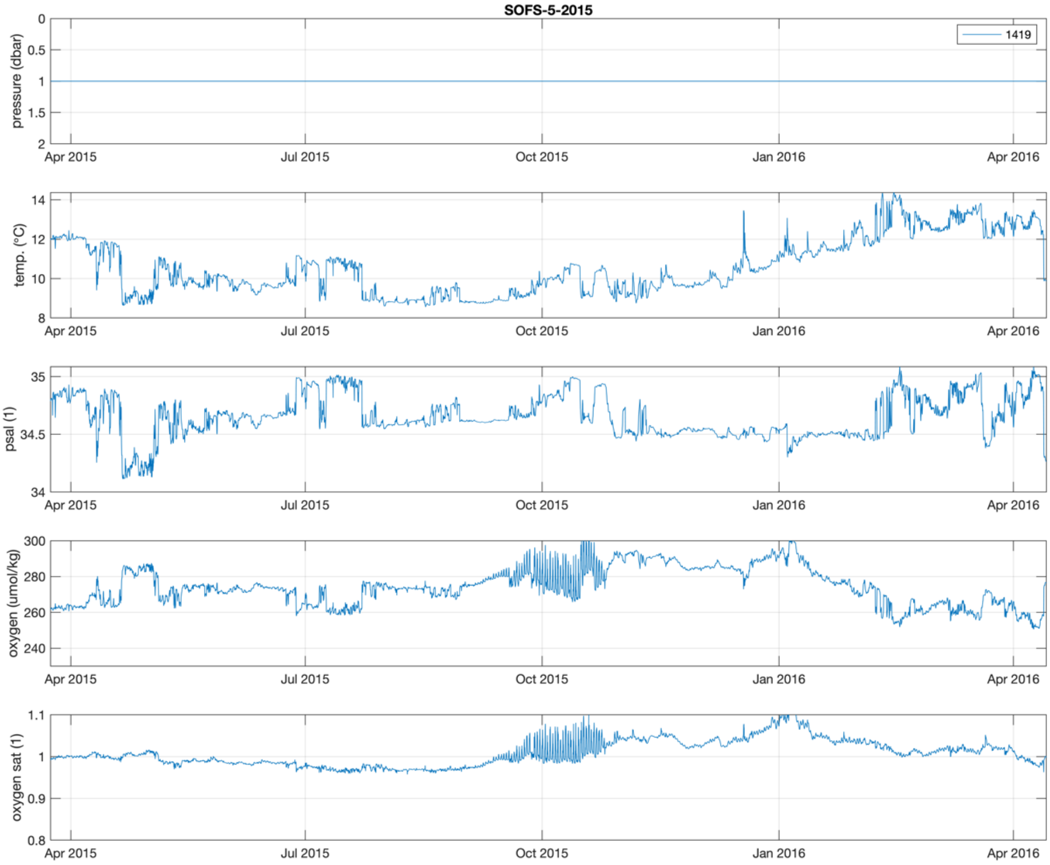
Jansen P, Wynn-Edwards CA, Shadwick EH and Trull TW (2023). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Oxygen Records Version 1.0. CSIRO, Australia. DOI: 10.26198/1te4-jq81



