



Integrated **Marine**
Observing System

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Acidification Moorings

System Description and Procedures for Moored Biogeochemical Measurements

Version 1.0

Bronte Tilbrook¹ and Erik van Ooijen¹
¹ CSIRO Environment, Hobart, Tasmania 7000

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Mooring locations

Australia's Integrated Marine Observing System (IMOS) supports surface biogeochemical moorings at three sites on the Australian shelf to provide baseline data to assess trends and variability in ocean acidification (OA), CO₂, salinity and temperature change. The three sites are at Wistari Channel, Heron Island, on the Great Barrier Reef (23.459°S, 151.927°E), off Maria Island, Tasmania (42.599°S, 148.234°E), and to the west of Kangaroo Island, South Australia (35.835°S, 136.451°E).

The sites are in regions where seawater CO₂ and related OA conditions are predicted to soon be outside ranges that ecosystems have experienced in the preindustrial era with concerns the changes will disrupt marine life. The site at Heron Island is the longest continuous coral reef time-series site in the Southern Hemisphere and one of a handful of long-term reef monitoring sites in the world. It delivers data that underpins research to determine OA exposure on the Great Barrier Reef and biological impacts of the changes. The Maria Island site is near the edge of the shelf in 95m water depth and provided data for the extension of the East Australian Current. This is a region undergoing major warming and ecosystem change. The Kangaroo Island mooring is near one of the few upwelling systems in Australian waters and in about 105m depth near the shelf edge. Both the Maria Island and Kangaroo Island sites monitor source waters that support the largest actively growing carbonate platform on earth along the Southern Australian coast.

Mooring design

The surface buoys have a 1.5m octagonal-shaped foam-filled fibreglass hull, with a polyurethane topcoat. The buoy is designed by the NOAA Pacific Marine Environmental Laboratory and extends about 0.9m above and 1.2m below the waterline. Instrumentation is fitted into moulded wells in the top of the buoy and on a centre pylon at the base of the buoy. The buoys are moored to the sea floor using a 700kg anchor made of two-stacked train wheels. Two acoustic releases are located above the anchors and are connected to the surface buoy via chain, swivels and heavy-duty bungee cord that is used to dampen wave action.

Each surface buoy is equipped with a Battelle M_{Ap}CO₂ monitoring system for fCO₂, a Sea-Bird Electronics SBE16plusV2 for salinity and temperature, a Sea-Bird Electronics SeaFET or SeapHOx for pH, and an Aanderaa optode (models 3835, 4175 and 4175C) for dissolved oxygen (see Sensor Specifications). Iridium communications are used to deliver data in near real-time and a GPS allows the position to be monitored continuously to ensure the mooring is remaining in place.

As part of regular maintenance and to minimise the effects of biofouling, the moorings are recovered about every six months, and the mooring line checked and replaced if necessary. A replacement surface buoy and calibrated sensors are swapped in at each recovery.

Measurement sequence

Fugacity of carbon dioxide (fCO₂)

The fCO₂ measurement by the M_{Ap}CO₂ system uses headspace equilibration with the equilibrator intake at 0.6m depth as described in Sutton et al. (2014). The system goes through an automated measurement sequence every 2 or 3 hours. Each sequence includes measurements of zero and span gas, equilibrator headspace, and air that occur over about 20 minutes, which includes time to flush the different gases through the system. The CO₂ mole

fraction in the gas streams is quantified using a LI-COR 820 non-dispersive infrared gas analyser and is converted to a fugacity at sea surface conditions.

