CDOM and FDOM full-depth Nisken profiles from high-resolution surveys of DOM optical properties conducted during the R/V Melville cruise MV1310 in the Gulf of Alaska (August 4–21, 2013)

Website: https://www.bco-dmo.org/dataset/820932
Version: 0
Version Date: 2020-08-14

Project
» Quantifying the Photochemical Reactivity of Deep Ocean Water (DORC PhotoChem)

Program
» United States Surface Ocean Lower Atmosphere Study (U.S. SOLAS)

Contributors	Affiliation	Role
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Coverage

Spatial Extent: **N**:59 **E**:-129 **S**:48 **W**:-153
Temporal Extent: 2013-08-04 - 2013-08-21

Dataset Description

CDOM and FDOM full-depth Nisken profiles from high-resolution surveys of DOM optical properties conducted during the R/V Melville cruise MV1310 in the Gulf of Alaska (August 4–21, 2013). CDOM and FDOM (w/5 EEMS/PARAFAC components).

This dataset page provides data access for optical data in a data table with select wavelengths and specific calculations. Text files containing each CDOM spectra for every scan used in the optical data table calculations are available in a zip file in the "Data Files" section on this page. [Note 2020-08-17, access to optical data table is pending]

CDOM = colored dissolved organic matter
FDOM = fluorescent dissolved organic matter
EEMS = excitation-emission matrix spectrum
PARAFAC = parallel factor analysis

Methods & Sampling

Location: North Pacific Gulf of Alaska: 48N to 59N and 129W to 153W

Methodology:

Methods are described in detail in the peer reviewed paper Cao et al. (2020).

Sampling and analytical procedures: From Cao et al. (2020):

Sampling: As part of the Deep Ocean Refractory Carbon (DORC) field campaign aboard the R/V Melville in the Gulf of Alaska (August 4–21, 2013) we performed high-resolution surveys of DOM optical properties, collecting samples from the sea surface down to ~5000 m using a 24 Niskin bottle rosette with a Sea-Bird CTD (conductivity-temperature-depth) sensor. Corresponding hydrographic (depth, T, S) and chemical (nitrate, nitrite, ammonia, silicate, phosphate, oxygen) data were collected for each cast and submitted to BCO-DMO (http://data.bco-dmo.org/jg/serv/BCO/NorthPacifi c_RDOC/CTD_Profiles.brev0) by co-chief scientist (D. Hansell, University of Miami). The DOC data corresponding with the optical measurements were also generated in the Hansell lab. For optical measurements, all labware was acid soaked in 2N HCl overnight with glass bottles subsequently precombusted (450C, 3 h minimum), and rinsed thoroughly with Milli-Q water (MQ; >18.2 MΩ·cm; Millipore) that was freshly produced on the ship (within 1 day) prior to sample collection. Seawater was gravity filtered directly from the Niskin bottle via silicon tubing through a pre-cleaned, 0.2 µm Whatman Polycap AS 75 nylon cartridge filter into the glass bottles. Filtered samples were analyzed for optical properties within 4 h after sampling to avoid potential long-term storage artifacts.

Fluorescent measurement of DOM and PARAFAC modeling:

A fluorescent excitation-emission matrix (EEM) spectrum was obtained for each sample with an Aqualog spectrofluorometer (HORIBA Jobin Yvon Inc., NJ, USA) using a 1-cm quartz cell with MQ as the blank. EEM fluorescence intensities were measured by scanning across an excitation range of 240–450 nm (5 nm intervals) and capturing emission spectra over a wavelengths range of 280–500 nm at 3.2 nm intervals. We optimized data quality by determining the integration time for each sample that maximized emission intensity detection at short excitation wavelengths without saturating the CCD at long excitation wavelengths (Gentry-Shields et al., 2013).

CDOM absorption measurement and spectral slope calculations:

CDOM absorption spectra were obtained with filtered samples at room temperature using a single-beam liquid waveguide capillary flow cell (World Precision Instruments Inc., measured at 92.2 cm pathlength), coupled with quartz fiber optic cables to a deuterium-tungsten light source (DT-mini GS) and a MAYA2000 PRO spectrophotometer (Ocean Optics, Inc.). To eliminate contamination from pump tubing, cleaning solutions and samples were pulled slowly through the system using Teflon lines and a peristaltic pump (~0.5 ml/min) located downstream from the waveguide.
The flow cell was cleaned at regular intervals (~every 10 samples) using a rotating valve that sequentially rinsed with a 20:80 vol/vol acetone:water mixture, 2N HCl, and fresh MQ water. In addition, to alleviate the common problem of microbubbles that accumulate on the interior surfaces of the flow cell when analyzing seawater samples, we dissolved bubbles off the cell walls back into degassed MQ supplied through a Liqui-CelTM MM-0.5x1 Series Membrane Contactor (3MTM) attached to an oilless vacuum pump. This was routine after the cleaning sequence and also used when blanks remained high after cleaning or between seawater samples. Removal of microbubbles was confirmed when no measurable change in absorbance was observed due to bubble compression after pressure was applied to the flow cell with MQ using a separate syringe. While this procedure proved excellent for removing attached microbubbles, the internal epoxy used to attach the membranes to the polycarbonate body of the Liqui-CelTM contributed an observable “CDOM-like” absorbance that could not be eliminated through cleaning the cartridge. Consequently, we flushed the system with MQ water after cleaning, degassing, and between samples until no change was observed in the UV portion of the blank spectrum with repeated “re-blanking” of the MAYA2000 signal. This re-blanked MQ reference accounted for instrument drift.

