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Southern Ocean Time Series (SOTS) Net Community Production (NCP) Calculation Procedure and MATLAB Code Version 1.0



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Executive summary

The Southern Ocean Time Series (SOTS) Observatory, located in Subantarctic waters near 141°E and 47°S, consists of autonomous moorings that provide high temporal resolution observations. 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 CO₂ 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 including solar radiation, chlorophyll fluorescence, optical backscatter, dissolved nitrate, dissolved oxygen, and total dissolved gases (using a total gas tension device). The oxygen and total gas tension observations can be combined to separate physical and biological contributions to surface mixed layer oxygen budgets and thus to yield estimates of net community production. This procedure, and the associated MATLAB code, are the subjects of this report. The code is currently enabled explicitly for the first three mooring deployments at SOTS with full suites of successful biogeochemical sensors required for the NCP calculations: Pulse-7, Pulse-9, and SOFS-7.5. It is constructed to allow expansion to future SOTS data sets, as well as other time series observations.

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/>.

1 Introduction

Net community production (NCP) is defined as the amount of photosynthetic primary production which is not immediately respired by phytoplankton or other organisms and can thus accumulate at the depths where it is produced, or be transferred to the deep ocean by mixing, advection, biological transport, or particle sinking. It is thus the important starting point of the biological carbon pump. There are many ways to estimate NCP including incubations, sinking particle flux measurements and dissolved nutrient mass balances. Each has advantages and shortcomings.

The focus here is on making a mass balance for oxygen (produced by photosynthesis and consumed by respiration) in surface waters to estimate NCP. This requires defining a surface layer over which the mass balance will be made – chosen here to be the surface mixed layer. This has the advantage that measurements at a single depth can be used to determine NCP. In the Subantarctic Southern Ocean, where the surface mixed layer depth (MLD) is almost always deeper than the euphotic zone (Rintoul and Trull, 2001) and phytoplankton biomass is generally confined above the MLD (Bowie et al., 2011), this approach also does a good job of capturing all the photosynthetic NCP.

The procedure described here is essentially that applied previously to SOTS seasonal records of oxygen and total gas tension observations (Trull et al., 2019, Weeding and Trull, 2014), which built on and slightly modified the earlier work of Emerson and colleagues (Emerson et al., 1991, Emerson and Stump, 2010b, Emerson et al., 2008a). It uses the total gas tension record to calculate inputs of oxygen to the mixed layer from the atmosphere, via two processes: i. diffusive gas exchange, and ii. bubble injection (for which the relative proportion of fully dissolving and partially dissolving bubbles must also be specified). Exchange with low oxygen waters below the mixed layer is also parameterized for two processes: i. eddy diffusion (for which the diffusivity must be specified), and ii. entrainment, as estimated from observed changes in mixed layer depth. These terms are then removed from the observed mixed layer oxygen time series to obtain NCP as a residual quantity.

This new version of the code enables records of atmospheric pressure and sub-mixed layer oxygen concentrations to be applied to refine the air-sea and sub-surface oxygen exchange terms (described in section 2), and allows the user to select various options (described in section 3) for the air-sea gas exchange algorithms and the terms (air-sea exchange, eddy diffusion, entrainment) used in the oxygen mass balance. The new code retains the 1-dimensional approach of our previous work in that it treats the time series as occurring in a single water mass. This is a simplification that requires evaluation; it may not be appropriate for all portions of the sensor records. Further discussion of this issue is available in previous works at SOTS that addressed NCP, carbon budgets, and nutrient depletion (Shadwick et al., 2015, Wang et al., 2001, Weeding and Trull, 2014).

NCP is estimated at each time step in units of $\text{mmol O}_2 \text{ m}^{-2}$, including their cumulative sum over the time series. Conversion to carbon units is also provided within the code, using the variable `ncp_oxygen2carbon`, for which the default ratio is 1.45 (Anderson and Sarmiento, 1994).