At the start of each measurement sequence a two-point calibration of the LI-COR 820 is made with a zero CO₂ gas and a high CO₂ span gas (typically 450-550 $\mu\text{mol mol}^{-1}$) that bracket the range of CO₂ mole fractions in seawater and air at the measurement sites. The zero CO₂ gas is generated by cycling air through soda lime and dried using the silica gel trap and nafion tubing. The CO₂ span gas is dry and is calibrated by NOAA/CMDL (<https://gml.noaa.gov/ccl/>) or CSIRO GASLAB and referenced to the WMO X2019 scale (Hall et al., 2021). The span gas can provide calibration data over the six-month deployments and has spare capacity to last for up to nine months if the measurement frequency is reduced using remote commands. The equilibrator headspace measurement occurs about 17 minutes after the zero and span calibration sequence and is followed by a measurement of air. The pressure of the equilibrator headspace gas and air are equal and measured using the LI-COR 820 pressure sensor. The gases are passed through silica gel and nafion tubing to remove water vapour prior to the measurement of CO₂ by the LI-COR 820. Residual water vapour in the gas stream is quantified using a Sensirion SHT71 relative humidity sensor and these values are used to correct to a dry CO₂ mole fraction. After flushing, each M_{Ap}CO₂ measurement is made over 30 seconds at 2Hz, and the high frequency data are stored internally with the average and standard deviation of each measurement. At the time of the equilibrator headspace measurements, a SBE16PlusV2 mounted on the surface buoy is polled for temperature, salinity, and dissolved oxygen sensor readings.

The M_{Ap}CO₂ and SBE 16PlusV2 data are stored internally and data are also transmitted to shore via iridium as daily near real-time data. The daily transmitted data contain diagnostic parameters that are used to monitor the performance of the sensors. The SeapHOx or SeaFET sensors used for pH measurements are mounted on the surface buoy and are logged independently of the M_{Ap}CO₂ system. The data from these sensors are stored internally for retrieval and processing after moorings are recovered.

Testing and Calibration Procedures

Pre- and post- deployment calibration checks are made on the sensors fitted to the moorings. The individual sensors used in the system are first checked to ensure the sensors meet performance requirements followed by a combined check of the equilibrator and M_{Ap}CO₂ detector in a seawater bath.

The LI-COR 820 in the M_{Ap}CO₂ system is used to measure the mole fraction of CO₂ and is first checked using a range of dry CO₂-in-air reference gases (0, 260, 370, 450 or 550 $\mu\text{mol mol}^{-1}$) at CSIRO, Hobart. The LI-COR 820 calibration is typically within $\pm 1 \mu\text{mol mol}^{-1}$ of the reference gas values and is accepted if the agreement is within $2 \mu\text{mol mol}^{-1}$. If the LI-COR 820 measurements and the CO₂-in-air reference gas values are different by more than $2 \mu\text{mol mol}^{-1}$, a correction is applied to the sensor output based the reference gas values. The LI-COR 820 response is rechecked over the reference gas range to ensure the measurements agree within $2 \mu\text{mol mol}^{-1}$. Measurements by the pressure sensor in the LI-COR 820 are checked against a Druck DPI142 pressure indicator, and verified to agree within 0.5 kPa before and after each deployment. The Sensirion SHT71 relative humidity sensor used to determine the water vapour content in the measured gas stream is reconditioned before deployments and recalibrated to an accuracy of <3% using a LI-COR 610 dew point generator. This sensor has a linear drift with time and post deployment checks using the dew point generator are used to apply a time dependent drift correction.

Once the individual sensors are calibrated, the MApCO₂ system response with the equilibrator is checked in a seawater bath operated over a range of temperatures and fCO₂ values expected in the field. These CO₂ measurements are compared to a General Oceanics 8050 CO₂ system (Pierrot et al. 2009) to ensure the systems agree within 2 μatm prior to deployment.

A SBE16plus V2 CTD is polled for temperature, salinity, and dissolved oxygen data for each MApCO₂ measurement sequence, with additional measurements made each hour. The temperature and salinity measurements use factory calibrations for initial deployments or annual calibrations performed at a certified National Australian Testing Authority facility at CSIRO, Hobart. Over the duration of deployments, the instruments meet manufacturer specifications for salinity of accuracy of ± 0.0066 PSU at S=35 PSU and stability of < 0.008 PSU/month, and for temperature an accuracy of 0.005°C and stability of < 0.0002 °C/month. A comparison between in-situ measurements made with the SBE16Plus V2 with occasional CTD measurements or water sample salinity measurements indicate a greater uncertainty of 0.03°C and 0.05 for sea surface temperature and salinity, respectively. The greater uncertainty could result from local variability around the sample site, sample storage artifacts, or mismatches in the time of CTD or water sampling. The larger uncertainties are used for propagation uncertainties in the CO₂ system calculations.

