Concentrations of Ne, Ar, Kr and Xe as measured by the gas equilibrator mass spectrometer (GEMS) in the SUSTAIN wind-wave tank in the summer of 2018

Website: https://www.bco-dmo.org/dataset/869295
Data Type: experimental
Version: 1
Version Date: 2022-02-03

Project
» Collaborative Research: RUI: Investigating Gas Exchange Processes using Noble Gases in a Controlled Environment (Gas Exchange at SUSTAIN)

Contributors	Affiliation	Role
Stanley, Rachel	Wellesley College	Principal Investigator
Haus, Brian	University of Miami Rosenstiel School of Marine and Atmospheric Science (UM-RSMAS)	Co-Principal Investigator
York, Amber D.	Woods Hole Oceanographic Institution (WHOI BCO-DMO)	BCO-DMO Data Manager

Abstract
Concentrations of Ne, Ar, Kr and Xe as measured by the gas equilibrator mass spectrometer (GEMS) in the SUSTAIN wind-wave tank in the summer of 2018. The results paper for these data was submitted to JGR-Oceans in December of 2021 and are in revision (Stanley et al., 2022).

Table of Contents

Coverage

Temporal Extent: 2018-07-10 - 2018-07-15

Methods & Sampling

Location: SUSTAIN wind-wave Tank, University of Miami

See Supplemental files section for "Noble Gas Ratios of Saturation Anomalies" data.

Methodology:

Noble gas ratios are measured using a Gas equilibator Inlet Mass Spectrometer (GEMS) according to Manning et al. (2016). O2/Ar ratios are measured using an Equilibator Inlet Mass Spectrometer (EIMS), similar to that of Cassar et al 2009 but with an equilibrator system as in the GEMS. O2 concentrations are measured by an

optode calibrated by Winkler. All of those data streams are combined to calculate noble gas concentrations.

Sampling and analytical procedures:

A full description of the sample collection and analysis is in Stanley et al., "Gas Fluxes and Steady State Saturation Anomalies at Very High Wind Speeds" Submitted to JGR-Oceans in Dec. 2021 (Stanley et al., 2022). Relevant paragraphs from the methodology can be found in the Supplemental Files section of this dataset page.

Data Processing Description

See Supplemental files section for "Noble Gas Ratios of Saturation Anomalies" data.

Codes written in matlab were used to convert the raw mass spectrometer data into noble gas ratios. The ratios were then calibrated using measurements in air taken before and after each experiment. Similar calibrations were done for the O2/Ar ratios. Optode data was calibrated with Winkler Samples measured periodically through the experiment. As described above, the noble gas ratios, O2/Ar ratios and optode concentrations were combined to calculate noble gas calculations – all those calculations were done in Matlab. Then the discrete copper tube samples were used as a final calibration of the noble gas concentrations.

BCO-DMO Data Manager Processing Notes:
* File ContinuousNobleGasData.txt imported into the BCO-DMO data system.
* Parameters (column names) renamed to comply with BCO-DMO naming conventions. See https://www.bco-dmo.org/page/bco-dmo-data-processing-conventions
* DateTime (UTC) column added in ISO 8601 format yyyy-mm-ddTHH:MM:SSZ.
* Sampling and Analytical methods summary saved as a pdf from the BCO-DMO metadata form so the formula can be read. The methodology section on this page is plain-text only.
* NGRatiosofSatAnom.txt file extension changed to csv and attached as a Supplemental File.

[table of contents | back to top]

Data Files

File
cont_noble_gas.csv(Comma Separated Values (.csv), 480.58 KB) MD5:e313476e799e9fb4cbdf005dd26fc8a3 Primary data file for dataset ID 869295

[table of contents | back to top]

Supplemental Files

File

Experimental Conditions in SUSTAIN wind wave tank

filename: ExperimentalConditions.csv

(Comma Separated Values (.csv), 1.55 KB)
MD5:4de26b79183f48ba3396e86728ccbf1c

Wind, wave and temperature conditions associated with each experiment in the SUSTAIN wind wave tank.