2 Required Input Data

Time series of the following variables (or default choices) are required (and in the MATLAB code are housed in the Structure `mooring_data`):

1. `mooring_data.time` = the times of the observations
2. `mooring_data.gastension_Pa` = GTD pressure in Pa
3. `mooring_data.dox2_umolkg` = Dissolved Oxygen concentration in $\mu\text{mol kg}^{-1}$
4. `mooring_data.mld_m` = mixed layer depth in meters
5. `mooring_data.temp_C` = mixed layer temperature in C
6. `mooring_data.psal_PSU` = mixed layer salinity in psu
7. `mooring_data.windspeed_ms` = wind speed at 10m height in m s^{-1}
8. `mooring_data.atmosphericpress_Pa` = atmospheric pressure at sea level in Pa
(a default value can be set if not available)
9. `mooring_data.dox2_submld_umolkg` = subsurface oxygen concentration
(a default value can be set if not available)

The MATLAB code is designed to read these from SOTS NetCDF files as archived at the AODN under the auspices of the IMOS Deep Water Moorings Facility / SOTS sub-facility, but other sources of input data can be used by placing it into these variables.

3 Algorithm options

The MATLAB code provides several choices for the oxygen mass balance algorithms:

Choice 1. Set the gas transfer velocity parameterisation for computation of air-sea gas exchange
`airsea_algorithm = 1;` 1 is the default, the full set of options are:

1. (Wanninkhof, 2014)
2. (Wanninkhof et al., 2002)
3. (Ho et al., 2006)
4. (Sweeney et al., 2007)
5. (Edson et al., 2011)

Choice 2. Set the parameter, `bubble_beta`, which is the ratio of fully to partially dissolving bubbles
`bubble_beta = 1;` 1 is the default, values of 0.1 and 10 are useful bounds to explore the sensitivity of NCP to this unknown aspect of the fate of injected bubbles. See Emerson et al. 2008 (eqn 7) for further information.

Choice 3. Set the vertical eddy diffusivity

`eddy_diff_coeff = 0.33E-4;`

The default eddy diffusivity coefficient is 0.33×10^{-4} , in m^2s^{-1} , in accord with Weeding and Trull, 2014. Exploring 3-fold variations around this value is recommended.

Choice 4. Set the time span over which the MLD estimates are smoothed prior to use

`mld_smooth_span = 24;`

The default value is 24 hours, to emphasize the time scales on which the mixed layer and sub mixed layer water masses are likely to have different oxygen contents.

Choice 5. Set the atmospheric pressure if the variable is not available

If there is an atmospheric pressure record, it is used by default.

To set a constant atmospheric pressure, set:

`atmospheric_pressure_manual_override=1`

and set your choice of atmospheric pressure in atmospheres, e.g. for 1 atm=101325Pa, set:

`atmospheric_pressure_choice = 1`

[the default value of `atmospheric_pressure_choice` is 0]

Choice 6. Set the subsurface oxygen concentration if the variable is not available

If there is a subsurface oxygen concentration, it is used by default.

To set a constant subsurface oxygen concentration, set:

`sub_mld_dox2_manual_override = 1`

and set your choice of subsurface oxygen concentration in mol m^{-3} , e.g. for 264 μM oxygen, set:

`sub_mld_dox2_choice = 0.264;`

[the default value of `sub_mld_dox2_choice` is 0]

Choice 7. Specify the oxygen inputs to be included in the mass balance:

`exchange_choice = 1;`

1: only air-sea exchange and bubbles

2: option 1 plus eddy diffusion

3: option 2 plus MLD based entrainment

4: option 2 plus and heat budget based entrainment (this code is not yet implemented)

In addition, choice of the input data quality from the AODN IMOS data files is allowed:

Choice 8. Selecting qc limits

Set this parameter to the lowest qc value you're not willing to accept.

Default value is 3, so that only data of qc values 1 and 2 are used by

`sots_ncp_select_acceptable_qc`.

```
qc_limit = 3;
```

Note that this code currently identifies the longest continuous period of data with this specified level of quality and calculates NCP for that period. Visualisation of the data flags is recommended prior to making the selection, to determine that this is appropriate for a given record, and/or to consider whether interpolation of other data is needed prior to the calculations.

4 MATLAB Scripts

The MATLAB code is organized as a single driver script, `sots_ncp_driver`, which call other scripts:

