Global reconstruction of surface oceanic N2O disequilibrium and its associated flux

Website: https://www.bco-dmo.org/dataset/810032
Data Type: model results, Cruise Results
Version: 1
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Project
» CAREER: Multiple Scales of Nitrogen Cycle in Oxygen Minimum Zones (Multiple Scales of Nitrogen Cycle in the Ocean)

Contributors	Affiliation	Role
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Abstract
Global reconstruction of surface oceanic N2O disequilibrium and its associated flux. The dataset consists of (1) a global compilation of observed nitrous oxide pressure, concentration, mixing ratio measurements and their associated disequilibrium in the surface ocean; (2) the globally mapped N2O disequilibrium predicted by a supervised learning algorithm, and (3) the reconstructed ocean to atmosphere N2O flux.

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Coverage

Spatial Extent: **N**:88.3943333 **E**:180 **S**:-77.177 **W**:-180
Temporal Extent: 1971-06-09 - 2018-06-04

Dataset Description

Global reconstruction of surface oceanic N2O disequilibrium and its associated flux. The dataset includes 3 files:
(1) **surfocean-n2o-compilation.csv**: available as a .csv/.tsv file via the "Get Data" button on the BCO-DMO landing page. A global compilation of observed surface ocean nitrous oxide pressure, concentration, mixing ratio measurements and their implied nitrous oxide disequilibrium used to train the supervised learning algorithm. Also attached as a .mat file (**surfocean-n2o-compilation.mat**) under "Data Files".
(2) **dn2o-mapped-Yang2020.nc**: available under "Data Files". Predicted N2O disequilibrium.
(3) **n2oFlux-Yang2020.nc**: available under "Data Files". The predicted ocean to atmosphere N2O flux.

This dataset contains a compilation of data from multiple sources. A list of all datasets and the associated information, including cruise name, is included in the associated Supplemental File, "SuppCruiseTable_dec11.xlsx".

Acquisition Description

We compiled surface (0m-12m depth) marine N2O concentrations and partial pressures measurements from a variety of sources. The core of the data is sourced from the MEMENTO database (Kock & Bange, 2015). We complement MEMENTO with additional published N2O measurements from the literature, and unpublished N2O measurements from 16 additional cruises (see Supplemental File "SuppCruiseTable_dec11.xlsx"), including 11 cruises from the Global Ocean Ship-Based Hydrographic Investigations Program (GO-SHIP). We do not perform any further quality control of the N2O data from published sources besides that performed by the individual contributors and the MEMENTO database administrators (Kock & Bange, 2015). A description of the quality control performed on new unpublished N2O data is reported as footnotes to the annotations labeled as qc1**, qc2**, or qc3** (see "SuppCruiseTable_dec11.xlsx"). We convert each marine N2O measurement to XwN2O (the N2O mixing ratio in seawater, in units of ppb) using, when needed, the N2O solubility coefficient (Weiss & Price, 1980). The coefficient is calculated using co-measured temperature,

and salinity, as well as sea level pressure from the ERA5 reanalysis (Copernicus Climate Change Service, 2017), at the time (month and year), and location of the measurement. If the measurement time is not available in the ERA5 reanalysis prediction, we instead use the climatological atmospheric pressure at sea level, calculated from the monthly predictions for the years from 1979 through 2018. We then calculated N2O disequilibrium as DN2O = XwN2O – XaN2O, where XaN2O is the atmospheric N2O mixing ratio estimated by linear interpolation of NOAA's flask measurement dataset (Hall et al., 2007) at the time and latitude of each marine N2O measurement.;

To convert sparse observations to a global climatology, we trained 100 ensembles of regressions trees (Random Forests) to predict DN2O based on its relationship to well-sampled physical and biogeochemical predictors. We note that, while the prediction of N2O disequilibrium is done in mixing ratio units (ppb), the results are reported in the more commonly used pressure units (natm): pN2O = XN2O . P, where P is the climatological atmospheric pressure at sea level in atm, predicted by ERA5, included as part of the relevant data file for easy conversion. (see Data File: dn2o-mapped-Yang2020.nc).

We calculate the N2O air-sea flux using two wind-speed dependent parameterizations: an updated version of a commonly-used quadratic formulation (Wanninkhof, 1992; Wanninkhof, 2014) and a recent formulation that explicitly accounts for the effect of bubble-mediated fluxes (Liang et al., 2013). We apply each parameterization to two high-resolution wind products (Copernicus Climate Change Service, 2017; Wentz et al., 2015), yielding four permutations of the piston velocity. In total, we obtain an ensemble of 400 global N2O air-sea flux estimates, from which we calculate a mean and uncertainty range (see Data File: n2oFlux-Yang2020.nc).

