Biological degradation rate constants for acetaldehyde and ethanol (and associated water quality parameters) in surface waters of the Upper Newport Back Bay estuary in California from May 2021 to July 2022

Website: https://www.bco-dmo.org/dataset/966895
Data Type: Other Field Results
Version: 1
Version Date: 2025-07-03

Project
» RUI: Collaborative Research: Cycling of ethanol and acetaldyhyde in coastal waters (Coastal Water Cycling)

Contributors	Affiliation	Role
Clark, Catherine	Western Washington University (WWU)	Principal Investigator, Contact
de Bruyn, Warren	Chapman University (CU)	Principal Investigator
Crosland, Jefferson	Western Washington University (WWU)	Scientist
Kodner, Robin	Western Washington University (WWU)	Scientist
Matsumoto, Maya	Western Washington University (WWU)	Scientist
Soenen, Karen	Woods Hole Oceanographic Institution (WHOI BCO-DMO)	BCO-DMO Data Manager

Abstract
These data are measurements of the biological degradation rate constants of the volatile organic carbon (VOC) species acetaldehyde and ethanol in near-shore surface waters of the Upper Newport Back Bay estuary in Southern California in 77 samples taken between May 2021 and July 2022. Water quality parameters, dissolved organic carbon concentrations, total bacteria counts and chlorophyll levels of the samples were also measured to help characterize the samples and identify environmental conditions affecting uptake rates. These data were collected by Dr. Warren De Bruyn of Chapman University. The goal of this project was to improve understanding of the cycling of the atmospheric pollutants ethanol and acetaldehyde in coastal seawater and surface waters.

Table of Contents

Coverage

Location: The Newport Back Bay (NBB) estuary in Orange County, Southern California, USA
Spatial Extent: **N**:33.650327 **E**:-117.8671967 **S**:33.6181867 **W**:-117.9051099
Temporal Extent: 2021-05-20 - 2022-10-04

Methods & Sampling

The Newport Back Bay (NBB) is an estuary in Orange County, Southern California, USA. It includes the Upper Newport Back Bay, a ~1000-acre ecological preserve managed by the U.S. Fish and Wildlife Service and the California Department of Fish and Game. This estuary includes salt marshes and mudflats. The primary freshwater input is the San Diego creek which drains a ~150 square mile watershed, with additional freshwater inputs from some storm-water drains. Water samples were collected from 3 sites: Site 1 (inlet; 33.650327, -117.8671967); site 2 (mid-estuary; 33.6302266, -117.8859726); site 3 (near the outlet into the Pacific Ocean; 33.6181867, -117.9051099). When freshwater inflow is significant, site 1 has lower salinity water with higher dissolved organic content.

Surface water (<5 cm) was sampled in the morning from the shore, stored in amber glass bottles and transported to the laboratory. Water quality measurements were made in-situ (Hanna Instruments HI 9829 multiparameter probe with a double junction pH/oxidation reduction potential (ORP) sensor (HI7609829-1), galvanic dissolved oxygen (DO) sensor (HI7609829-2), conductivity/turbidity sensor (HI7609829-4) and a temperature sensor.

Absorbance was measured to assess the dissolved organic content of the sample and allow for calculations of estimated photochemical production rates of ethanol and acetaldehyde. Samples were first filtered through 0.2 micron Durapore filters to remove microorganisms. Spectra were obtained in a 1 cm quartz cell using a Horiba Aqualog spectrofluorometer. Excitation-emission matrices (EEMs) were also collected (excitation 250-450 nm; emission 250 to 830 nm). Nanopure water was used as the blank. Raw absorbance data were used to calculate absorption coefficients (Juetten et al., 2025).

Aerobic bacterial counts were measured by adding 1 mL of a 1:100 mL mixture of seawater and artificial seawater to Petrifilm Aerobic Count Plates (3M Corporation), incubating at 37oC for 48 hours and then counting the number of colony-forming units on the plates. This provides a measurement of culturable colonies and would be expected to underestimate the true aerobic microbial population. For total bacteria counts, 20 mL was filtered through black 0.2 µm polycarbonate filters (Whatman Cyclopore), fixed with glutaraldehyde (2% in 0.1 M phosphate buffer; pH 7.4; Poly Scientific) and stored in aluminum foil packets at 4oC. These filters were shipped on dry ice to Western Washington University where they were placed on microscope slides, DAPI stained and particles counted using a fluorescence microscope.

Filtered samples were acidified to pH <2 using 6 M hydrochloric acid before measuring DOC concentrations with a Shimadzu TOC analyzer.