0. `sots_ncp_driver` % the parent script, where algorithm choices are set
1. `sots_ncp_1_addpath` % modify to add and save the path specific to your computer
2. `sots_ncp_2_constants` % loads scientific constants, and also includes some parameters which users may wish to alter, such as the conversion factor `ncp_oxygen2carbon`.
3. `sots_ncp_3_extractor` % loads data from SOTS NetCDF files into structure mooring data. This routine is currently written explicitly for 3 deployments (Pulse-7, Pulse-9, and SOFS-7.5), and is likely to need refinement for other data sets.
4. `sots_ncp_4_select_acceptable_qc` % selects the longest continuous data period with specified QC flags
5. `sots_ncp_5_mooring_plot` % makes plots to check that data is correct
6. `sots_ncp_6_dox2_converter` % converts input O_2 and solubility to mol m^{-3} , calculates saturation
7. `sots_ncp_7_dox2_sat_plot` % plots O_2 saturation vs temperature and gas tension
8. `sots_ncp_8_gas_records` % calculates Henry's law constants, water vapour, and N_2 time series
9. `sots_ncp_9_gas_transfer_velocity_X` % calculates gas transfer velocity according to user Choice 7 in the driver, as labelled by X – the placeholder for the individual gas exchange algorithm scripts.
10. `sots_ncp_10_N2_exchange` % calculates air-sea exchange and bubble processes to match N_2 time series. This script also includes the calculation of changes in mixed layer depths which is used to calculate oxygen entrainment. It is present in this script to enable possible future inclusion on nitrogen entrainment, which is currently assumed to be negligible and is not calculated.
11. `sots_ncp_11_O2_exchange_X` % calculates O_2 exchange processes to produce physical O_2 timeseries (X indicates the gas exchange algorithm selected in the driver script at Choice 7)
12. `sots_ncp_12_atmospheric_exchange_visualisation` % creates plots to compare N_2 and physical O_2 exchange processes
13. `sots_ncp_13_net_com_prod_calc` % calculates net community production
14. `sots_ncp_14_net_com_prod_visualisation` % creates plots to compare NCP time series with relevant variables
15. `sots_ncp_15_workspace_cleanup` % deletes unwanted variables and assigns the variables described in 'Outputs'

The input input files and these scripts must be in the MATLAB Path.

All the scripts are required except the visualization scripts 5, 7, 12, and 14, and the Path script (if set separately).

5 Outputs from calculations

The scripts create outputs in the MATLAB workspace. The important ones to save from a run are all the choices (as listed in section 3), and the calculated results, as follows:

1. NCP % hourly timeseries of net community production in moles of O₂ per cubic metre
2. NCP_qc % QC values for NCP, calculated as the maximum QC flag from the mooring inputs
3. Bubble_injected_oxygen % hourly timeseries of bubble injected oxygen in moles per cubic metre
4. Entrained_oxygen % hourly timeseries of entrained oxygen (from below MLD) in moles per cubic metre
5. Eddy_diff_oxygen % hourly timeseries of eddy diffused oxygen (from below MLD) in moles per cubic metre
6. Gas_exchange_oxygen % hourly timeseries of oxygen exchanged into water from atmosphere in moles per cubic metre

In addition, cumulatively summed timeseries of NCP are available as new variables in the mooring_data structure, in units of both oxygen and carbon:

- mooring_data.ncp_O2_umm2_cumsum
- mooring_data.ncp_C_mgm2_cumsum

The conversion to carbon units uses the C/O₂ ratio for NCP set by the parameter *ncp_oxygen2carbon* in the script *sots_ncp_2_constants* (default value 1.45).

Because these rate variables are determined over a time interval, n-1 rate values are obtained from the n state observations. To provide for easy plotting and other manipulations, a final fill value of NaN is added at the end of the rate variables, so that all variables have the same length. This choice means that the NCP at time step i applies to the forward interval between time steps i and i+1.

6 Details of Net Community Production calculations

Net community production (per square metre) is calculated following the work of Emerson et al. (2010a, 2008b), as developed for the SOTS site by Weeding and Trull, 2014.

Unless otherwise stated, each parameter is calculated or obtained with an hourly timestamp, using the instruments situated together at ~30 m depth (known as the RAS package on the Pulse moorings, and the instrument package on the SOFS moorings).

For gas calculations, a standard atmosphere (1atm) of 101.325 kPa is used, unless a time series of atmospheric pressures has been provided.

1. Oxygen solubility

Oxygen solubility in micromoles per kilogram of seawater (at 1 atm total atmospheric pressure, including saturated water vapour, and an atmospheric O₂ concentration of 20.946%) is calculated using the work of Garcia and Gordon (1992), from temperature and salinity.

2. Nitrogen solubility

Nitrogen solubility in micromoles per kilogram of seawater (at 1 atm total atmospheric pressure, including saturated water vapour, and an atmospheric N₂ concentration of 78.084%) is calculated from temperature and salinity, using the work of Hamme and Emerson (2004).

