Total alkalinity from an experiment testing the suitability of high-density polyethylene (HDPE) for collection and long-term storage of total alkalinity samples using laboratory-manipulated oligotrophic Atlantic surface water

Website: https://www.bco-dmo.org/dataset/957694
Data Type: experimental
Version: 1
Version Date: 2025-04-03

Project
» US GEOTRACES GP17-OCE and GP17-ANT: Inorganic Carbon Cycling in the South Pacific and Southern Oceans by Direct Measurement (GP17-OCE and GP17-ANT Inorganic Carbon)

Contributors	Affiliation	Role
Woosley, Ryan J.	Massachusetts Institute of Technology (MIT)	Principal Investigator
Neithardt, Daina	Massachusetts Institute of Technology (MIT)	Student
Bruno, Jessica A.	Massachusetts Institute of Technology (MIT)	Technician
Rauch, Shannon	Woods Hole Oceanographic Institution (WHOI BCO-DMO)	BCO-DMO Data Manager

Abstract
Total alkalinity plays an important role in buffering seawater and determining how much anthropogenic carbon dioxide the oceans can absorb and mitigate the rise in atmospheric concentrations. Total alkalinity varies with location, depth, and time making it an important variable needed to quantify and monitor ocean acidification, and potentially for ocean alkalinity enhancement interventions. Currently, best practices are to use expensive high quality borosilicate glass bottles for collecting and storing these samples. However, unlike other carbon system variables, total alkalinity is not affected by gas exchange meaning plastic bottles may be suitable for total alkalinity sample storage. Plastic bottles are lighter, cheaper, and less prone to breakage making them easier to handle and ship. Here, we test the suitability of high-density polyethylene (HDPE) for collection and long-term storage of total alkalinity samples through laboratory experiments where HDPE bottles were treated to different cleaning methods and then filled with surface seawater and stored for 15-17 months before analyzing for total alkalinity. It was determined that HDPE is not suitable for long-term storage of total alkalinity samples as there were large changes in total alkalinity over time and precision of duplicate samples was very poor. We hypothesize that HDPE plastic is slightly porous leading to leaching of alkalinity either into or out of the bottle over time impacting the value of the sample. Use of HDPE bottles for total alkalinity samples is not recommended for long term sample storage.

Table of Contents

- Coverage
- Dataset Description
  - Methods & Sampling
  - Data Processing Description
  - BCO-DMO Curation Notes
  - Problem Description
- Data Files
- Related Publications
- Related Datasets
- Parameters
- Instruments
- Project Information
- Funding

Coverage

Location: Laboratory experiment

Temporal Extent: 2025-01-07 - 2025-01-24

Methods & Sampling

125-milliliter (mL) high-density polyethylene (HDPE) oblong wide-mouth bottles certified to meet EPA performance-based standards for metals, cyanide, and fluoride (Fisher Scientific product number 05-721-147) were used. The bottles had been previously used on GP17-OCE (R/V Roger Revelle cruise RR2214). Bottles were pretreated in one of five treatments: 1.) no further conditioning, 2.) 1-week soak in low nutrient surface seawater, 3.) 2-week soak in low nutrient surface seawater 4.) 1-week soak in milli-Q water or 5.) a 2-week soak in milli-Q water.

After the treatment, the bottles were rinsed with milli-Q water 3 times and allowed to dry in a fume hood. All of the bottles were then filled with low-nutrient surface seawater collected from the North Atlantic (39˚ 46.406' N, 70˚ 53.065' W on October 10, 2019). A 20-liter (L) carboy was filled with the seawater (that had previously been poisoned to ~0.04% HgCl2) by filtering through a 0.8/0.2-micrometer (um) AcroPak™ 1000 filter (Pall Laboratories, Port Washington, New York USA, product number 1515-002). After filtering, the carboy was shaken vigorously to ensure it was well mixed and allowed to equilibrate overnight. The practical salinity of the water was 34.992, and the initial TA was determined to be 2299.68 ±0.59 (N=5). More details can be found in Woosley et al. (submitted).

Instrumentation:
Samples were analyzed in the lab for total alkalinity using a custom-designed open cell titration with non-linear least squares fitting designed and built by the laboratory of Andrew G. Dickson (University of California, San Diego) and described in detail in Dickson et al. (2003).

Data Processing Description

Data were quality controlled and flagged for any known analytical issues that occurred for a given sample.

BCO-DMO Curation Notes

- Imported original file "HDPE Lab Test Submit to BCODMO.xlsx" into the BCO-DMO system.
- Marked "-999" as a missing data value (missing data are empty/blank in the final csv file).
- Renamed fields to comply with BCO-DMO naming conventions.
- Converted the date-time column to ISO 8601 format.
- Saved final file as "957694_v1_ta_hdpe_bottle_storage_test.csv".

Problem Description

No known issues occurred aside from changes in sample total alkalinity during storage, which is what the experiment was meant to determine.

WOCE quality flags were used (2 = good, 3 = questionable, 4 = bad, 5 = missing, 6 = average of two duplicates, 9 = not sampled).

For laboratory experiments, flags are indicative of analytical quality and not storage quality.