Chlorophyll *a* levels were determined with EPA method 445.0. Briefly, 200 mL were buffered saturated magnesium carbonate solution, filtered through GF/F filters (Cytiva), sealed in aluminum foil packets and stored at -80oC in the dark. Samples were shipped on dry ice to Western Washington University's Institute for Watershed Studies laboratory where the GF/F filters were ground and chlorophyll extracted with acetone before determining chlorophyll levels by measuring fluorescence before and after acidification with 0.1 N HCl using a Turner Designs TD700 or 10 AU.

The measurement of acetaldehyde and ethanol uptake rates has been described in detail in de Bruyn et al. (2021). Briefly, samples were split into two aliquots; one aliquot was filtered through 0.2 µm filters (Millipore) to remove abiotic particles and microorganisms to serve as abiotic controls for biological uptake. About 150 mL from the other unfiltered aliquot was placed in a glass syringe, spiked with deuterated acetaldehyde or ethanol (d-4; Aldrich 98% deuterated; 40-100 nM)) and used to measure acetaldehyde or ethanol biological degradation rates. Syringes were kept in the dark in a water bath set to the temperature of the water when sampled. Degradation rates were determined from changes in deuterated acetaldehyde or ethanol concentrations over 4 to 5-hours. Every ~45 minutes, samples were removed from the syringe and deuterated acetaldehyde or ethanol measured by purge and trap gas chromatography mass spectrometry (Shimadzu GC-14A/HP5973MSD). Details of this measurement are given in de Bruyn et al. (22021). In brief, deuterated acetaldehyde or ethanol is sparged using ultrapure He, trapped in a glass bead trap at liquid nitrogen temperatures, thermally desorbed, and analyzed on a Poroplot Q column (Shimadzu, 14A) with MS detection (Agilent 5973).

Data Processing Description

Acetaldehyde and ethanol concentrations in unfiltered incubations decreased exponentially with time consistent with first-order or pseudo-first-orde rkinetics. For first order or pseudo first order kinetics the rate of reaction depends only on the concentration of a single species, in this case acetaldehyde or ethanol: Reaction rate = - dA/dt = k [A] where [A] is the acetaldehyde or ethanol concentration and k is the first order rate constant. Separating variables and integrating results in the integrated rate law: ln [A]t/[A]t=0 = - kt Where [A]t is

the concentration of acetaldehyde or ethanol at time t and [A]t=0 is the concentration of acetaldehyde or ethanol at t=0. Therefore a plot of the natural log of the acetaldehyde concentration at time t divided by the concentration at time t=0 is linear and the slope is the first-order rate constant with units of time-1. This is summarized from De Bruyn et al. (2021).

Absorbance was converted to absorption coefficient at a particular wavelength by dividing the absorbance by 0.01 and multiplying by 2.303. This is described in Juetten et al. (2025).

BCO-DMO Processing Description

* adjusted parameter names to comply with database requirements
* added lat/lon of sampling sites to dataset
* converted sampling date to ISO format

[table of contents | back to top]

Related Publications

Juetten, K., De Bruyn, W. J., Landram, Z., Jansen, C. D. R., Harrison, A. W., Strecker, A., & Clark, C. D. (2025). Production of dissolved organic matter from lily pads (Nymphaea odorata) in a mesotrophic freshwater lake. Aquatic Sciences, 87(2). https://doi.org/10.1007/s00027-025-01180-4
Methods

de Bruyn, W. J., Clark, C. D., Harrison, A. W., Senstad, M., & Hok, S. (2021). The degradation of acetaldehyde in estuary waters in Southern California, USA. Environmental Science and Pollution Research, 28(27), 35811–35821. https://doi.org/10.1007/s11356-021-13232-x
Methods

[table of contents | back to top]

Parameters

Parameter	Description	Units
date	date sample taken	unitless
site	location sample was taken	unitless
Latitude	Sampling latitude, south is negative	decimal degrees
Longitude	Sampling longitude, west is negative	decimal degrees
PH	in situ pH of surface water sample	unitless
Temp	temperature of in situ surface water sample	degrees Celsius (°c)
Salinity	salinity of in situ surface water sample	practical salinity units (PSU)

ORP	oxidation-reduction potential of in situ surface water sample	millivolts (mV)
abs_300	absorbance at 300 nm	unitless
abs_350	absorbance at 350 nm	unitless
abscoefficient300	absorption coefficient at 300 nm	inverse meters (m-1)
abscoefficient350	absorption coefficient at 350 nm	inverse meters (m-1)
Aerobic_counts	total number of bacteria that were culturable in aerobic conditions	number per milliliter (mL-1)
Total_bacteria	total number of bacteria observed under a microscope	number per milliliter (mL-1)
DOC	dissolved organic carbon concentration	milligrams per liter (mg L-1)
Chloro	concentration of chlorophyll pigments	micrograms per liter (microg/L)
K1_ethanol	rate constant for biological degradation of ethanol	inverse minutes (min-1)
K2 _acetaldhyde	rate constant for biological degradation of acetaldehyde modelled from the rate constant for biological degradation of ethanol	inverse minutes (min-1)
K2_acetaldhyde_meas directly	rate constant for biological degradation of acetaldehyde mesaured directly	inverse minutes (min-1)

[table of contents | back to top]

Instruments

Dataset-specific Instrument Name	Shimadzu TOC analyzer
Generic Instrument Name	Elemental Analyzer
Dataset-specific Description	Shimadzu TOC analyzer was used to measure DOC concentrations
Generic Instrument Description	Instruments that quantify carbon, nitrogen and sometimes other elements by combusting the sample at very high temperature and assaying the resulting gaseous oxides. Usually used for samples including organic material.