3. Argon solubility

Argon solubility in micromoles per kilogram of seawater (at 1 atm total atmospheric pressure, including saturated water vapour, and an atmospheric Ar concentration of 0.934%) is calculated from temperature and salinity, using the work of Hamme and Emerson (2004).

4. Water vapour pressure of seawater

The water vapour pressure of seawater is calculated from temperature and salinity, using a Wagner polynomial (Wagner and Pruß, 2002), modified to account for salinity as described in Dickson, Sabine et al. (2007). The result is available in both kPa and atm.

5. Conversion of GTD pressure to dissolved nitrogen concentration, via Henry's Law.

The GTD sensor provides the total pressure contributed by all dissolved gases. Conversion to dissolved N₂ allows the air-sea exchange of N₂ to be tracked and in turn air-sea exchange of O₂ to be estimated. To achieve this, other contributions to the GTD pressure are removed as follows:

- water vapour pressure, using measured temperature and salinity

- trace gases, assuming atmospheric composition (this covers all trace gases in the chosen standard atmosphere rather than just Ar and CO₂, following the modification of the Emerson et al., 2008 procedure as introduced by Weeding and Trull, 2014).
- Oxygen, using the measured optode oxygen record

The procedure uses Henry's law in the form $c_i = p_i k_H$, with the constant k_H describing the concentration c of gas i that will be dissolved in a liquid, for a given partial pressure p_i (in atm) of that gas.

The code first calculates the Henry's law coefficient for O₂, using calculated oxygen solubility (as a function of temperature and salinity read from the input file), atmospheric gas fractions from Glueckauf (1951), and adjusts these dry gas fractions for use with the wet atmosphere that applies to the solubility algorithms. It then repeats this process for N₂. It then calculates the observed partial pressure of N₂, by taking the pressure measured by the GTD, subtracting from it the calculated water vapour pressure and measured O₂ partial pressure, and corrects it for the presence of minor gases by multiplying by the ratio of N₂ to the sum of N₂ and other minor gases (Argon, CO₂, etc., again using Glueckauf (1951)). Finally, it calculates the concentration of N₂ in micromoles per kilogram, using the N₂ Henry's law constant and partial pressure.

6. Schmidt numbers

The Schmidt number is the ratio of momentum diffusivity (kinematic viscosity) to mass diffusivity for a fluid, indicating which process is dominant. Schmidt numbers are highly temperature dependent (but have much smaller salinity dependence), and are used to calculate rates of air sea gas exchange for one gas relative to another. Schmidt numbers are calculated for oxygen and nitrogen from temperature following Wanninkhof (1992), and are normalized to a value of 660 to express them relative to CO₂ at 20 C and salinity 35.

7. Expression of gas measurements in moles per cubic metre

The oxygen records are available from IMOS/AODN in units of moles of gas per unit mass (kilogram). Because the mixed layer mass balance is made in volume units (m³) the input dissolved oxygen gas data is converted into moles per cubic metre of seawater. Dissolved nitrogen concentration (as obtained from the GTD data, see item 5 in this section above) is converted to the same units.

8. Calculation of gas transfer velocity

Gas transfer velocities are estimated from wind speeds, using the user's choice of parameterisation (as described in section 2 above). This requires wind speeds at a standard height of 10 m, and accordingly the wind speeds measured by the SOFS surface buoys at approximately 2.5m are scaled to 10 m height, using COARE algorithms (Fairall et al., 2003). This conversion is done outside this code and the 10 m data are read in from the IMOS/AODN code. Previous implementations of the code used satellite derived wind speeds, which showed negligible differences from the SOFS observations (Weeding and Trull, 2014).

These 10 m windspeeds are combined with the user selected gas transfer parameterisation, relevant Schmidt numbers, gas concentrations, solubilities, and measured atmospheric pressure to calculate the rate of gas exchange between the atmosphere and ocean for both oxygen and nitrogen.

9. Gas exchange via injected bubbles and molecular diffusion

Molecular diffusion coefficients for oxygen and nitrogen are calculated from observed temperature and salinity, using the exponential activation energy formulation of Ferrell and Himmelblau (1967).

10. Smoothing and rectification of Mixed Layer Depth (MLD) to estimate entrainment

The hourly MLD estimates are smoothed using a running mean applied over the period specified by the user (24 hours is the default choice).

This record is then rectified so that only times of deepening are used to estimate entrainment. This is done by differentiating MLD and setting the negative values, indicating shoaling, to zero.

