# Nutrient, CTD Profile, and Nitrous oxide data from the Southern Benguela Upwelling System (Integrated Environmental Programme, February 2017)

Website: https://www.bco-dmo.org/dataset/969121

**Data Type**: Cruise Results

Version: 1

Version Date: 2025-08-12

#### **Project**

» <u>Collaborative Research</u>: <u>Exploring the dynamics of nitrous oxide in the Southern Benguela Upwelling System</u> (SBUS N2O)

Contributors	Affiliation	Role
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#### **Abstract**

This dataset includes the CTD profile data, nutrients, and N2O concentration and isotope data for the 2017 IEP (Integrated Ecosystem Programme) off the west coast of South Africa in the Southern Benguela Upwelling system, on board the R/V Mirabilis. Data were collected using the following instruments: a rosette equipped with Sea-Bird SBE 911 CTD and oxygen (Sea-Bird SBD 43) sensors and 12 6-liter Niskin bottles, a Lachat QuickChem® flow injection auto-analysis (FIA) platform, a Turner Designs Trilogy fluorometer equipped with a UV module, and a Gas Chromatography (GC)-IRMS analyser. Low oxygen zones are hotspots for N2O production. We assessed the mechanisms of N2O production using isotope data in the Southern Benguela Upwelling System. Measurements took place in the Marine Biogeochemistry Lab at the University of Cape Town and the Bourbonnais Lab at the University of South Carolina.

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# Coverage

Location: Southern Benguela Upwelling System

**Spatial Extent: N:-32.3022 E:18.30633333 S:-32.7433 W:16.43233333** 

**Temporal Extent**: 2017-02-23 - 2017-02-24

## Methods & Sampling

Seawater samples were collected during a South African Department of Forestry, Fisheries and Environment (DFFE) Integrated Ecosystem Programme cruise aboard the *FRV Mirabilis* in February 2017 along 14 stations across the St Helena Bay Monitoring Line ( $\sim$ 32.5°S) and the Columbine upwelling cell. Hydrographic profiles were obtained using a Sea-Bird SBE 911 CTD with oxygen sensors and 12 x 6-liter (L) Niskin bottles. Oxygen sensors were calibrated against discrete Winkler titrations. Seawater for nutrient analysis ( $NO_3^-+NO_2^-$ ,  $NO_2^-$ ,  $PO_4^{3-}$ , Si(OH)<sub>4</sub>) was collected following GO-SHIP protocols, frozen at -20 degrees Celsius (°C), and analyzed using flow injection analysis (FIA) and manual colorimetric methods.  $NH_4^+$  was determined fluorometrically using OPA derivatization immediately after collection.

 $N_2O$  samples were collected in 125-milliliter (mL) gas-tight glass bottles, preserved with saturated HgCl<sub>2</sub>, and stored inverted at room temperature. Concentrations and isotopic compositions ( $\delta^{15}N-N_2O$  and  $\delta^{18}O-N_2O$ ) were determined using a continuous-flow isotope ratio mass spectrometer (CF-MC-IRMS) following Bourbonnais et al. (2017) and McIlvin & Casciotti (2011). Calibration included internal seawater standards and  $N_2O$  reference gases spanning a wide isotopic range. Derived variables include apparent oxygen utilization (AOU), N-deficit (based on AOU- $NO_3^-$  stoichiometry), and  $N_2O$  saturation disequilibrium ( $\Delta N_2O$ ), with equilibrium concentrations estimated from Weiss & Price (1980) using atmospheric  $N_2O$  histories from Liu & Tanhua (2024).

## **Data Processing Description**

Data were processed using Ocean Data View (Schlitzer, 2016).

## **BCO-DMO Processing Description**

- Imported original file "Wallschuss data.xlsx" into the BCO-DMO system.
- Marked "#N/A" as a missing data value (note that missing data are empty/blank in the final CSV file).
- Renamed fields to comply with BCO-DMO naming conventions.
- Converted Date column to YYYY-MM-DD format.
- Created date-time column in ISO 8601 format.
- Saved the final file as "969121 v1 n2o isotopes.csv".