Sampling and analytical prodcedures:
The data is compiled from multiple sources, published and unpublished. Refer to the associated Supplemental File "SuppCruiseTable_dec11.xlsx" for a detailed description of sampling and analytical methods associated with new data and references associated with published data. "qc" refers to "qualtiy control and methods"; see related references and descriptions in the Supplemental File.

GOSHIP (qc1): N2O was measured using shipboard gas chromatography-electron capture detection (GC-ECD) using analytical techniques modified from those described in Bullister and Wisegarver (2008). N2O was purged from 200 mL seawater samples using N2 carrier gas and trapped onto a trap that included MS5A held at -60°C. The trap was subsequently heated to 175°C to release N2O, which was further separated and purified via two precolumns before being quantified using electron capture detection. (The carrier gas for the N2O analyses was a 95%Ar/5% CH4 mix) The analytical system was calibrated frequently using internal standards of known N2O compositions or standards from Working Group no. 143 of the Scientific Committee on Oceanic Research (SCOR) (Wilson et al. 2018). Concentrations of N2O in seawater samples and gas standards are reported relative to the SIO98 calibration scale.

SPOT (qc3): Dissolved N2O concentrations were measured using a headspace equilibration method modified from Laperriere et al. (2019). A 30-mL ultra-high purity N2 headspace was introduced into 160 mL seawater samples using a 30-mL syringe with a second empty 30-mL syringe inserted into the septum to collect displaced sample water. Each headspace was overpressured with 10 mL of ultra high purity N2 to minimize atmospheric contamination. Samples were analyzed on an SRI 8610 Greenhouse Gas Monitoring Gas Chromatograph (GC) equipped with an electron capture detector (ECD), dual HayeSep D packed columns, and a 1-mL sample loop (SRI Instruments, Torrance, California, USA). Ultra-high purity N2 gas was used as the carrier with the sample loop kept at 60 °C and the column oven kept at 100 °C. Two certified standards, 0.1 ppm and 1 ppm N2O (Matheson Tri-Gas) were used for daily calibration using a linear calibration scheme.

Others (qc2): N2O concentrations were measured with a GV IsoPrime Continuous Flow Isotope-Ratio Mass Spectrometer (CF-IRMS) as described in Bourbonnais et al. (2017). Briefly, seawater was pumped from sample bottles and completely extracted using a gas-extractor continuously sparged with He. N2O was then concentrated and purified in a purge-trap system. CO2 and H2O were removed with chemical and cryogenic traps. N2O was cryofocused with liquid N2 traps and passed through a gas chromatography (GC) column before IRMS analysis. N2O concentrations were calculated from relative peak heights between the samples and seawater standards of known N2O concentration equilibrated with the atmosphere at 5C and 20C. Equilibrium surface N2O concentrations were calculated based on the global mean atmospheric N2O dry mole fraction at the time of the cruise. The data were inter calibrated with samples also measured using purge-trap gas extraction systems coupled with either a GC-Electron Capture Detector (ECD) or a GC-quadrupole mass spectrometer (Fenwick et al., 2017) when available (e.g., P18 GO-SHIP, ArcticNet 2017 expedition) and yielded comparable N2O concentrations (generally less than 5% difference).

The data is compiled from multiple sources, published and unpublished. Refer to the Supplemental File, "SuppCruiseTable_dec11.xlsx", for a detailed description of sampling and analytical methods associated with new data and references associated with published data.

Processing Description

Data Processing:
The N2O disequilibrium at the location of each measurement is estimated following: _DXN2O = XN2O_ocean – XN2O_atm. Here, XN2O_ocean is the ocean-side N2O measurement converted to mixing ratios, and XN2O_ atm is the atmospheric N2O mixing ratio estimated by interpolating the National Oceanic and Atmospheric Administration atmospheric N2O flask dataset at the latitude and time of the oceanic measurements.

BCO-DMO Processing:
added "date" column as YYYY-MM-DD.

