Data Documentation

Dataset Information

Dataset Title:

NCCOS Assessment: Water Quality Data to Assess Eutrophication Effects on Coral Ecosystem Health in Vatia Bay, American Samoa from 2015-05-13 to 2018-08-28

Description:

This dataset represents three years of water quality data collected in Vatia Bay, American Samoa. A standard suite of nutrient parameters (nitrate, nitrite, ammonium, urea, total nitrogen, orthophosphate, total phosphorus and silica), as well as tracers of human waste (sucralose and caffeine) were quantified at sixteen randomly selected sites (surface and bottom samples) monthly from 2015 to 2017.

Purpose:

American Samoa's reefs are considered to be among the most pristine in the United States. These reefs host approximately 950 species of fish, 240 species of algae, 330 species of coral and many other species of invertebrates. Vatia Bay is located on the north shore of the island of Tutuila, the largest and most populous island of the U.S. territory of American Samoa. The Bay has been designated as a priority area by the American Samoa Coral Reef Advisory Group. There have been local concerns about the impacts of land based sources of pollution and water quality on the coral reef ecosystems of Vatia Bay, due to the prevalence of benthic algae. Excess nutrient loads can affect coral health both directly (*e.g.*, lowering fertilization and calcification rates) and indirectly (increasing benthic algal growth which can outcompete corals for space). Nutrients can come from a variety of sources, but the two likely largest sources for this system as human waste and piggeries. The objectives of this study where to: quantify the magnitude and spatiotemporal variability of surface water nutrients in the Bay; establish a baseline of nutrient conditions against which to measure changes in the future; link observed concentrations of nutrients to hydrologic forcing factors and possible nutrient sources; and use human dietary chemical indicators to evaluate if human waste is reaching Vatia Bay. Environmental data, such as the dataset presented here, serve as a baseline of current conditions, which are needed determine the efficacy of management efforts, *i.e.*, measuring change over time. The data presented here can be utilized by coastal managers to best prioritize management strategies in a way to maximize success in decreasing stressors on coral reef ecosystems. Partners included: American Samoa's Coral Reef Advisory Group, American Samoa Environmental Protection Agency (ASEPA), National Park Service (NPS) and American Samoa Community College.

Methods:

Four strata were operationally articulated within the Bay based on proximity to the stream/shore and geography. Within each strata, four sites were randomly selected (using ArcGIS) in order to capture the spatial variability within the Bay. This stratified random sampling design allows for statistical comparisons among the articulated strata. Additionally, one targeted site was selected at the largest stream channel input to the Bay (just upstream from the largest

bridge in the village Sites were accessed by either sea kayak or wading. At wading sites, care was taken to sample away from the person's body and on an incoming swell/wave to minimize the potential for contamination. Surface water (0.1 m below surface) and bottom water (via Niskin bottle, just above bottom) were collected for water quality analysis; exceptions to this were very shallow sites where only surface water was collected. From 2015 to 2017, each of these sites was visited monthly to collect grab samples. In 2018, sampling efforts focused on capturing precipitation events, so the sampling was conducted at less regular intervals. High density polyethylene (HDPE) bottles were used for nutrient collections. The bottles were rinsed three times with site water prior to sampling. Nitrile or latex gloves were worn by field personnel to avoid contamination of the samples during handling. Samples were stored on ice, in the dark while in the field, frozen at -20°C upon returning to the lab and not thawed until immediately prior to analysis. Samples were not filtered so that total nutrient levels could be analyzed, rather than only dissolved levels. During some sampling months, extra sample volume was collected (into amber glass vials) for analysis of caffeine and sucralose. These were sampled concurrently with the nutrient samples at the same sites. Chemical analyses were conducted using previously published methods at NOAA contract laboratories (Geochemical Environmental Research Group at Texas A&M University for nutrients; and Florida International University for caffeine/sucralose).

For a complete description of the process and analyses see Whitall *et al*. (2019).