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## **Data Files**

File

**969121\_v1\_n2o\_isotopes.csv**(Comma Separated Values (.csv), 439.64 KB)

MD5:f8c69a33521c9d03b31827df67415254

Primary data file for dataset ID 969121, version 1

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### **Related Publications**

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 <a href="https://doi.org/10.1002/2016GB005567">https://doi.org/10.1002/2016GB005567</a> Methods

Liu, M., & Tanhua, T. (2024). Water masses in the Atlantic Ocean: water mass ages and ventilation. https://doi.org/ $\frac{10.5194}{egusphere-2024-1362}$ Methods

McIlvin, M. R., & Casciotti, K. L. (2011). Technical Updates to the Bacterial Method for Nitrate Isotopic Analyses. Analytical Chemistry, 83(5), 1850–1856. doi:10.1021/ac1028984

Methods

Schlitzer, R. (2014) Ocean Data View. http://odv.awi.de <a href="https://odv.awi.de/software">https://odv.awi.de/software</a>

Wallschuss, S. (2024). The role of sediments in modulating nitrous oxide production in the Southern Benguela Upwelling System: insights from stable isotopic tracers [Data set]. Zenodo. https://doi.org/10.5281/ZENODO.14410840 https://doi.org/10.5281/zenodo.14410840 lsRelatedTo

Wallschuss, S., Granger, J., Bourbonnais, A., Flynn, R., Burger, J., Pillay, K., & Fawcett, S. (2025). The Role of Sediments in Modulating Nitrous Oxide Production in the Southern Benguela Upwelling System: Insights From Stable Isotopic Tracers. Global Biogeochemical Cycles, 39(8). Portico. https://doi.org/10.1029/2024gb008463 Results

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 Methods

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## **Parameters**

Parameter	Description	Units
Cruise_ID	Internal Cruise name	unitless
Station_ID	Sampling Station	unitless
ISO_DateTime_GMT	Date and time in ISO 8601 format	unitless
Date	Date of station	unitless
Time	Time of station	unitless
Latitude	Latitude	Degrees North
Longitude	Longitude	Degrees East
Bottom_depth	Depth of water colum	meters (m)
Pressure	Pressure	decibars (db)
Depth	Depth of sample	meters (m)

Temperature	Temperature	degrees Celsius
Salinity	Salinity	practical salinity units (PSU)
Oxygen_mL_L	Dissolved oxygen	milliliters per liter (mL/L)
Oxygen_umol_kg	Dissolved oxygen	micromole per kg
Nitrate	Nitrate concentration	micromolar (uM)
Nitrite	Nitrite concentration	micromolar (uM)
Phosphate	Phosphate concentration	micromolar (uM)
Silicate	Silicate concentration	micromolar (uM)
N2O_equilibrium	Gas equilibrium concentration of N2O at specific temperature/salinity/pressure	nanomolar (nM)
N2O	Measured N2O concentration	nanomolar (nM)
D_N2O	N2O equilibrium - measured N2O concentration	nanomolar (nM)
d15N_N2O	d15N-(bulk) value of N2O (vs. AIR)	per mille (‰)
d18O_N2O	d18O value of N2O (vs. VSMOW)	per mille (‰)
d15N_Nitrate	d15N value of Nitrate (vs. AIR)	per mille (‰)
d18O_Nitrate	d18O value of Nitrate (vs. VSMOW)	per mille (‰)

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# Instruments

Dataset- specific Instrument Name	Sea-Bird Electronics SBE 911plus CTD system
Generic Instrument Name	CTD Sea-Bird SBE 911plus
Dataset- specific Description	CTD Rosette: Sea-Bird Electronics SBE 911plus CTD system equipped with a Sea-Bird SBE 43 dissolved oxygen sensor and a 12-bottle rosette sampler (12 $\times$ 6-L Niskin bottles). Temperature and conductivity sensors were calibrated annually by the manufacturer. The oxygen sensor was calibrated against discrete Winkler titration measurements.
Description	The Sea-Bird SBE 911 plus is a type of CTD instrument package for continuous measurement of conductivity, temperature and pressure. The SBE 911 plus includes the SBE 9plus Underwater Unit and the SBE 11plus Deck Unit (for real-time readout using conductive wire) for deployment from a vessel. The combination of the SBE 9 plus and SBE 11 plus is called a SBE 911 plus. The SBE 9 plus uses Sea-Bird's standard modular temperature and conductivity sensors (SBE 3 plus and SBE 4). The SBE 9 plus CTD can be configured with up to eight auxiliary sensors to measure other parameters including dissolved oxygen, pH, turbidity, fluorescence, light (PAR), light transmission, etc.). more information from Sea-Bird Electronics