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Data Files

File	Version
dn2o-mapped-Yang2020.nc - Predicted N2O disequilibrium (NetCDF, 170.65 MB) MD5:88d77b3149edd5cad2d39781ec4cc8f7 *Predicted N2O disequilibrium. The N2O disequilibrium at the location of each measurement is estimated following: _DXN2O = XN2O_ocean – XN2O_atm . Here, XN2O_ocean is the ocean-side N2O measurement converted to mixing ratios, and XN2O_atm is the atmospheric N2O mixing ratio estimated by interpolating the National Oceanic and Atmospheric Administration atmospheric N2O flask dataset at the latitude and time of the oceanic measurements. To convert sparse observations to a global climatology, we trained 100 ensembles of regressions trees (Random Forests) to predict dN2O based on its relationship to well-sampled physical and biogeochemical predictors.* *File contents:* *latitude_2d = enter-cell latitude; degrees north* *longitude_2d = center-cell longitude; degrees east* *cellArea_m2 = Cell area in m^2* *n2oFlux_EnsMean_g-pm2-pyr = dn2o_EnsMean_natm; natm* *n2oFlux_EnsStd_g-pm2-pyr = dn2o_EnsStd_natm; natm* *n2oFluxSeas_g-pm2-pyr = dn2o_griddedobs_mean_natm; natm* *atm-press = Sea Level Pressure -- ERA5 climatological average; atm* *biomes_masks = ocean biomes masks (1:Tropical ocean, 2:Coastal upwelling systems, 3:Polar ocean, 4: Mid-latitudes, 5: Deep mixed layer systems, 6: Subtropical gyres)* *coastal_upwellSys_masks = coastal upwelling systems masks (1:Peru, 2:Benguela, 3:Costa-Rica, 4:Chile, 5:California current, 6: Canary, 7:Arabian sea , 8: Bay of Bengal)*	1
n2oDataYang2020PNAS.mat - Surface N2O Compilation (MATLAB Data (.mat), 9.90 MB) MD5:c8ddb77538e77dbb6486ff3a9c887cf9 *Surface N2O Compilation in .mat format*	1

File	Version
n2oFlux-Yang2020.nc - Predicted ocean to atmosphere N2O flux (NetCDF, 357.95 MB) MD5:35620fa745a5a6a5c823cab32efbf3df *We calculate the N2O air-sea flux using two wind-speed dependent parameterizations: an updated version of a commonly-used quadratic formulation, and a recent formulation that explicitly accounts for the effect of bubble-mediated . We apply each parameterization to two high-resolution wind products yielding four permutations of the piston velocity. In total, we obtain an ensemble of 400 global N2O air-sea flux estimates, from which we calculate a mean and uncertainty range.* *File contents:* *latitude_2d = center-cell latitude; degrees north* *longitude_2d =center-cell longitude; degrees east* *cellArea_m2 =Cell area in m^2* *n2oFlux_EnsMean_g-pm2-pyr =n2o flux -- ensemble mean prediction; g m^(-2) y^(-1)* *n2oFlux_EnsStd_g-pm2-pyr =n2o flux -- ensemble standard-deviation; g m^(-2) y^(-1)* *n2oFluxSeas_g-pm2-pyr = n2o flux seasonality (sum of components); g m^(-2) y^(-1)* *n2oFluxSeas_fromWind_g-pm2-pyr = wind component of the n2o flux; g m^(-2) y^(-1)* *n2oFluxSeas_fromXn2o_g-pm2-pyr = dn2o component of the n2o flux; g m^(-2) y^(-1)* *n2oFluxSeas_fromIcePress_g-pm2-pyr = sea-ice and atmospheric pressure component of the n2o flux; g m^(-2) y^(-1)* *n2oFluxSeas_fromCovar_g-pm2-pyr = covariations component of the n2o flux; g m^(-2) y^(-1)* *biomes_masks =ocean biomes masks (1:Tropical ocean, 2:Coastal upwelling systems, 3:Polar ocean, 4: Mid-latitudes, 5: Deep mixed layer systems, 6: Subtropical gyres)* *coastal_upwellSys_masks = coastal upwelling systems masks (1:Peru, 2:Benguela, 3:Costa-Rica, 4:Chile, 5:California current, 6: Canary, 7:Arabian sea , 8: Bay of Bengal)*	1

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Related Publications

Bange, H. W., Bell, T. G., Cornejo, M., Freing, A., Uher, G., Upstill-Goddard, R. C., & Zhang, G. (2009). MEMENTO: a proposal to develop a database of marine nitrous oxide and methane measurements. Environmental Chemistry, 6(3), 195. doi:10.1071/en09033 https://doi.org/10.1071/EN09033 [details],
Methods

Bourbonnais, A., Letscher, R. T., Bange, H. W., Échevin, V., Larkum, J., Mohn, J., … Altabet, M. A. (2017). N2 O production and consumption from stable isotopic and concentration data in the Peruvian coastal upwelling system. Global Biogeochemical Cycles, 31(4), 678–698. doi:10.1002/2016gb005567 https://doi.org/10.1002/2016GB005567 [details],
Methods