Aanderaa optodes used for dissolved oxygen are logged by the SBE16PlusV2 and are calibrated before and after deployments at CSIRO, Hobart, using a purpose-built calibration system, referenced to dissolved oxygen measurements made using modified Winkler titrations (Culberson, 1991). The calibrations cover a range of temperatures and oxygen concentrations that occur in the field and are used to fit coefficients to the Stern-Volmer equation (Uchida et al. 2008). Calibrations made before deployments and after sensor retrieval are used to check for sensor drift, which is typically $< 1\%$ and is linear over a six-month deployment and a time-dependent drift correction is applied. The uncertainty of measurements is typically within $\pm 1 \mu mol l^{-1}$, based on pre- and post-deployment calibrations with occasional field measurements of dissolved oxygen on water samples used to compare with the optode measurements.

Measurements of pH by SeaFET or SeapHOx sensors are made with a Honeywell Durafet pH electrode following the calibration procedures of Bresnehan et al. (2014). The sensors are preconditioned in seawater prior to deployment.

Quality Control (QC)

Realtime QC

All sensor data apart from pH are transmitted daily from the mooring when a satellite iridium connection is possible. These near real-time data use pre-deployment sensor calibrations for fCO₂, sea surface temperature, sea surface salinity, and dissolved oxygen. Matlab code is used to automatically range check and flag data using the WOCE flag convention (good=2, questionable =3, and bad = 4). Error propagation is applied following the data reduction method described in the Calculations and Data Reduction section. These daily data files are converted to a NetCDF file for each platform and sent daily to the AODN portal.

Delayed mode QC

The high-frequency measurements stored on the sensors are downloaded on recovery, and the sensors returned for post-deployment calibration and maintenance. Pre- and post-deployment

calibrations are compared to determine if the level of sensor drift is within an acceptable range and data are recalculated with final calibration coefficients as described in the Calculation and Data Reduction section below.

The data are first checked automatically with bad measurements identified either as measurement gaps, measurements outside acceptable ranges, or as outliers identified using the Thomson Tau method (Thompson, 1985). Data are then automatically checked based on parameter range checking and sensor diagnostics information, followed by a manual check. A final quality check is made by comparing the air CO₂ measurements to historical air CO₂ data for each mooring and by comparison to the Globalview CO₂ dataset (Dlugokencky et al., 2015). Globalview data are smoothed over latitude bands of a few degrees with limited data to constrain atmospheric boundary-layer CO₂ measurements in coastal regions of the Southern Hemisphere where local sources and sinks of CO₂ can cause variability in air CO₂. Consequently, this check is to confirm there no large step changes or discrepancies in the measured air CO₂ that might indicate an instrumental issue. The final delayed mode data has WOCE quality flags assigned (good=2, questionable=3, and bad=4), is converted to a NetCDF file and sent to the AODN portal.

Calculation and Data Reduction

Fugacity of CO₂

For each measurement cycle, the zero and span gas are analysed immediately before equilibrator air and atmospheric gas to calibrate the LI-COR 820 NDIR response and provide a measurement of the CO₂ mole fraction in the gas stream. The gas stream analysed by the NDIR is only partially dried by flowing the gas through silica gel and nafion tubing, and a dilution correction is applied to account for the presence of water vapour (LI-COR Application note 129).

$$xCO_2(\mu mol mol^{-1}) = \frac{xCO_2^{raw}}{\left(1 - \frac{w}{1000}\right)}$$

where, w is the calculated water vapour mole fraction and xCO_2^{raw} is the raw data value for the CO₂ mole fraction measured in the gas stream by the LI-COR 820 NDIR.

The partial pressure of CO₂ in the water is calculated at total pressure, P (atm), with a correction for water vapour pressure (pH_2O ; Weiss and Price, 1980) calculated at the sea surface temperature, T (K), and sea surface salinity, S :

$$pCO_2(\mu atm) = xCO_2(P - pH_2O)$$

where,

$$pH_2O(atm) = \exp\left(24.4543 - 67.4509 \frac{100}{T} - 4.8489 \ln \frac{T}{100} - 0.000544S\right)$$