Instruments:

FDOM: Aqualog spectrofluorometer (HORIBA Jobin Yvon Inc., NJ, USA)
CDOM: Single-beam liquid waveguide capillary flow cell (World Precision Instruments Inc., measured at 92.2 cm pathlength), coupled with quartz fiber optic cables to a deuterium-tungsten light source (DT-mini GS) and a

MAYA2000 PRO spectrophotometer (both from Ocean Optics, Inc.).

Data Processing Description

Data processing:

Fluorescent DOM processing and PARAFAC modeling: Post-processing EEM spectra to correct and calibrate the spectra was conducted following Murphy et al. (2010) and included four steps: (1) manufacturer-provided spectral correction parameters were applied to each EEM, (2) inner filter effects were corrected for sample EEMs following Lakowicz (2013), (3) spectra were normalized to the MQ Raman peak area at an excitation wavelength of 350 nm, and (4) MQ Raman and Rayleigh scatter signals were removed using an interpolation method following protocols developed by Bahram et al. (2006). Fluorescence intensities (FI) are herein reported in Raman Units (RU).
A total of 518 samples were pooled for PARAFAC analysis using the DOMFluor toolbox in MATLAB (Stedmon and Bro, 2008). These included survey samples taken directly from vertical profile casts (N = 504) and from shipboard irradiations (see section 2.2) to capture potential components from photo-degraded EEMs measurements (N = 14). Due to higher fluorescent intensities in surface waters relative to deep samples, all EEM spectra were first normalized to unit intensity (i.e., individual fluorescence intensity maxima for each sample was set to 1.0) prior to the modeling process (Murphy et al., 2008). PARAFAC was then applied to the scaled EEM spectra and the model was constructed and further validated using split-half analysis. Once the modeling process was complete, fluorescence intensities were multiplied by their maximum intensities to obtain actual, non-normalized fluorescence intensities for each component in a given sample.

CDOM processing:

Baseline corrections for CDOM absorbance spectra were made by subtracting an offset value that corrects for scattering and refractive index differences between seawater and the MQ blank as described in Reader and Miller (2011). Our capillary waveguide produced a small, reproducible optical resonance (~0.002 m-1) centered close to zero absorbance at the longer wavelengths typically used for blank corrections (e.g., 700–800 nm). We chose to determine our offset value by fitting the raw absorbance spectra between 630 and 640 nm with a nonlinear fitting routine (“nlinfit” function, MATLAB® 2016 Statistics Toolbox; MathWorks, MA) to (Reader and Miller, 2011): $A = Fe\text{-}s\lambda + O$
where A is the CDOM absorbance, F is a fitting parameter, S is the spectral slope coefficient, and O is a specific offset value obtained for each sample. We then calculated the corrected CDOM absorbance spectrum by normalizing the raw absorbance spectrum using this offset value and converting to a Napierian absorption coefficient spectrum according to: $ag(\lambda) = 2.303 \times A(\lambda) / L$
where $ag(\lambda)$ (m-1) is the Napierian absorption coefficient of CDOM at wavelength λ, $A(\lambda)$ (unitless) is the offset-corrected CDOM absorbance at λ, and L (m) is the pathlength (0.922 m).
The specific ultraviolet absorbance (SUVA254, L mg-1 m-1) can be calculated by dividing ag(254) by the DOC concentration (Weishaar et al., 2003), reported by Hansell and associated with this project as cited above. The CDOM spectral slope coefficient (S) for the spectral range 275–295 nm, hereafter referred to as S275-295, can be determined by calculating the slope of the log-transformed linear regression over the wavelength interval of 275–295 nm (Helms et al., 2008).

BCO-DMO data manager processing notes:
* Spectra text files attached to Dataset Landing page in the "Data Files" section
* Optical data table is not yet available from this page, communicating with data submitter about parameter descriptions and content.