Bullister, J. L., & Wisegarver, D. P. (2008). The shipboard analysis of trace levels of sulfur

hexafluoride, chlorofluorocarbon-11 and chlorofluorocarbon-12 in seawater. Deep Sea Research Part I: Oceanographic Research Papers, 55(8), 1063–1074. doi:10.1016/j.dsr.2008.03.014 [details],
Methods

Copernicus Climate Change Service (C3S) (2017): ERA5: Fifth generation of ECMWF atmospheric reanalyses of the global climate . Copernicus Climate Change Service Climate Data Store (CDS), accessed in March 2019. https://cds.climate.copernicus.eu/cdsapp#!/home [details],
Methods

Fenwick, L., Capelle, D., Damm, E., Zimmermann, S., Williams, W. J., Vagle, S., & Tortell, P. D. (2017). Methane and nitrous oxide distributions across the North American Arctic Ocean during summer, 2015. Journal of Geophysical Research: Oceans, 122(1), 390–412. doi:10.1002/2016jc012493 https://doi.org/10.1002/2016JC012493 [details],
Methods

Hall, B. D., Dutton, G. S., & Elkins, J. W. (2007). The NOAA nitrous oxide standard scale for atmospheric observations. Journal of Geophysical Research, 112(D9). doi:10.1029/2006jd007954 https://doi.org/10.1029/2006JD007954 [details],
Methods

Kock, A., & Bange, H. (2015). Counting the Ocean's Greenhouse Gas Emissions. Eos, 96. doi:10.1029/2015eo023665 https://doi.org/10.1029/2015EO023665 [details],
Methods

Laperriere, S. M., Nidzieko, N. J., Fox, R. J., Fisher, A. W., & Santoro, A. E. (2018). Observations of Variable Ammonia Oxidation and Nitrous Oxide Flux in a Eutrophic Estuary. Estuaries and Coasts, 42(1), 33–44. doi:10.1007/s12237-018-0441-4 [details],
Methods

Liang, J.-H., Deutsch, C., McWilliams, J. C., Baschek, B., Sullivan, P. P., & Chiba, D. (2013). Parameterizing bubble-mediated air-sea gas exchange and its effect on ocean ventilation. Global Biogeochemical Cycles, 27(3), 894–905. doi:10.1002/gbc.20080 [details],
Methods

Wanninkhof, R. (1992). Relationship between wind speed and gas exchange over the ocean. Journal of Geophysical Research, 97(C5), 7373. doi:10.1029/92jc00188 https://doi.org/10.1029/92JC00188 [details],
Methods

Wanninkhof, R. (2014). Relationship between wind speed and gas exchange over the ocean revisited. Limnology and Oceanography: Methods, 12(6), 351–362. doi:10.4319/lom.2014.12.351 [details],
Methods

Weiss, R. F., & Price, B. A. (1980). Nitrous oxide solubility in water and seawater. Marine Chemistry, 8(4), 347–359. doi:10.1016/0304-4203(80)90024-9 [details],
Methods

Wentz, F.J. et al. (2015). Remote Sensing Systems Cross-Calibrated Multi-Platform (CCMP) 6-hourly Ocean Vector Wind Analysis Product on 0.25 Deg Grid (Version 2.0, Remote Sensing Systems, Santa Rosa, CA, 2015). Accessed in March 2019 via www.remss.com. [details],
Methods

Wilson, S. T., Bange, H. W., Arévalo-Martínez, D. L., Barnes, J., Borges, A. V., Brown, I., … Rehder, G. (2018). An intercomparison of oceanic methane and nitrous oxide measurements. Biogeosciences, 15(19), 5891–5907. doi:10.5194/bg-15-5891-2018 [details],
Methods

Yang et al. 2020. Global reconstruction reduces the uncertainty of oceanic nitrous oxide emissions and reveals a vigorous seasonal cycle. Proceedings of the National Academy of Sciences (in press) [details],
Results

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Parameters

Parameter	Description	Units
cruise	Cruise name	unitless
date	Date; format: YYYY-MM-DD	unitless
year	Measurement year; format: YYYY	unitless
month	Measurement month; format: MM	unitless
day	Measurement day; format: DD	unitless
latitude	Measurement latitude	degrees North
longitude	Measurement longitude	degrees East
depth	Measurement depth	meters (positive down)
n2o_ppb	Ocean n2o mixing ratio	ppb
n2o_nM	Ocean n2o mixing ratio	nmol/L
dn2o_ppb	Estimated n2o disequilibrium	ppb
atmPressure	Sea level pressure estimated at observed time and location	atm
temperature	Co-measured temperature	degrees Celsius
salinity	Co-measured salinity (or estimated from climatology if absent)	g/kg