Dataset-specific Instrument Name	GC/MS; Shimadzu GC-14A/HP5973MSD
Generic Instrument Name	Gas Chromatograph Mass Spectrometer
Dataset-specific Description	Purge and trap gas chromatography mass spectrometry (GC/MS; Shimadzu GC-14A/HP5973MSD) was used to measure acetaldehyde concentrations
Generic Instrument Description	Instruments 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 by a mass spectrometer.

Dataset-specific Instrument Name	Hanna Instruments HI 9829
Generic Instrument Name	Multi Parameter Portable Meter
Dataset-specific Description	Hanna Instruments HI 9829 multiparameter probe was used to measure water quality parameters
Generic Instrument Description	An analytical instrument that can measure multiple parameters, such as pH, EC, TDS, DO and temperature with one device and is portable or hand-held.

Dataset-specific Instrument Name	Horiba Aqualog
Generic Instrument Name	Spectrometer
Dataset-specific Description	Horiba Aqualog spectrometer was used to measure absorbance
Generic Instrument Description	A spectrometer is an optical instrument used to measure properties of light over a specific portion of the electromagnetic spectrum.

[table of contents | back to top]

Project Information

RUI: Collaborative Research: Cycling of ethanol and acetaldyhyde in coastal waters (Coastal Water Cycling)

Coverage: Upper Newport Back Bay estuary in Orange County, Southern California

NSF Award Abstract

Ethanol is added to gasoline to increase octane levels and lower the concentrations of carbon monoxide and surface ozone in the atmosphere. As a renewable fuel, ethanol may also help decrease our dependence on gasoline. Increased use of ethanol in the United States and globally as a fossil fuel substitute and additive is expected to increase ethanol levels in the atmosphere. Atmospheric ethanol is converted to acetaldehyde which is a hazardous pollutant. To understand the impact of increasing ethanol usage, it is important to understand the cycling of ethanol and acetaldehyde in the environment--how they are produced, consumed, and interconverted. Because these compounds can cross from air into water, this requires understanding what happens to these compounds in both the atmosphere and in seawater and other surface waters. This proposal focuses on improving our understanding of processes that produce and consume ethanol and acetaldehyde in coastal seawater and other coastal surface waters like estuaries and salt marshes. This project

will measure the rates of photochemical production of ethanol and acetaldehyde, as well as their chemical and biological degradation rates. The project will also measure the rate and efficiency of the biological production of acetaldehyde from ethanol by microbial organisms in these waters. The scientists have an excellent track record of involving undergraduate students, including underrepresented minorities, in their research and as co-authors on publications, a trend they plan to continue with this project. These students would be trained in analytical chemistry and environmental research and would present their research findings at local and national conferences. Lastly, the PIs also plan outreach activities with high school STEM programs to improve student diversity in environmental research.

The primary sink for ethanol in the troposphere is reaction with OH to produce acetaldehyde. Acetaldehyde levels in the troposphere are also expected to increase with increased use of ethanol. Changes in the atmospheric concentrations of these species are expected to have a significant impact on the oxidative capacity of the troposphere. To understand future impacts, it is important to understand current tropospheric budgets which have significant uncertainties for both species. One of the largest sources of uncertainty is the role of the oceans and surface waters in cycling these species into and out of the troposphere. The current understanding is limited by the very small database of ambient concentration measurements in both air and water and an incomplete insight into the processes that control concentrations in seawater and surface waters; these processes represent a complex interplay between biological and photochemical sources and sinks, and air-water exchange. To improve the current understanding of the cycling of ethanol and acetaldehyde in coastal seawater and surface waters, this project will measure: 1) chemical and biological degradation rates of ethanol and acetaldehyde in coastal waters; 2) the rate and efficiency of the biological production of acetaldehyde from ethanol by microbial organisms; 3) ethanol and acetaldehyde concentrations in air and surface waters; 4) the ethanol and acetaldehyde source strength of estuary and saltmarsh sediments; and 5) ethanol and acetaldehyde photochemical production rates in surface waters.

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-2022112
NSF Division of Ocean Sciences (NSF OCE)	OCE-2022184

[table of contents | back to top]