Cited Publications:

- Whitall, D., M. Curtis, A. Mason, and B. Vargas-Angel. 2019. Excess Nutrients in Vatia Bay, American Samoa: Spatiotemporal Variability, Source Identification and Impact on Coral Reef Ecosystems. NOAA Technical Memorandum NOS NCCOS 266. Silver Spring, MD. 69 pp. https://doi.org/10.25923/j8cp-x570
- Armstrong, F., and C. Stearns. 1967. The measurement of upwelling and subsequent biological processes by means of the Technicon Autoanalyzer and associated equipment. Deep-Sea Research, 14:381-389. https://doi.org/10.1016/0011-7471(67)90082-4
- Batchu, S., C. Ramirez, and P. Gardinali. 2015. Rapid ultra-trace analysis of sucralose in multiple-origin aqueous samples by online solid-phase extraction coupled to high-resolution mass spectrometry. Analytical and Bioanalytical Chemistry, 407:3717-25. https://doi.org/10.1007/s00216-015-8593-6
- Hansen, H., and F. Koroleff. 1999. Determination of Nutrients. In: Grasshoff, K., K. Kremling, and M. Ernhardt [Eds.], Methods of Seawater Analysis. New York, Wiley-VCH. ISBN 3-527-29589-5
- Harwood, J., and A. Kuhn. 1970. A colorimetric method for ammonia in natural waters. Water Research, 4:805-811. https://doi.org/10.1016/0043-1354(70)90037-0
- Wang, C. 2012. Assessment of the Occurrence and Potential Effects of Pharmaceuticals and Personal Care Products in South Florida Waters and Sediments. Florida International University Electronic Theses and Dissertations, 689. https://digitalcommons.fiu.edu/etd/689

Associated Accessions:

- Coral Reef Ecosystem Program; Pacific Islands Fisheries Science Center. 2016. Benthic Surveys in Vatia, American Samoa: benthic images collected during belt transect surveys from 2015-11-2 to 2015-11-12 (NCEI Accession 0146680). NOAA National Centers for Environmental Information. Dataset. https://accession.nodc.noaa.gov/0146680

- Coral Reef Ecosystem Program; Pacific Islands Fisheries Science Center. 2017. Benthic Surveys in Vatia, American Samoa: comprehensive assessment of coral demography (adult and juvenile corals) from belt transect surveys between 2015-11-02 and 2015-11-12 (NCEI Accession 0165016). NOAA National Centers for Environmental Information. Dataset. https://accession.nodc.noaa.gov/0165016
- Coral Reef Ecosystem Program; Pacific Islands Fisheries Science Center. 2018. Benthic cover derived from photo transects in Vatia, American Samoa from 2015-11-02 to 2015-11-12 (NCEI Accession 0169726). NOAA National Centers for Environmental Information. Dataset. https://accession.nodc.noaa.gov/0169726

People & Projects

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- Greg Piniak, NCCOS

Funding:

- US DOC; NOAA; NOS; National Centers for Coastal Ocean Science (NCCOS)
- US DOC; NOAA; NOS; Coral Reef Conservation Program (CRCP)

Associated Projects:

- NCCOS Project #245, Nutrient Dynamics and Changes to Benthic Communities in Vatia, American Samoa, https://coastalscience.noaa.gov/project/nutrient-dynamics-changes-benthic-communities-vatia-american-samoa/
- CRCP Project #31090, Eutrophication Impacts on Coral Ecosystem Health in Vatia, American Samoa

Extents

Start Date:	2015-05-13
End Date:	2018-08-28

Northern Boundary: -14.244537
Southern Boundary: -14.250670
Western Boundary: -170.6754
Eastern Boundary: -170.66831

Keywords

Sea Areas, Water Bodies, Marine Protected Areas:

- Coastal Ocean
- American Samoa
- Tutuila
- Vatia Bay

NCCOS Keywords:

- NCCOS Research Priority > Stressor Impacts and Mitigation
- NCCOS Research Topic > Biological Effects of Contaminants and Nutrients
- NCCOS Research Location > Region > Pacific Ocean
- NCCOS Research Location > U.S. States and Territories > American Samoa
- NCCOS Research Data Type > Field Observation

CoRIS Keywords:

CoRIS Discovery Thesaurus:

- Numeric Data Sets > Water Quality

CoRIS Theme Thesaurus:

- EARTH SCIENCE > Oceans > Ocean Chemistry > Chemistry Monitoring and Assessment

CoRIS Place Country/Territory Keywords:

- COUNTRY/TERRITORY > United States of America > American Samoa > Tutuila Island > Vatia Bay (14S170W0028)

CoRIS Place Ocean/Seas Keywords:

- OCEAN BASIN > Pacific Ocean > Tutuila Island > Vatia Bay (14S170W0028)

File Information

Total File Size: 471 KB total, 6 files in 1 folder (410 KB unzipped)
Data File Format(s): Comma-separated value (.CSV)
Data File Compression: no compression