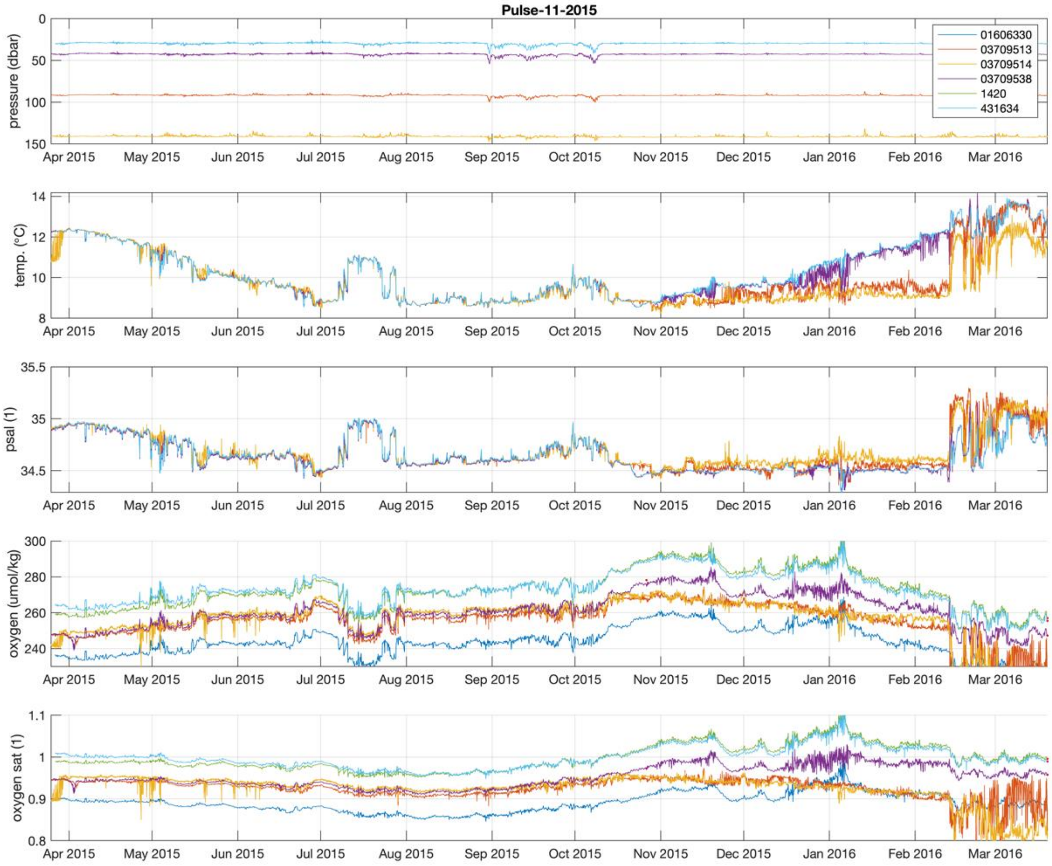
Jansen P, Wynn-Edwards CA, Shadwick EH and Trull TW (2023). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Oxygen Records Version 1.0. CSIRO, Australia. DOI: 10.26198/1te4-jq81



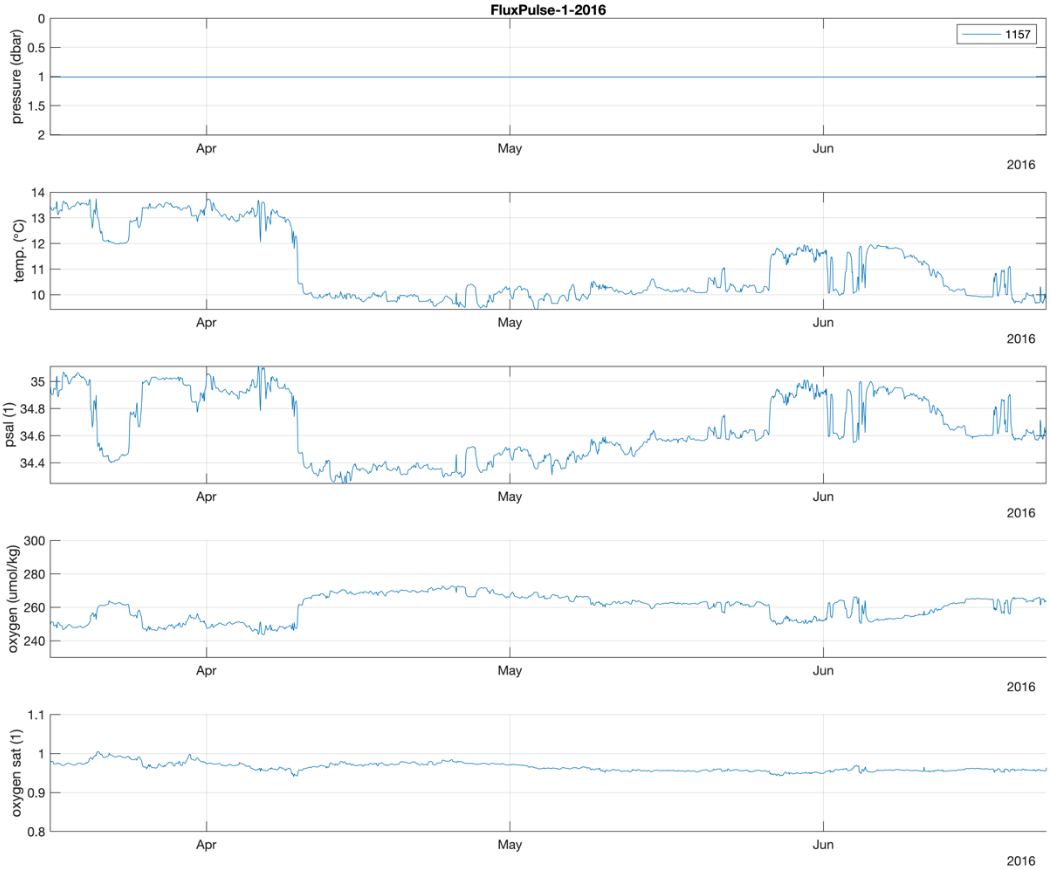
Pulse-10-2013 SBE37SMP-ODO 9513 failed in June 2013.