Parameter (column) inforation (Name, Description, Units):

ExptNumber, Number of experiment, used to cross ref to discrete noble gas table, none

Start_date, date on which that set of experimental conditions started in format M/D/YYYY (GMT), none

Start_time, time on which that set of experimental conditions started in format M/D/YYYY (GMT), none

End_date, date on which that set of experimental conditions ended in format hh:mm (GMT), none

End_time, time on which that set of experimental conditions ended in format hh:mm (GMT), none

Wavetype, 0 denotes monochromatic waves, 1 denotes short crested JONSWAP, none

WaterTemp, temperature of the water (nominal – actualy temperature fluctuated within 1 deg), deg C

U10, wind speed, at 10 m above surface, that was produced for the experiment, m/s

Noble Gas Ratios of Saturation Anomalies

filename: NGRatiosofSatAnom.csv

(Comma Separated Values (.csv), 455.27 KB)
MD5:12bfa116ea7d49f583449ed028ee4e3c

Ratios of the saturation anomalies (percent departure from equilibrium) of the noble gases as determined by the Gas Equilibrator Mass Spectrometer.

Parameter (Column) information (Name, Description, Units):

Del(Ne/Xe), "ratio of Ne/Xe in water compared to air, expressed as a percent deviation from 1. = ((Ne/Xe)meas / (Ne/Xe)air -1) x100", %

Del(Ar/Xe), "ratio of Ne/Xe in water compared to air, expressed as a percent deviation from 1",   %

Del(Kr/Xe), "ratio of Ne/Xe in water compared to air, expressed as a percent deviation from 1",   %

Del(Ne/Kr), "ratio of Ne/Xe in water compared to air, expressed as a percent deviation from 1",   %

Del(Ne/Xe), "ratio of Ne/Xe in water compared to air, expressed as a percent deviation from 1",   %

Del(Ne/Xe), "ratio of Ne/Xe in water compared to air, expressed as a percent deviation from 1",   %

Del(Ne/Xe), "ratio of Ne/Xe in water compared to air, expressed as a percent deviation from 1",   %

Temp,   "Water temperature ",   degrees Celsius

Salinity,   "water salinity (interpolated from discrete samples)"   psu ,

Sampling and Analytical Summary for ContinuousNobleGasData

filename: SamplingAnalytical_summary_continuousNG.pdf

(Portable Document Format (.pdf), 246.72 KB)
MD5:21bcfcc8937664ef6489331546edc552

Sampling and Analytical Summary from Stanley et al. (2022) relevant to dataset "ContinuousNobleGasData."

Stanley et al. (2022), "Gas Fluxes and Steady State Saturation Anomalies at Very High Wind Speeds " Submitted to JGR-Oceans in Dec. 2021.

Related Publications

Cassar, N., Barnett, B. A., Bender, M. L., Kaiser, J., Hamme, R. C., & Tilbrook, B. (2009). Continuous High-Frequency Dissolved O2/Ar Measurements by Equilibrator Inlet Mass Spectrometry. Analytical Chemistry, 81(5), 1855–1864. doi:10.1021/ac802300u

Methods

Manning, C. C., Stanley, R. H. R., & Lott, D. E. (2016). Continuous Measurements of Dissolved Ne, Ar, Kr, and Xe Ratios with a Field-Deployable Gas Equilibration Mass Spectrometer. Analytical Chemistry, 88(6), 3040–3048. https://doi.org/10.1021/acs.analchem.5b03102
Methods

Stanley, R. H. R., Kinjo, L., Smith, A. W., Aldrett, D., Alt, H., Kopp, E., Krevanko, C., Cahill, K., & Haus, B. K. (2022). Gas Fluxes and Steady State Saturation Anomalies at Very High Wind Speeds. Journal of Geophysical Research: Oceans, 127(10). Portico. https://doi.org/[10.1029/2021jc018387](10.1029/2021jc018387)
Results

[<u>table of contents</u> | <u>back to top</u>]

Related Datasets

IsRelatedTo

Stanley, R., Haus, B. (2022) **Concentrations of He, Ne, Ar, Kr and Xe collected in copper tube samples in the SUSTAIN wind-wave tank in the summer of 2018.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2022-02-03 doi:10.26008/1912/bco-dmo.869304.1 [<u>view at BCO-DMO</u>]
Relationship Description: Datasets were collected concurrently during the same experiments and measure the same water.

[<u>table of contents</u> | <u>back to top</u>]

Parameters

Parameter	Description	Units
date	Date and time (UTC) sample was collected in format %d-%b-%Y %H:%M:%S (e.g. 10-Jul-2018 14:14:19)	unitless
NeConc	Concentration of Neon in the SUSTAIN tankwater	micromoles per kilogram (umol/kg)
ArConc	Concentration of Argon in the SUSTAIN tankwater.	micromoles per kilogram (umol/kg)
KrConc	Concentration of Krypton in the SUSTAIN tankwater.	micromoles per kilogram (umol/kg)
XeConc	Concentration of Xenon in the SUSTAIN tankwater.	micromoles per kilogram (umol/kg)
Temp	Water temperature of the SUSTAIN tankwater.	degrees Celsius
Salinity	water salinity (interpolated from discrete samples) of the SUSTAIN tankwater.	Practical Salinity Units (PSU)
ISO_DateTime_UTC	Date and time (UTC) sample was collected in ISO 8601 format %Y-%m-%dT%H:%M:%SZ (e.g. 2018-07-10T14:14:19Z)	unitless