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Data Files

File
CDOM spectral scan text files filename: DORC_CDOM_Survey_Data.zip (ZIP Archive (ZIP), 13.18 MB) MD5:7613c5e079505730f434f8d7aa4b7916 NOTES FOR CDOM DATA (SpectraSuite Data Files): Each spectral scan is a txt file identified with an 11 character string as follows: xxyyzzcdom#.txt xx = station number yy = cast number (some stations had multiple casts as noted in CTD data set; either 01 or 02) zz = bottle number cdom = designator for absorbance spectrum # = replicate scan (range 1-4) Each scan contains spectral data from 198.46 to 1125.99 (full spectral scan 2068 pixels) data begins on line 18 The header (lines 1-17) provide a date and time stamp, as well as settings for the Ocean Optics Maya spectrometer.

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Related Publications

Bahram, M., Bro, R., Stedmon, C., & Afkhami, A. (2006). Handling of Rayleigh and Raman scatter for PARAFAC modeling of fluorescence data using interpolation. Journal of Chemometrics, 20(3-4), 99–105. doi:10.1002/cem.978
Methods

Cao, F., Zhu, Y., Kieber, D. J., & Miller, W. L. (2020). Distribution and photo-reactivity of chromophoric and fluorescent dissolved organic matter in the Northeastern North Pacific Ocean. Deep Sea Research Part I: Oceanographic Research Papers, 155, 103168. doi:10.1016/j.dsr.2019.103168
Results

Gentry-Shields, J., Wang, A., Cory, R. M., & Stewart, J. R. (2013). Determination of specific types and relative levels of QPCR inhibitors in environmental water samples using excitation–emission matrix spectroscopy and PARAFAC. Water Research, 47(10), 3467–3476. doi:10.1016/j.watres.2013.03.049
Methods

Helms, J. R., Stubbins, A., Ritchie, J. D., Minor, E. C., Kieber, D. J., & Mopper, K. (2008). Absorption spectral slopes and slope ratios as indicators of molecular weight, source, and photobleaching of chromophoric dissolved organic matter. Limnology and Oceanography, 53(3), 955–969. doi:10.4319/lo.2008.53.3.0955
Methods

Lakowicz, J. R. (2013). Principles of Fluorescence Spectroscopy. New York, NY: Springer. https://isbnsearch.org/isbn/9781461576587
Methods

Murphy, K. R., Butler, K. D., Spencer, R. G. M., Stedmon, C. A., Boehme, J. R., & Aiken, G. R. (2010). Measurement of Dissolved Organic Matter Fluorescence in Aquatic Environments: An Interlaboratory Comparison. Environmental Science & Technology, 44(24), 9405–9412. doi:10.1021/es102362t
Methods

Reader, H. E., & Miller, W. L. (2011). Effect of estimations of ultraviolet absorption spectra of chromophoric dissolved organic matter on the uncertainty of photochemical production calculations. Journal of Geophysical

Research, 116(C8). doi:10.1029/2010jc006823 https://doi.org/10.1029/2010JC006823
Methods

Stedmon, C. A., & Bro, R. (2008). Characterizing dissolved organic matter fluorescence with parallel factor analysis: a tutorial. Limnology and Oceanography: Methods, 6(11), 572–579. doi:10.4319/lom.2008.6.572b
Methods

Weishaar, J. L., Aiken, G. R., Bergamaschi, B. A., Fram, M. S., Fujii, R., & Mopper, K. (2003). Evaluation of Specific Ultraviolet Absorbance as an Indicator of the Chemical Composition and Reactivity of Dissolved Organic Carbon. Environmental Science & Technology, 37(20), 4702–4708. doi:10.1021/es030360x
Methods

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Related Datasets

IsSupplementedBy

Hansell, D. (2014) **CTD profile data from R/V Melville cruise MV1310 in the North Pacific Gulf of Alaska; 48N to 59N and 129W to 153W in 2013 (North Pacific RDOC project).** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2014-09-02
http://lod.bco-dmo.org/id/dataset/527102 [view at BCO-DMO]
Relationship Description: Corresponding hydrographic (depth, T, S) and chemical (nitrate, nitrite, ammonia, silicate, phosphate, oxygen) data for each cast.

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Parameters

Parameters for this dataset have not yet been identified

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Instruments

Dataset-specific Instrument Name	Aqualog spectrofluorometer (HORIBA Jobin Yvon Inc., NJ, USA)
Generic Instrument Name	Fluorometer
Dataset-specific Description	FDOM: Aqualog spectrofluorometer (HORIBA Jobin Yvon Inc., NJ, USA)
Generic Instrument Description	A fluorometer or fluorimeter is a device used to measure parameters of fluorescence: its intensity and wavelength distribution of emission spectrum after excitation by a certain spectrum of light. The instrument is designed to measure the amount of stimulated electromagnetic radiation produced by pulses of electromagnetic radiation emitted into a water sample or in situ.