Data Files:

- NCCOS-Vatia-Water-Quality_Data-01_Inorganic-Nutrients.CSV
- NCCOS-Vatia-Water-Quality_Data-02_Total-Nutrients.CSV
- NCCOS-Vatia-Water-Quality_Data-03_Tracers.CSV

Documentation Files:

- NCCOS-Vatia-Water-Quality_BrowseGraphic.JPG
- NCCOS-Vatia-Water-Quality_DataDocumentation.PDF
- NCCOS-Vatia-Water-Quality_DataDocumentation_Site-Info.CSV

Table 1: Inorganic Nutrients Data Dictionary

Column	Variable	Label	Definition	Units	Range
1	Sample ID and Depth	Sample Designation	Site name and sample depth	n/a	n/a
2	Date	Collection Date	Day of the year sample was collected and depth (surface or bottom)	MM/DD/YYYY	5/13/15 to 8/28/18
3	Nitrate	NO3-	Water concentration	mg N/L	0 to 0.52
4	Orthophosphate	HPO4=	Water concentration	mg P/L	0 to 0.37
5	Silica	HSiO3-	Water concentration	mg Si/L	0 to 33.95
6	Ammonium	NH4+	Water concentration	mg N/L	0 to 0.29
7	Nitrite	NO2-	Water concentration	mg N/L	0 to 0.02
8	Urea	Urea	Water concentration	mg N/L	0 to 0.05

Table 2: Total Nutrients Data Dictionary

Column	Variable	Label	Definition	Units	Range
1	Sample ID and Depth	Sample Designation	Site name and sample depth	n/a	n/a
2	Date	Collection Date	Day of the year sample was collected and depth (surface or bottom)	MM/DD/YYYY	5/13/15 to 8/28/18
3	Total Nitrogen	Total N	Water concentration	mg N/L	0.03 to 1.40
4	Total Phosphorus	Total P	Water concentration	mg P/L	0.01 to 0.59

Table 3: Tracers Data Dictionary

(ND indicates no data/missing or damaged sample)

Column	Variable	Label	Definition	Units	Range
1	Sample ID and Depth	Sample Designation	Site name and sample depth	n/a	n/a
2	Date	Collection Date	Day of the year sample was collected and depth (surface or bottom)	MM/DD/YYYY	6/13/16 to 8/28/18
3	Sucralose	Sucralose	Water concentration	ng/L	2.88 to 369.82
4	Caffeine	Caff	Water concentration	ng/L	1.09 to 343.04

Table 4: Site Information Data Dictionary

Column	Variable	Label	Definition	Units	Range
1	Latitude	Latitude	Latitude of site	decimal degrees	-14.244537 to -14.250670
2	Longitude	Longitude	Longitude of site	decimal degrees	-170.668315 to -170.6754
3	Stratum	Stratum	Site stratum: Central, Inner, North, South, Stream	n/a	n/a
4	Site Name	Site_Name	Site Name	n/a	n/a

Parameter Information

Major parameters:

- Nutrients:
  - Nitrate, Nitrite, Ammonium, Urea, Total Nitrogen
  - Orthophosphate, Total Phosphorus
  - Silica
- Caffeine
- Sucralose

Parameter Description:

Parameter: Nutrients
Property Type: measured
Units: mg/L
Observation Category: laboratory analysis
Sampling Instrument: Niskin bottle
Sampling and Analyzing Method:

- Nitrate and nitrite analyses were based on the methodology of Armstrong *et al.* (1967).
- Ammonium analysis was based on the method of Harwood and Kuhn (1970) using dichloro-isocyanurate as the oxidizer.
- Urea was measured using diacetyl-monoximine and themicarbozide with colorimetric analysis.
- The total concentration of nitrogen was determined after an initial decomposition step. This method involves persulfate oxidation while heating the sample in an autoclave (115°C, 20 minutes) (Hansen and Koroleff, 1999). After oxidation of the samples, nitrogen determination was conducted on the Astoria Pacific analyzer for nitrate.
- The total concentration of phosphorus were determined after an initial decomposition step. This method involves persulfate oxidation while heating the sample in an autoclave (115°C, 20 minutes) (Hansen and Koroleff 1999). After oxidation of the samples, phosphorus determination was conducted on the Astoria Pacific analyzer for orthophosphate.
- Silicate determination was accomplished using the methods of Armstrong *et al*. (1967) using stannous chloride.