Dataset- specific Instrument Name	GV Instruments IsoPrime Continuous Flow Multi-Collector Isotope Ratio Mass Spectrometer (CF-MC-IRMS)
Generic Instrument Name	GV Instruments IsoPrime Isotope Ratio Mass Spectrometer
Dataset- specific Description	$N_2O$ Isotopic and Concentration Analysis: GV Instruments IsoPrime Continuous Flow Multi-Collector Isotope Ratio Mass Spectrometer (CF-MC-IRMS), coupled to a custom-built automated gas extraction and cryogenic purification system, used for $\delta^{15}N$ and $\delta^{18}O$ analysis of dissolved $N_2O$ .
Generic Instrument Description	The GV Instruments IsoPrime Isotope Ratio Mass Spectrometer is a laboratory benchtop isotope ratio mass spectrometer (IRMS), that operates in dual inlet or continuous flow modes. It forms part of the IsoPrime system which has a range of sample preparation and purification modules that can be coupled with the IsoPrime IRMS. The modules can analyse a range of samples (solids, liquids or gases) and each prepares the sample to be introduced into the IRMS as purified gases. The resultant prepared gases such as H2, CO2, CO, N2, SO2 or N2O are then ionised and analysed for their isotopic content by the IRMS. The instrument was originally manufactured GV instruments as part of the IsoPrime series, but this part of the business was sold to Isoprime Ltd (a group member of Elementar Analysensysteme GmbH) and this instrument has been superseded by more recent models.

Dataset- specific Instrument Name	Lachat QuickChem® 8500 Series 2
Generic Instrument Name	Lachat QuikChem 8500 flow injection analysis system
Dataset- specific Description	Flow Injection Autoanalyzer: Lachat QuickChem® 8500 Series 2, used for nitrate + nitrite (NO <sub>3</sub> <sup>-</sup> +NO <sub>2</sub> <sup>-</sup> ) and silicic acid (Si(OH) <sub>4</sub> ) analysis. Standards and a certified reference material (JAMSTEC) were used for drift correction and validation.
Instrument	The Lachat QuikChem 8500 Series 2 Flow Injection Analysis System features high sample throughput and simple, but rapid, method changeover. The QuikChem 8500 Series 2 system maximises productivity in determining ionic species in a variety of sample types, from sub-ppb to percent concentrations. Analysis takes 20 to 60 seconds, with a sample throughput of 60 to 120 samples per hour.

Dataset- specific Instrument Name	6-L Niskin bottles
Generic Instrument Name	Niskin bottle
Dataset- specific Description	CTD Rosette: Sea-Bird Electronics SBE 911plus CTD system equipped with a Sea-Bird SBE 43 dissolved oxygen sensor and a 12-bottle rosette sampler (12 $\times$ 6-L Niskin bottles). Temperature and conductivity sensors were calibrated annually by the manufacturer. The oxygen sensor was calibrated against discrete Winkler titration measurements.
Instrument	A Niskin bottle (a next generation water sampler based on the Nansen bottle) is a cylindrical, non-metallic water collection device with stoppers at both ends. The bottles can be attached individually on a hydrowire or deployed in 12, 24, or 36 bottle Rosette systems mounted on a frame and combined with a CTD. Niskin bottles are used to collect discrete water samples for a range of measurements including pigments, nutrients, plankton, etc.