The partial pressure of CO₂ is converted to fugacity after Weiss (1974):

$$fCO_2(\mu atm) = pCO_2 \exp \left[\frac{P(B(CO_2, T) + 2\delta(CO_2, T))}{RT} \right]$$

where,

$$R = 82.0578 \text{ cm}^3 \text{ mol}^{-1} \text{ K}^{-1},$$

$$B(CO_2, T) = -1636.75 + 12.0408T - 3.27957 \cdot 10^{-2}T^2 + 3.162528 \cdot 10^{-5}T^3 \text{ cm}^3 \text{ mol}^{-1}$$

$$\delta(CO_2, T) = 57.7 - 0.118T \text{ cm}^3 \text{ mol}^{-1}$$

Dissolved oxygen

The bphase (Bp , degrees) and the temperature ($Topt$, °C) values from the Aanderaa optode are used to calculate pre- and post-calibrated dissolved oxygen values, DO_{raw} , using the Stern-Volmer equation (Uchida et al., 2008), and corresponding calibration coefficients, c1 to c7:

$$DO_{raw}(\mu mol \text{ l}^{-1}) = \frac{\frac{c4 + c5Topt}{c6 + c7Bp} - 1}{c1 + c2Topt + c4Topt^2}$$

The optode salinity is set to zero and a correction is applied to dissolved oxygen at seawater salinity using coefficients of Garcia and Gordon (1992, 1993) calculated from Benson and Krause (1984) data:

$$DO_{sw}(\mu mol \text{ l}^{-1}) = DO_{raw} \exp(S(B0 + B1T_s + B2T_s^2 + B3T_s^3) + C0S^2)$$

where the salinity, S , and seawater temperature, T (°C) are measured by the SBE16plusV2 with,

$$T_s = \ln \frac{298.15 - T}{273.15 + T}$$

The coefficients are:

$$B0 = -6.24523e-3$$

$$B1 = -7.37614e-3$$

$$B2 = -1.03410e-2$$

$$B3 = -8.17083e-3$$

$$C0 = -4.88682e-7$$

The percent saturation in dissolved oxygen, $DOXS$, is calculated as

$$DOXS (\%) = 100 \left(\frac{DO_{sw}}{DO_{satn}} \right)$$

Where DO_{satn} is the concentration of dissolved oxygen in surface waters at sea surface temperature and salinity in equilibrium with air at one atmosphere total pressure. DO_{satn} is calculated using equation 8 of Gordon and Garcia (1992, 1993) and applying a conversion factor of 44.6596 to convert from $ml \text{ l}^{-1}$ to $\mu mol \text{ l}^{-1}$

$$DO_{satn}(\mu mol l^{-1}) = 44.6596 \cdot \exp(A0 + A1T_s + A2T_s^2 + A3T_s^3 + A4T_s^4 + A5T_s^5) + S(B0 + B1T_s + B2T_s^2 + B3T_s^3) + C0S^2$$

where,

$$\begin{aligned} A0 &= 2.00907 \\ A1 &= 3.22014 \\ A2 &= 4.05010 \\ A3 &= 4.94457 \\ A4 &= -2.56847e-1 \\ A5 &= 3.88767 \\ B0 &= -6.24523e-3 \\ B1 &= -7.37614e-3 \\ B2 &= -1.03410e-2 \\ B3 &= -8.17083e-3 \\ C0 &= -4.88682e-7 \end{aligned}$$

pH

Raw DuraFET voltages measured by the seaFET or SeapHOx instrument are calibrated on the total pH scale (pHt) at in-situ temperature and salinity following Bresnehan et al. (2014). The pHt calibration values are obtained from CO2SYSv3 (Sharp et al., 2023) using total dissolved inorganic carbon (DIC) and total alkalinity (TA) sampled next to the pH sensor and at the time of a pH measurement. The water samples are analysed at CSIRO, Hobart, for DIC and TA using coulometry and open-cell potentiometric titration, respectively (Dickson et al. 2007). Reference seawater material from the Dickson laboratory at the Scripps Institution of Oceanography was used to verify the measurement precision of $\pm 2 \mu mol kg^{-1}$ for both variables. The CO2SYSv3 calculations use Lueker et al. (2000) K1/K2 dissociation constants, the bisulfate (HSO4-) dissociation constant of Dickson (1990), the hydrofluoric acid dissociation constant of Perez and Fraga (1987), and the boron-salinity ratio of Uppstrom (1979). Surface measurements at these sites show total phosphate and silicate concentrations are less than 0.5 and 1.8 $\mu mol kg^{-1}$, respectively, which causes less than a 0.001 reduction in pHt and are assumed zero for the calculation. The uncertainty in the pH measurement is calculated in CO2SYSv3 using the uncertainties of input parameters listed in Table 1.