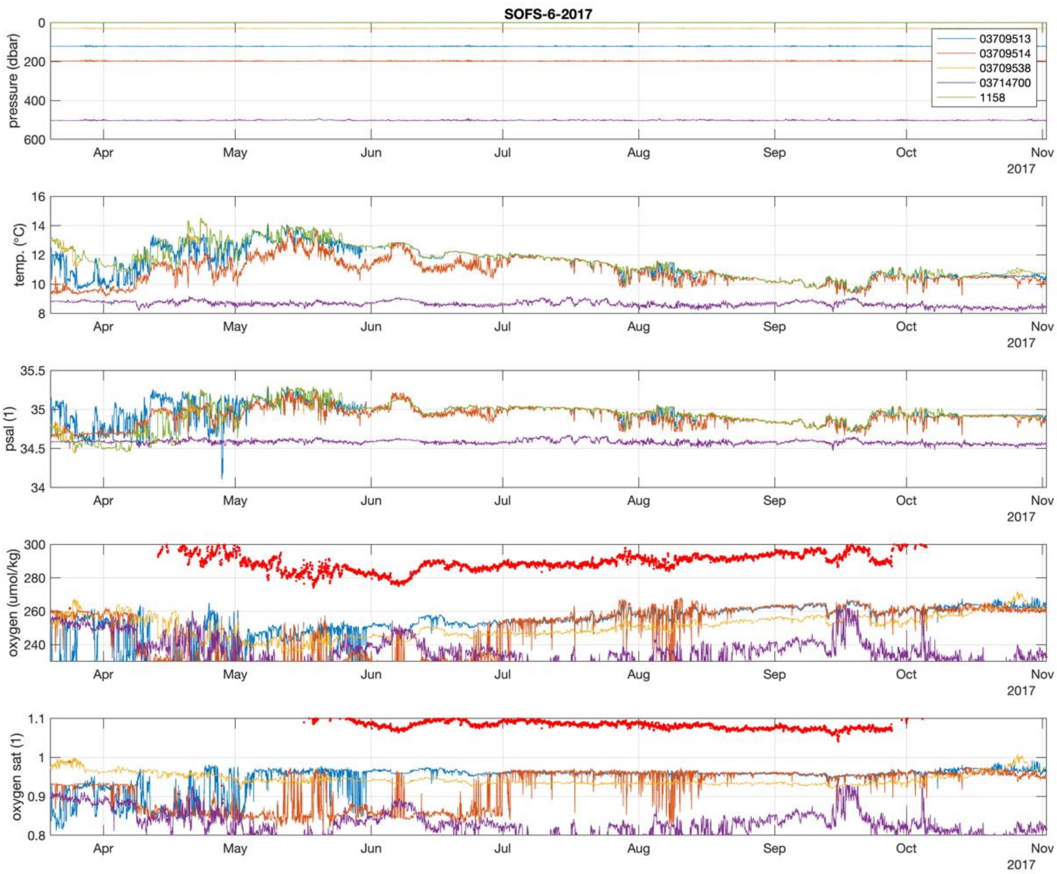


Jansen P, Wynn-Edwards CA, Shadwick EH and Trull TW (2023). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Oxygen Records Version 1.0. CSIRO, Australia. DOI: 10.26198/1te4-jq81