Dataset-specific Instrument Name	MAYA2000 PRO spectrophotometer
Generic Instrument Name	Spectrophotometer
Dataset-specific Description	CDOM: Single-beam liquid waveguide capillary flow cell (World Precision Instruments Inc., measured at 92.2 cm pathlength), coupled with quartz fiber optic cables to a deuterium-tungsten light source (DT-mini GS) and a MAYA2000 PRO spectrophotometer (both from Ocean Optics, Inc.).
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	MAYA2000 PRO spectrophotometer (Ocean Optics, Inc.)
Generic Instrument Name	Spectrophotometer
Dataset-specific Description	CDOM: Single-beam liquid waveguide capillary flow cell (World Precision Instruments Inc., measured at 92.2 cm pathlength), coupled with quartz fiber optic cables to a deuterium-tungsten light source (DT-mini GS) and a MAYA2000 PRO spectrophotometer (both from Ocean Optics, Inc.).
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.

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Deployments

MV1310

Website	https://www.bco-dmo.org/deployment/526876
Platform	R/V Melville
Report	http://dmoserv3.whoi.edu/data_docs/NorthPacific_RDOC/MV1310_Preliminary_Report_2.pdf
Start Date	2013-08-04
End Date	2013-08-23
Description	Original data are available from the NSF R2R data catalog

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Project Information

Quantifying the Photochemical Reactivity of Deep Ocean Water (DORC PhotoChem)

Coverage: Sub-Arctic Pacific, Gulf of Alaska, Line P

NSF award abstract:

NSF award abstract:
Because 70% of marine dissolved organic carbon (DOC) is found in the deep ocean, it is important to determine its sources and sinks to understand its role in the global carbon cycle. Unfortunately, the sinks for DOC at depth remain largely unknown; however, limited data has suggested that photochemistry may influence the removal of deep refractory DOC. A scientist from the University of Georgia will use field and laboratory irradiation experiments to quantify the photochemical rates controlling (1) direct loss of DOC and photoproduction of carbon monoxide, a significant product resulting from DOC oxidation, (2) common optical tracers of organic carbon such as colored dissolved organic matter and fluorescent dissolved organic matter fading; and (3) two reactive oxygen species (hydrogen peroxide and superoxide) that reflect the role of oxygen in DOC photochemistry. The study will focus on the north Pacific, where the lowest deep ocean DOC concentrations are found which most likely reflect the presence of an aged and refractory carbon pool. Layered in the top 1000m above this deep DOC is a concentration gradient that will allow comparison of waters with different DOC concentrations, ages and apparent refractivity. Results from the study will be used to quantitatively reevaluate this basic question that now constrains global DOC models: Does photochemistry have a significant role in the removal of the massive amount of refractory DOC that is pooled in the deep sea?

In terms of the broader impacts, based on established links with K-12 teachers, the scientist and his students plan visits to local schools to present their science, as well as have a website entitled "ask the oceanographer" and maintain a live blog during their cruise. Results from this study will be included into class materials dealing with the carbon cycle. One graduate and three undergraduate students would be supported and trained as part of this project. It is anticipated that undergraduate students from historically underrepresented groups would be recruited via the University of Georgia's Summer Undergraduate Research Program.

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Program Information

United States Surface Ocean Lower Atmosphere Study (U.S. SOLAS)

Website: http://www.us-solas.org/

Coverage: Global

The Surface Ocean Lower Atmosphere Study (SOLAS) program is designed to enable researchers from different disciplines to interact and investigate the multitude of processes and interactions between the coupled ocean and atmosphere.

Oceanographers and atmospheric scientists are working together to improve understanding of the fate, transport, and feedbacks of climate relevant compounds, and also weather and hazards that are affected by processes at the surface ocean.

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Physical, chemical, and biological research near the ocean-atmosphere interface must be performed in synergy to extend our current knowledge to adequately understand and forecast changes on short and long time frames and over local and global spatial scales.

The findings obtained from SOLAS are used to improve knowledge at process scale that will lead to better quantification of fluxes of climate relevant compounds such as CO2, sulfur and nitrogen compounds, hydrocarbons and halocarbons, as well as dust, energy and momentum. This activity facilitates a fundamental understanding to assist the societal needs for climate change, environmental health, weather prediction, and national security.

The US SOLAS program is a component of the International SOLAS program where collaborations are forged with investigators around the world to examine SOLAS issues ubiquitous to the world's oceans and atmosphere.

Â» International SOLAS Web site

Science Implementation Strategy Reports

US-SOLAS (4 MB PDF file)
Other SOLAS reports are available for download from the US SOLAS Web site

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1234388

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