11. Calculation of the amount of gas injected by bubbles

Because dissolved N_2 is assumed to be constant and saturated in the sub-surface, only air-sea exchange of N_2 significantly affects its concentration in the mixed layer, as estimated from the GTD record. There are two processes involved: i. exchange at the air-sea interface at atmospheric pressure (computed using a choice of gas transfer velocity parameterization), and ii) exchange at higher pressure via injected bubbles. Estimating the relative importance of these improves the use of N_2 to estimate O_2 exchange, in particular because bubbles which fully dissolve will inject these gases at their atmospheric concentration ratio, rather than at their atmospheric ratios s further modified by the square root of the ratio of their diffusivities. Thus, the relative importance of 'small' bubbles (that completely dissolve once injected underwater) to 'large' bubbles (from which gases dissolve according to their relative diffusivities into the water before resurfacing) must be estimated (Emerson et al., 2008b). This is done by trial and error and sensitivity tests, using the parameter "bubble_beta", which describes the ratio complete to partial dissolution. The default value for bubble_beta is 1, and exploration of 10-fold variations around this value is advised. For a given value, the amount of injected bubbles (V_{inj} , in moles m^{-3}) at each timestep is calculated as the amount sufficient to complete the N_2 mass balance. For example, the rate of gas exchange from the first timestamp is used to predict the exchange of gas between the atmosphere and ocean that would appear in the nitrogen concentration at the second timestamp. This change in concentration is compared with the measured change in nitrogen over that timestep based on the GTD data, and any difference is attributed to bubbles. Because the underlying gas exchange formulations parameterized as a function of windspeed have been derived from observations which may include bubble injection, it is useful to examine the interactions of the choice of gas transfer parameterization and the choice of bubble_beta in developing NCP error estimates.

12. Calculation of physical oxygen records

Following whatever choice was selected by the user, the expected changes in oxygen in the mixed layer are estimated, by beginning with the conditions of the first timestamp, and modelling how oxygen would change via:

- i. only air-sea gas exchange
as described above at items 8-10.
- ii. air-sea exchange and eddy diffusion
with eddy diffusion specified as the product of the chosen eddy diffusivity and the gradient in oxygen concentration at the base of the mixed layer. This is determined by the estimate of the sub-surface oxygen concentration and a length scale (`eddy_gradient_thickness_m`), for which the default value is 50 m based on O₂ profiles as reviewed in Weeding and Trull, 2014.
- iii. air-sea exchange, eddy diffusion, and entrainment.
with entrainment specified as the amount of oxygen brought into the mixed layer when it deepens, using the estimate of the sub-surface oxygen concentration.

The calculations are initially performed in moles per cubic metre, and then once complete, converted into micromoles per kilogram.

The change in the amount of oxygen in the mixed layer at each time step (in mol m⁻²) is calculated, and after subtracting inputs from the atmosphere (via diffusive gas exchange and bubble injection) and from below the mixed layer (via eddy diffusion and entrainment), the proportion of this change resulting from biology is estimated. The user can choose which of these terms can be removed in any given run.

13. Estimation of net community production

Net community production (NCP) is equated to the change oxygen mediated by biology as calculated in the oxygen exchange routines (`O2_exchange_eddy` or `O2_exchange_eddy_and_entrainment`).