Jansen P, Wynn-Edwards CA, Shadwick EH and Trull TW (2023). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Oxygen Records Version 1.0. CSIRO, Australia. DOI: 10.26198/1te4-jq81

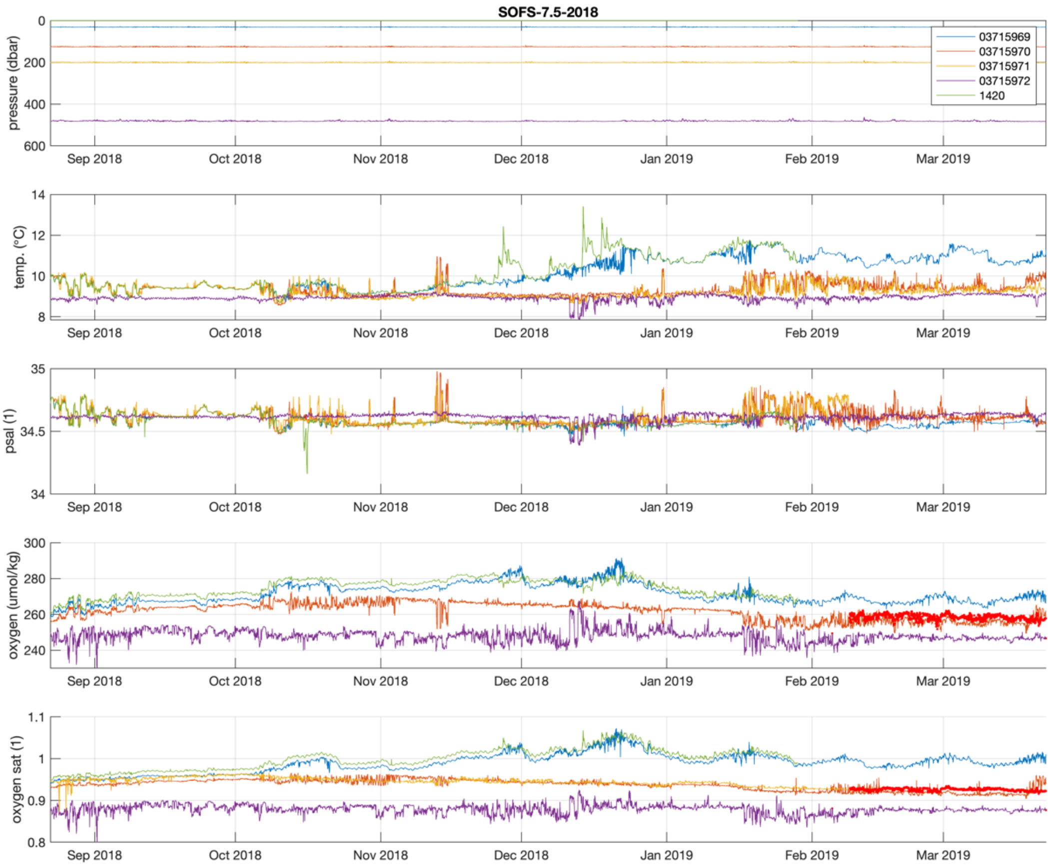

FluxPulse-1-2016
1157
pressure (dbar)
temp. (°C)
psal (1)
oxygen (umol/kg)
oxygen sat (1)
Apr
May
Jun
2016



SOFS-6-2017 Optode 1158 reading high, marked bad by manual QC

Jansen P, Wynn-Edwards CA, Shadwick EH and Trull TW (2023). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Oxygen Records Version 1.0. CSIRO, Australia. DOI: 10.26198/1te4-jq81

Jansen P, Wynn-Edwards CA, Shadwick EH and Trull TW (2023). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Oxygen Records Version 1.0. CSIRO, Australia. DOI: 10.26198/1te4-jq81



SOFS-7.5-2018, SBE37SMP-ODO 15971 salinity cell failed in February 2019.