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Instruments

Dataset-specific Instrument Name	GV IsoPrime Continuous Flow Isotope-Ratio Mass Spectrometer
Generic Instrument Name	Isotope-ratio Mass Spectrometer
Dataset-specific Description	Others (see qc2): GV IsoPrime Continuous Flow Isotope-Ratio Mass Spectrometer (CF-IRMS)
Generic Instrument Description	The Isotope-ratio Mass Spectrometer is a particular type of mass spectrometer used to measure the relative abundance of isotopes in a given sample (e.g. VG Prism II Isotope Ratio Mass-Spectrometer).

Dataset-specific Instrument Name	Shipboard gas chromatography-electron capture detection
Generic Instrument Name	Gas Chromatograph
Dataset-specific Description	GOSHIP: Shipboard gas chromatography-electron capture detection (GC-ECD) SPOT: SRI 8610 Greenhouse Gas Monitoring Gas Chromatograph (GC) equipped with an electron capture detector (ECD), dual HayeSep D packed columns, and a 1-mL sample loop (SRI Instruments, Torrance, California, USA).
Generic Instrument Description	Instrument separating gases, volatile substances, or substances dissolved in a volatile solvent by transporting an inert gas through a column packed with a sorbent to a detector for assay. (from SeaDataNet, BODC)

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Project Information

CAREER: Multiple Scales of Nitrogen Cycle in Oxygen Minimum Zones (Multiple Scales of Nitrogen Cycle in the Ocean)

Coverage: Global

NSF Award Abstract: The nitrogen cycle in the ocean is key to ocean productivity, carbon storage, and emissions of nitrous oxide, a potent greenhouse gas, to the atmosphere. The chemical processes that connect nitrogen species in the ocean are sensitive to the amount of oxygen dissolved in seawater. These reactions become more intense within oxygen minimum zones, areas of the ocean with little or no dissolved oxygen. Oxygen minimum zones are affected by currents that range in scale from hundreds to less than few kilometers. These currents create microhabitats where nitrogen cycling and nitrous oxide emissions are higher. This project investigates the interaction between small-scale ocean circulation, oxygen availability, and the nitrogen cycle. It uses a series of increasingly finer-scale numerical simulations of the Pacific Ocean, where two of the largest oxygen minimum zones are found. These simulations provide information about nitrogen transformations and nitrous oxide emissions on timescales from less than one year to several decades, and spatial scales from a few kilometers to the basin scale. This research will increase our ability to simulate and predict ocean responses to natural and human disturbances, with implications for society. The educational component of the project establishes a series of ocean-going chemical oceanography activities for approximately 100 undergraduate students at the University of California at Los Angeles each year. The field trips involve half-day cruises in the Santa Monica Bay, where students sample a variety of biogeochemical properties. Observations collected during the field trips will be used as a resource in classroom activities and student research projects. The field trips and educational materials offer opportunities to explore cutting-edge questions in ocean biogeochemistry, increase student interest in ocean sciences and access to research, and enhance student learning and self-efficacy, ultimately promoting retention in oceanography and STEM. Oxygen minimum zones host major nitrogen transformations, including denitrification, anammox, and nitrous oxide production, which are essential for biogeochemistry and climate. These reactions are strongly partitioned along oxygen gradients in the suboxic range, making them sensitive to ventilation and chemical heterogeneity driven by variable ocean currents. However, the nature of this sensitivity is poorly understood. The objective of this project is to test the hypothesis that physical circulation at scales from tens of kilometers (mesoscale) to less than one kilometer (submesoscale) is critical in shaping these nitrogen cycle transformations. To test the hypothesis and investigate its implications, we will optimize a new model of the nitrogen cycle against a range of recent observations, and implement it in a realistic three-dimensional hydrodynamic-biogeochemical model. We will adopt a nesting strategy to downscale a Pacific-wide historical simulation to a series of regional domains at resolutions down to few kilometers or less, resolving the oxygen minimum zone boundaries and their fine-scale variability. By analyzing these model solutions, we will: (1) constrain the sensitivity of the microbial nitrogen cycle to oxygen, ventilation, and chemical heterogeneity; (2) in light of this sensitivity, quantify the role of mesoscale and submesoscale processes in shaping nitrogen transformations and transport across oxygen

minimum zone boundaries; and (3) investigate the response of the nitrogen cycle to climate variability, in particular fixed-nitrogen losses and nitrous oxide emissions to the atmosphere.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1847687

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