Dataset- specific Instrument Name	Sea-Bird SBE 43
Generic Instrument Name	Sea-Bird SBE 43 Dissolved Oxygen Sensor
Dataset- specific Description	CTD Rosette: Sea-Bird Electronics SBE 911plus CTD system equipped with a Sea-Bird SBE 43 dissolved oxygen sensor and a 12-bottle rosette sampler (12 $\times$ 6-L Niskin bottles). Temperature and conductivity sensors were calibrated annually by the manufacturer. The oxygen sensor was calibrated against discrete Winkler titration measurements.
Generic Instrument Description	The Sea-Bird SBE 43 dissolved oxygen sensor is a redesign of the Clark polarographic membrane type of dissolved oxygen sensors. more information from Sea-Bird Electronics

Dataset-specific Instrument Name	Thermo Scientific Genesis 30 Visible
Generic Instrument Name	Spectrophotometer
Dataset-specific Description	Spectrophotometer: Thermo Scientific Genesis 30 Visible, used for colorimetric determination of nitrite ( $NO_2^-$ ) and phosphate ( $PO_4^{3-}$ ).
Generic Instrument Description	An instrument used to measure the relative absorption of electromagnetic radiation of different wavelengths in the near infra-red, visible and ultraviolet wavebands by samples.

Dataset- specific Instrument Name	Turner Designs Trilogy
Generic Instrument Name	Turner Designs Trilogy fluorometer
Dataset- specific Description	Ammonium Analysis: Turner Designs Trilogy fluorometer with a UV module, used for NH <sub>4</sub> + detection via OPA derivatization.
Generic Instrument Description	

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# **Project Information**

Collaborative Research: Exploring the dynamics of nitrous oxide in the Southern Benguela Upwelling System (SBUS N2O)

**Coverage**: Southern and Northern Benguela Upwelling System

#### NSF Award Abstract:

Nitrous oxide is a long-lived and powerful greenhouse gas. It is also a driver of ozone depletion in the stratosphere. Natural sources of nitrous oxide include production by bacteria through processes called nitrification and denitrification. The ocean is a major source of nitrous oxide to the atmosphere, and areas of high biological productivity like eastern boundary upwelling systems have been shown to generate particularly high nitrous oxide emissions to the atmosphere. The Southern Benguela Upwelling System (SBUS) is arguably the most productive eastern boundary upwelling system, yet there are no published measurements of nitrous oxide from this region. In addition, the relative importance of the major biological pathways of nitrous oxide production in the SBUS is not well established. A team of scientists from the University of Connecticut and the University of South Carolina will investigate nitrous oxide cycling in the SBUS, estimate nitrous oxide fluxes to the atmosphere, and explore what drives changes in nitrous oxide cycling across seasons and in different locations. This study will improve understanding of an important greenhouse gas and how its cycling might change in response to changing ocean conditions. Funding from the proposed work will sponsor the training of a graduate student at the University of Connecticut and an undergraduate student at the University of South Carolina. It will also provide a postdoctoral fellow the opportunity to apply computational skills in regional modeling and machine learning, offering preparation for a career in academia or industry. The project will contribute to undergraduate education and communication of climate change science to the general public and policymakers through the incorporation of the study methodology into an undergraduate Service Learning course at the University of Connecticut.

This work seeks to provide estimates of the regional flux of nitrous oxide to the atmosphere, to examine seasonal dynamics, to assess the biological pathways to nitrous oxide production and consumption, and to query regional and large scale forcings on nitrous oxide dynamics in the SBUS. To this end, the team will (a) measure nitrous oxide concentrations in samples collected in the SBUS during seasonal surveys, measure surface nitrous oxide continuously underway, and derive robust estimates of the sea-to-air flux of nitrous oxide from coincident windspeed; (b) query nitrous oxide production and consumption pathways from measurements of the nitrogen and oxygen isotope ratios of nitrous oxide and nitrate, and investigate environmental correlates of nitrous oxide cycling; (c) develop regional machine learning models for nitrous oxide from these measurements to investigate environmental drivers of seasonal and inter-annual nitrous oxide dynamics, predicting nitrous oxide in the SBUS with historical data and with hydrographic fields derived from a regional dynamical ocean model. The work will give insights into pathways of nitrous oxide production

and consumption in an eastern boundary upwelling system bounded by a broad continental shelf – contrasting the greater body of knowledge obtained from active margins. The statistical nitrous oxide models borne of machine learning will ultimately serve to predict nitrous oxide from climate projections of the SBUS, and to anticipate the regional response of nitrous oxide to global ocean de-oxygenation.

This award reflects NSF's statutory mission and has been deemed worthy of support through evaluation using the Foundation's intellectual merit and broader impacts review criteria.

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# **Funding**

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-2241432
NSF Division of Ocean Sciences (NSF OCE)	OCE-2241433

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