Data Quality Method:

All laboratory data contained blanks, spikes and percent recoveries. Data were QA/QC'd using National Status and Trends protocols.

Parameter Description:

Parameter: Caffeine
Property Type: measured
Units: ng/L
Observation Category: laboratory analysis
Sampling Instrument: Niskin bottle
Sampling and Analyzing Method:

Caffeine was quantified at Florida International University (sub-contract to TDI Brooks) using previously published methods (Wang 2012). The caffeine procedure is based on the combined performance of an Equan MAX Plus online Solid Phase Extraction (SPE) preconcentration system coupled to a high pressure liquid chromatography (LC) system equipped with resolution mass spectrometry detection using a QExactive orbitrap-based mass spectrometer (SPE-LC-HRMS). The analytical separation was carried out using a Hypersil Gold aQ column (100×2.1 mm, 1.9 µm) while the SPE pre-concentration column was a Hypersil Gold aQ (0.5×50 mm; Thermo Scientific, West Palm Beach, FL, USA). The automated online SPE clean-up and pre-concentration step was performed using only 10 mL of filtered water samples. The online procedure consists of a divertion valve on the mass spectrometer which is programmed by the data system to control the loading and elution of the two LC columns. In the load position, 10 mL of sample was injected into a 10-mL loop and then loaded onto a SPE column by the loading LC pump, followed by a wash step with 98:2 0.1% formic acid: acetonitrile to remove interferences (flow rate 2 mL/min). The target compounds were retained in the SPE column and the matrix that is not retained during the extraction process was directed to waste while simultaneously the analytical pump equilibrated the analytical column in the starting gradient conditions. After 5 min, when the valve was switched to inject position, the solvent flow through the SPE column was reversed, and the analytes were then backflushed with a gradient of acetronitrile and 0.1% formic acid onto a Hypersil Gold aQ column for separation and quantitation by heated electrospray ionization source (HESI)-MS/MS. After 7 min, the switching valve was returned to the loading position to allow the extraction column to be re-equilibrated with water. The samples were kept at 10 °C in the autosampler. The total run time per sample was 13 min. The analyte was detected on a Q-Exactive Mass spectrometer equipped with an HESI source operated in the positive mode. The capillary temperature was 350 °C with a discharge current of 4 kV and S-lens RF level of 80 %. Sheath gas and auxiliary gas (N2) were used at a flow rate of 30 and 20 arbitrary units, respectively. The analysis was performed in Parallel Reaction Monitoring (PRM) (with an inclusion list of the exact mass of the target compounds) at a resolution of 35,000. Quantitation is performed by the internal standard approach (concentrations are calculated based on area ratio between the analyte and labeled internal standard) to correct for matrix effects and any losses in the online extraction step. The monitoring ions for caffeine were 195.0877 and 138.0662 and for the labelled caffeine (13C3 caffeine) was 198.0977.

Data Quality Method:

All laboratory data contained blanks, spikes and percent recoveries. Data were QA/QC'd using National Status and Trends protocols.

Parameter Description:

Parameter: Sucralose
Property Type: measured
Units: ng/L
Observation Category: laboratory analysis
Sampling Instrument: Niskin bottle
Sampling and Analyzing Method:

Sucralose was quantified at Florida International University (sub-contract to TDI Brooks) using previously published methods (Batchu *et al*. 2015). The methodology for sucralose quantification is based on automated online solid-phase extraction (SPE) and high-resolving-power orbitrap mass spectrometer (MS) detection. Operating in full scan (no collision-induced dissociation), detection of the unique isotopic pattern (100:96:31 for [M-H](-), [M-H+2](-), and [M-H+4](-), respectively) was used for ultra-trace quantitation and analyte identification. The method offers fast analysis (14 min per run) and low sample consumption (10 mL per sample) with method detection limits (MDLs) and method confirmation limits (MCLs) of 1.4 and 5.7 ng/L in seawater, respectively.

Data Quality Method:

All laboratory data contained blanks, spikes and percent recoveries. Data were QA/QC'd using National Status and Trends protocols.

Document Information

Date:	2019-12-02
Resource Provider:	NCCOS Data Manager, nccos.data@noaa.gov, US DOC; NOAA; NOS; National Centers for Coastal Ocean Science (NCCOS)
Comment:	This data documentation describes data files archived as a NOAA NCEI data accession, and is intended to provide dataset-level metadata for the purposes of discovery, use, and understanding.
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