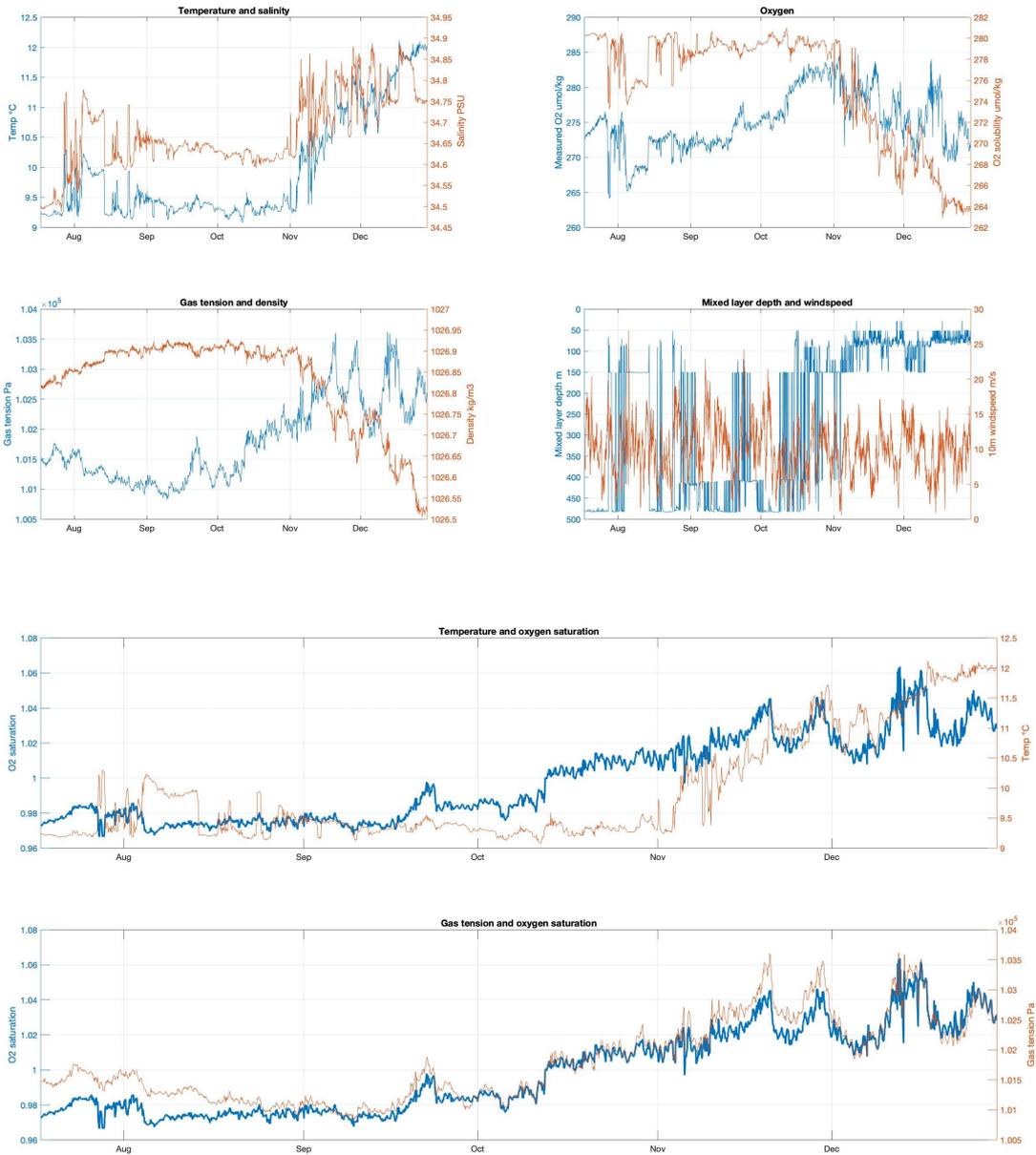
This yields NCP at each time in the series, in the following forms:

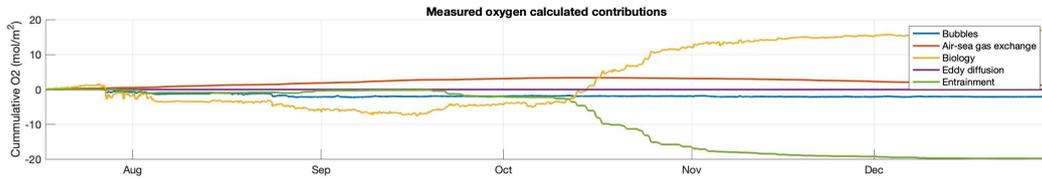
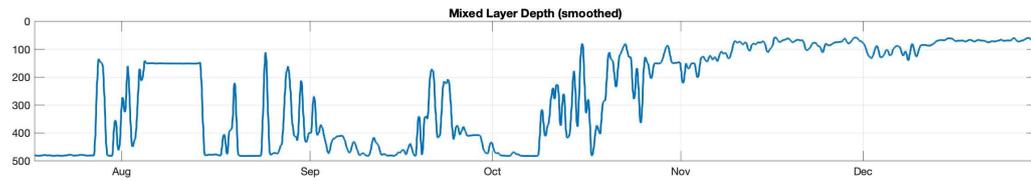
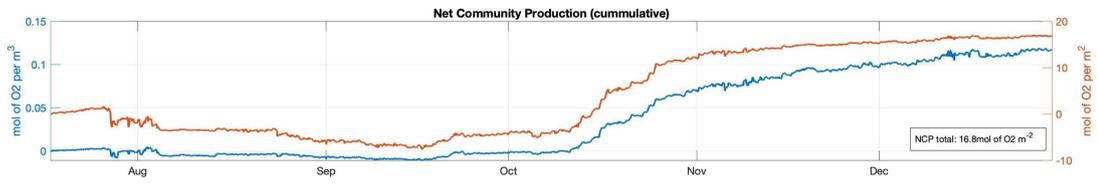
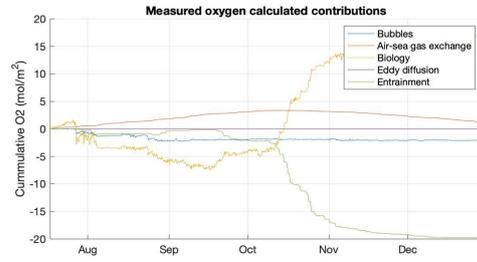
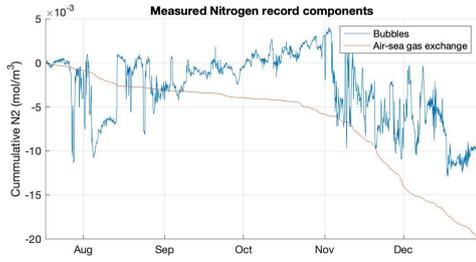
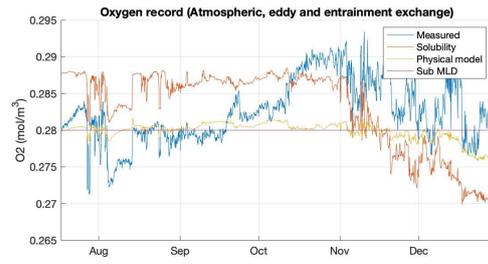
- i. in mol O₂ m⁻² hr⁻¹, directly.
- ii. in mol O₂ m⁻³ hr⁻¹, by dividing by the mixed layer depth
- iii. in umol O₂ kg⁻¹ hr⁻¹, by multiplying by the mixed layer depth and the density
- iv. in mg C m⁻² hr⁻¹ by further multiplying by the conversion parameter `ncp_oxygen2carbon`, with default value of 1.45 (Anderson and Sarmiento, 1994) .

Cumulative sums over the full time series are provided for i. and iv.

7 Example Outputs

For the Pulse-9 data and the parameter default choices selected in the code on Github, the following visualization outputs are obtained, and can be used to check that the scripts and data have run correctly.





8 Accessing SOTS 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 (good) and 2 (probably good).

The URL for data access is:

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

9 Accessing NCP MATLAB Code

The MATLAB code is freely available via Github, in the open public directory:

`bweeding/SOTS-Net-community-production`

10 Perspectives and Concluding Remarks

We remind users that the code has significant limitations, including:

1. Horizontal advective inputs are not assessed. This could be addressed by adding a separate script to calculate them from surface velocity and regional gas gradient estimates, and then subtracting this further term from the measured O₂ concentration changes in this NCP script.
2. The assumption of negligible N₂ gradients in the ocean may not hold, and if not then the use of the GTD derived N₂ record to assess bubble inputs may be in error. Calculation of possible N₂ inputs from below the mixed layer (assuming reasonable gradients) relative to the bubble inputs can give an idea of the scale of potential errors.
3. The assumption that the mixed layer is well mixed on the timescales of the observations, and/or that entrainment brings in water with different O₂ levels may be in error. For example, production during a sunny day in the euphotic zone (~ top 50m) as recorded by the sensors at ~30 m depth, may not be homogenized throughout the mixed layer until convection occurs at night. In spring in deep mixed layers this would manifest as a large positive NCP estimate in the day followed by a large negative estimate at night. Similarly, shoaling of the mixed layer via insolation on that day followed by deepening at night may not transfer much oxygen at all, if the subsurface values have changed by advection. We advise exploration of the sensitivity of NCP estimates to smoothing of the time series as a first step to gauge the scope of these issues.
4. Because the entrainment term is large, especially in spring, exploration of the sensitivity of NCP to the sub-surface oxygen concentration estimate is recommended.

Finally, we note that new approaches to estimating the roles of bubbles, entrainment, and advection continue to be developed, and thus advise careful consultation of recent literature to assess the fitness for purpose and the utility of refinements.

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