Aragonite Saturation State (Omega_Ar)

For surface sample where both pHt and fCO₂ measurements are made independently, the saturation state of aragonite is calculated using CO2SYSv3. The uncertainty of the calculation uses uncertainty estimates of input parameters in Table 1 and accounts for fCO₂ and pH covariance. Future calculations using fCO₂ or pHt paired with TA will reduce the uncertainty in Omega_Ar by almost 50%.

Table 1. Delayed-mode quality-controlled data with uncertainty.

Parameter	Unit	Description	Uncertainty
TIME	YYYY-MM-DDThh:mm:ssZ	ISO8601, UTC	
LATITUDE	decimal degrees	Latitude	0.0001
LONGITUDE	decimal degrees	Longitude	0.0001
XCO2EQ_PPM	micromol/mol	Dry mole fraction of CO ₂ in the equilibrator head space	2
XCO2ATM_PPM	micromol/mol	Dry mole fraction of CO ₂ in the atmosphere	2
fCO2SW_UATM	microatm	Fugacity of carbon dioxide at surface water in water saturated air at sea surface temperature and salinity	2
DfCO2	microatm	Delta fCO ₂ = (fCO ₂ _WET_SW - fCO ₂ _WET_AIR)	
Press_ATM	kPa	Barometric pressure	0.05
TEMP	degC	Sea surface temperature	0.03
PSAL	PSS	Sea surface salinity	0.05
DOX1	micromol/l	Concentration dissolved oxygen in surface seawater	1
†DOXS	%	Concentration of dissolved oxygen expressed as a percentage of the oxygen concentration in water that is in equilibrium with the atmosphere	
††pHt		Total pH scale when measured	0.015
OMEGA_A		Saturation state of aragonite by computation	0.26
quality_control	QC flag	QC flag for reported parameters 2=good; 3=questionable; 4=bad	
SUB_FLAG	24-bit number	Internal QC parameter	

† 1 atmosphere total pressure and at sea surface temperature and salinity

†† calculated using fCO₂ and pH paired surface samples at sea surface temperature and salinity

Sensor specifications

CO₂: Battelle M_{AP}CO₂, using a LI-COR 820 NDIR

Equilibrator: Vented bubble equilibrator, intake depth 1m

Equilibrator volume: 100 ml of air equilibrating with an unlimited volume of seawater

Headspace gas flowrate: $\sim 600 \text{ cc min}^{-1}$

Resolution: $0.01 \mu\text{mol mol}^{-1}$

Accuracy: $< 2 \mu\text{mol mol}^{-1}$, based on laboratory calibrations and field comparisons

Equilibrator and Air Pressure Sensors: LI-COR 820 internal pressure sensor

Resolution: 0.01 kPa

Accuracy: $< 0.5 \text{ kPa}$, based on laboratory comparison against a Druck DPI 142 sensor

Relative Humidity Sensor: Sensirion Humidity Sensor SHT71

Measurement range: 0-100%

Resolution: 1%

Accuracy: $\pm 3\%$ (20-80% Relative Humidity), factory calibration or CSIRO calibrated using LICOR-610

O₂ Sensor: Aanderaa Optode 3835, 4175, 4175C

Resolution: $0.01 \mu\text{mol l}^{-1}$

Accuracy: $< 1 \mu\text{mol l}^{-1}$, based on Winkler oxygen titrations at CSIRO, Hobart

CTD Sensor (Equilibrator and Sea Surface): Sea-Bird Electronics SBE16plusV2, depth of 1m

Resolution: $0.0001 \text{ }^\circ\text{C}$; 0.00005 S m^{-1}

Accuracy: $0.005 \text{ }^\circ\text{C}$; 0.0005 S m^{-1}

pH Sensor: Sea-Bird Electronics SeaFET or SeapHOx

Resolution: 0.001

Accuracy: ± 0.015

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