Jansen P, Wynn-Edwards CA, Shadwick EH and Trull TW (2023). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Oxygen Records Version 1.0. CSIRO, Australia. DOI: 10.26198/1te4-jq81

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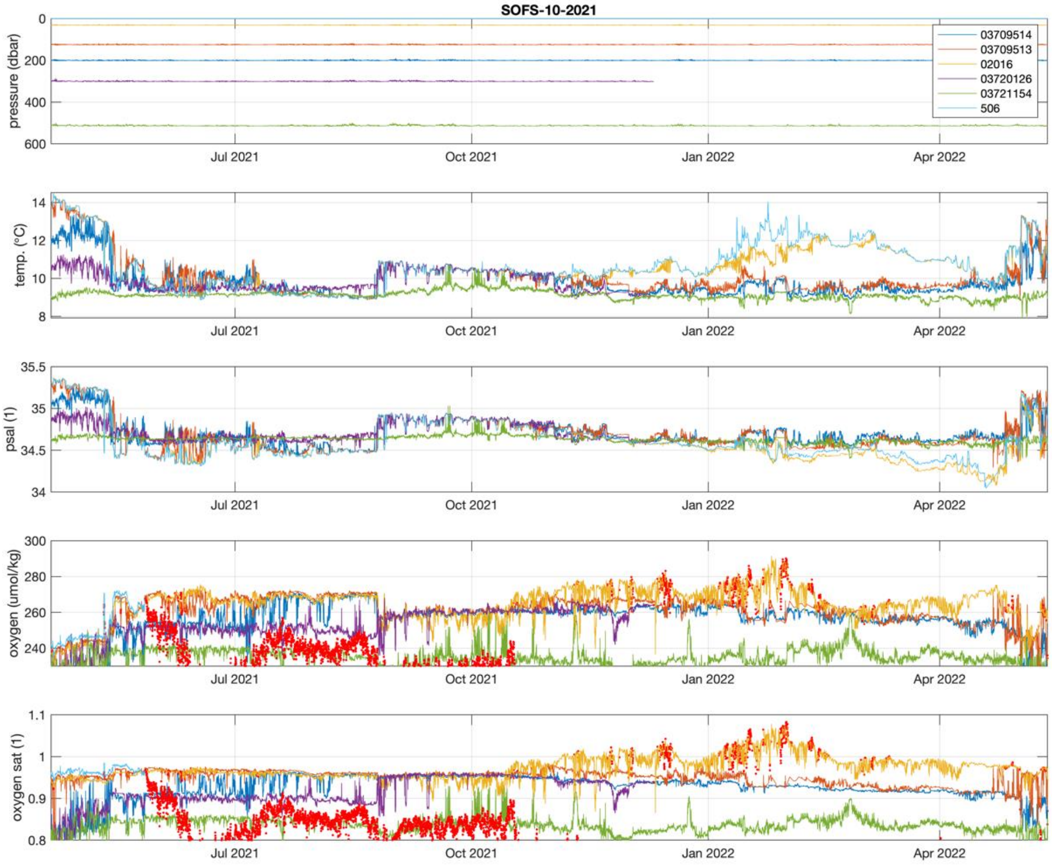
SOFS-9-2020 Optode 1420 manually marked bad (red) bio fouled after November 2020.



SOFS-10-2021, Optode 506, manually marked bad (red) bio fouled in June 2021.

Jansen P, Wynn-Edwards CA, Shadwick EH and Trull TW (2023). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Oxygen Records Version 1.0. CSIRO, Australia. DOI: 10.26198/1te4-jq81

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Version	**Date**	**Change Description**	**Revision Author**
1.0	01 Mar 2023	Original version	Jansen, Wynn-Edwards, Shadwick and Trull