[table of contents | back to top]

Data Files

File	
957694_v1_ta_hdpe_bottle_storage_test.csv	(Comma Separated Values (.csv), 5.05 KB) MD5:e8b48d918c445aa3cc7103bb4a1cd70d
Primary data file for dataset ID 957694, version 1	

[table of contents | back to top]

Related Publications

Dickson, A. G., Afghan, J. D., & Anderson, G. C. (2003). Reference materials for oceanic CO2 analysis: a method for the certification of total alkalinity. Marine Chemistry, 80(2), 185–197. https://doi.org/10.1016/S0304-4203(02)00133-0
Methods

Woosley, R.J., J.A. Bruno, D. Neithardt, Z.A. Wang, N. Fujiki, and A. Murata. (submitted, 2025) Comparison of open cell and single-step total alkalinity titration methods and implications for organic alkalinity. Limnol. Ocenogr. Meth.
Results

[table of contents | back to top]

Related Datasets

IsRelatedTo

Woosley, R., Bruno, J. A., Neithardt, D. (2025) **Open cell and single-step method for total alkalinity titrations from samples collected on R/V Mirai cruises MR23-06C and MR23-07 in the North Pacific and Western Arctic from September to November 2023.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 2) Version Date 2025-07-29 doi:10.26008/1912/bco-dmo.957527.2 [view at BCO-DMO]

Woosley, R., Neithardt, D., Lahn, L. (2025) **Total alkalinity determined through experiments comparing usage of high-density polyethylene (HDPE) and borosilicate glass bottles for collection and storage of water samples collected on the GEOTRACES GP17-OCE cruise (R/V Roger Revelle RR2214).** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2025-04-02 doi:10.26008/1912/bco-dmo.957644.1 [view at BCO-DMO]

[table of contents | back to top]

Parameters

Parameter	Description	Units
Bottle_ID	Bottle identifier (label given to sample)	unitless
Soak_solution	Solution used for pre-treatment soak (None, Milli-q water, or Seawater)	unitless
Soak_Duration	Soak duration (number of weeks)	weeks
Bottle_Number	Number of bottle for each treatment	unitless
Analysis_Date_Time_EST	Analysis date and time in Eastern Standard Time in ISO8601 format	unitless
Total_Alkalinity	Total Alkalinity	micromoles per kilogram seawater (umol/kg_sw)
Analysis_Flag	WOCE QC flagging scheme	unitless

[table of contents | back to top]

Instruments

Dataset-specific Instrument Name	high-density polyethylene (HDPE) oblong wide-mouth bottles
Generic Instrument Name	High density polyethylene water bottle
Dataset-specific Description	125 mL HDPE oblong wide-mouth bottles certified to meet EPA performance-based standards for metals, cyanide, and fluoride (Fisher Scientific product number 05-721-147) were used.
Generic Instrument Description	A high density polyethylene (HDPE) water bottle. Often used for surface sampling from small boats. HDPE has a somewhat higher chemical resistance than low density polyethylene (LDPE). HDPE is also somewhat harder and more opaque and it can withstand higher temperatures (120 degrees Celsius for short periods, 110 degrees Celsius continuously).

Dataset-specific Instrument Name	custom designed open cell titration
Generic Instrument Name	Titrator
Dataset-specific Description	Samples were analyzed in the lab for total alkalinity using a custom designed open cell titration with non-linear least squares fitting designed and built by the laboratory of Andrew G. Dickson (University of California, San Diego) and described in detail in Dickson et al. (2003).
Generic Instrument Description	Titrators are instruments that incrementally add quantified aliquots of a reagent to a sample until the end-point of a chemical reaction is reached.

[table of contents | back to top]

Project Information

US GEOTRACES GP17-OCE and GP17-ANT: Inorganic Carbon Cycling in the South Pacific and Southern Oceans by Direct Measurement (GP17-OCE and GP17-ANT Inorganic Carbon)

Coverage: South Pacific and Amundsen Sea

NSF Award Abstract
The oceans help to slow climate change by absorbing about a quarter of the carbon dioxide (CO2) produced by burning of fossil fuels and other human activities. The Pacific and Southern Oceans are known to take up and store significant amounts of anthropogenic CO2, but many questions regarding the amount, variability, and biogeochemical and ecological impacts remain unanswered. This research will focus on answering some of those questions in two areas of the Pacific by analyzing samples for total CO2, total alkalinity, and pH on two GEOTRACES cruises, GP17-OCE and GP17-ANT. The project will support several undergraduate student researchers and create educational modules on ocean acidification for general public and K-12 students.

On the GP17-OCE expedition in the south Pacific, sub-decadal scale variability in the uptake of CO2 and resulting decrease in pH (termed ocean acidification) will be examined by comparing data collected on this expedition with data from prior occupations of the line in 1991, 2005 and 2014. An extended multilinear regression technique will be used to separate natural variability from human induced changes. The second expedition, GP17-ANT, covers the Amundsen Sea, an area with few prior carbon measurements. This sea is perennially ice-covered with several seasonal polynyas (areas of open water surrounded by sea ice) and exhibits complex water circulation making the contribution to the global carbon cycle uncertain. The data collected from this expedition will examine several hypotheses regarding how carbon is taken up, mixed, and recirculated in the region, how glacial ice melt, sea ice, and biological productivity influence the carbon cycle, and provide baseline measurements against future data to determine changes in the carbon cycle of the region over time. Both expeditions will leverage the myriad of other parameters being measured, particularly trace metals such as iron and zinc, to examine how cycling of carbon and trace metals are interlinked through pH.

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.

[table of contents | back to top]

Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-2148468

[table of contents | back to top]