[<u>table of contents</u> | <u>back to top</u>]

Instruments

Dataset-specific Instrument Name	Andaerra Optode
Generic Instrument Name	Aanderaa Oxygen Optodes
Dataset-specific Description	Andaerra Optode for temperature
Generic Instrument Description	Aanderaa Oxygen Optodes are instrument for monitoring oxygen in the environment. For instrument information see the Aanderaa Oxygen Optodes Product Brochure.

Dataset-specific Instrument Name	Hiden Hal 3F Quadrupole Mass Spectrometer
Generic Instrument Name	Mass Spectrometer
Generic Instrument Description	General term for instruments used to measure the mass-to-charge ratio of ions; generally used to find the composition of a sample by generating a mass spectrum representing the masses of sample components.

Dataset-specific Instrument Name	Pfeiffer Prismaplus
Generic Instrument Name	Mass Spectrometer
Dataset-specific Description	Pfeiffer Prismaplus for O2/Ar
Generic Instrument Description	General term for instruments used to measure the mass-to-charge ratio of ions; generally used to find the composition of a sample by generating a mass spectrum representing the masses of sample components.

Project Information

Collaborative Research: RUI: Investigating Gas Exchange Processes using Noble Gases in a Controlled Environment (Gas Exchange at SUSTAIN)

Coverage: SUSTAIN wind-wave tank at University of Miami

NSF Abstract:

An exact description of gas exchange between the atmosphere and the ocean is not fully developed, yet it is a critical process for understanding climate change and ecosystem dynamics. This is particularly problematic when evaluating the important role of bubbles in air-sea gas exchange, especially in remote ocean locations where high winds and waves make direct measurements extremely difficult. This project seeks to provide needed fundamental, high wind/wave gas-exchange measurements by using a large, state-of-the-art, wind-wave tank. Here the PIs can apply their novel measurements of noble gases (neon, argon, krypton, and xenon) to calculate overall gas fluxes under precisely controlled conditions. This tank setting allows a systematic approach to define the physical and chemical parameters (temperature, salinity, pH, wind speed,

turbulence, bubble size distribution, etc.) required to construct more accurate models without the great uncertainties inherent in making similar measurements from a ship in storm conditions. A significant outcome of this study, beyond improved understanding of air-sea gas exchange, could be greatly improved estimates of the critical ecological balance between photosynthesis and respiration. Current methods use carbon dioxide and oxygen dissolved in seawater as an indication of biological activity, but cannot distinguish between biological processes and atmospheric exchange, and estimates are especially inaccurate under high wind and wave conditions with strong bubble injection. This study will improve our ability to separate biological and physical processes in evaluation of dissolved gasses in seawater.

Also, this project will provide 15 female undergraduate students at Wellesley College with an exciting, on-site research experience using a state-of-the-art tank facility at the University of Miami, and results will be incorporated into general and advanced chemistry classes. The production of student-created, short format videos, and other public outreach activities will also be supported to disseminate information on the importance of marine gas exchange.

The study of gas exchange processes between the ocean and the atmosphere has been hindered by the lack of data required to define quantitative relationships that account for bubble processes under a variety of wind, wave, and temperature conditions. Current gas exchange models tend to be highly unreliable in their parameterization of bubble processes. In large part, this is due to the difficulty of making traditional measurements at sea in remote locations within well-defined conditions, especially with high winds and waves. By using the large SUSTAIN wind-wave tank (23 m x 6 m x 2 m), the researchers in this project plan to greatly advance our understanding of the effect of wind, wave, and temperature variability on gas transfer. The use of a recently developed, field-portable equilibrator mass spectrometer that allows nearly continuous measurements of noble gas ratios (Ne, Ar, Kr, and Xe) will result in these SUSTAIN tank experiments providing precisely characterized gas flux data under varying wind speeds from 10 to 40 m/s. In addition, an underwater shadowgraph system will image bubbles, allowing the researchers to quantify bubble size distributions, a key factor missing from bubble models. Current models use a greatly simplified, two size-class representation of bubbles; an approach that this research will re-evaluate in hopes of creating better parameterizations of the role of bubble size on gas flux, and consequently improved air-sea gas exchange models for oceanic and climatic applications.

Funding