Estimation of the parameters of a simple model of thorium and particle cycling in the ocean water column, based on a fit to radionuclide and particle data from the US GEOTRACES North Atlantic Section (GA03)

Website: https://www.bco-dmo.org/dataset/721940
Data Type: model results
Version:
Version Date: 2018-02-26

Project
» Selecting and Applying an Inverse Method to Infer Particle Dynamics from GEOTRACES Data (GEOTRACES Particle Dynamics)

Contributors	Affiliation	Role
Marchal, Olivier	Woods Hole Oceanographic Institution (WHOI)	Principal Investigator
Lam, Phoebe J.	University of California-Santa Cruz (UCSC)	Co-Principal Investigator
Lerner, Paul	Woods Hole Oceanographic Institution (WHOI)	Co-Principal Investigator, Contact
York, Amber D.	Woods Hole Oceanographic Institution (WHOI BCO-DMO)	BCO-DMO Data Manager

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Dataset Description

This dataset contains model code and output from a thorium and particle cycling model.

The model code and documentation are available for download as a .zip file: Lerner_Th_P_InverseModel.zip (2.6 MB)

Model output data are available by clicking the "Get Data" button above. These data are parameter estimates from fitting the model to radionuclide and particle data from the US GEOTRACES North Atlantic Section, not samples collected in the field.

Both the model and inverse method are described in detail in the model manual "Manual of Matlab Code: Nonlinear Inversion of Thorium and Particle Data," as well as in Lerner et al., 2017. This document describes how to use the routine submitted here to fit a 1-d thorium and particle cycling model to radionuclide and particle data

These data and model were published in:

Lerner, P., Marchal, O., Lam, P. J., Buesseler, K., and Charette, M. (2017). Kinetics of thorium and particle cycling along the US GEOTRACES North Atlantic Transect. Deep Sea Research Part I: Oceanographic Research Papers, 125, 106-128, Fig. 12, Supplementary Figs. S1-S3. doi: 10.1016/j.dsr.2017.05.003

Methods & Sampling

Location: The model is fit to 228,230,234Th, 234,238U, 228Ra, and particle concentration data collected from a section from Bermuda to a station just off the coast of Mauritania. The section crosses the Mid-Atlantic Ridge and the southeastern portion of the North Atlantic Subtropical gyre. The locations and depth ranges of data used to estimate model parameters are listed below (Table 1 of Lerner et al., 2017).

Data: The thorium and particle cycling model is fit to radionuclide and particle data from the US GEOTRACES North Atlantic Section (GA03). The following lists these data, along with their associated references, in which analytical methods associated with these data are published. The subscript "p" denotes particulate data and "d" denotes "dissolved" data, where particulate and dissolved material are separated by filters with a pore size of 0.8 µm. These data have all been submitted to BCO-DMO, and all except 228Th are published. These data are also available as part of the GEOTRACES Intermediate Data Product (Mawji et al., 2014).

234,238U (obtained from salinity) - Owens et al., 2011 (available in datasets of project: https://www.bco-dmo.org/project/2066)

234Thd,p (dpm m-3) - Owens et al., 2015 (available in datasets of project: https://www.bco-dmo.org/project/2066)

230Thd (dpm m-3) - Hayes et al., 2015a (available in dataset https://www.bco-dmo.org/dataset/3847)

230Thp (dpm m-3) - Hayes et al., 2015b (available in dataset https://www.bco-dmo.org/dataset/3847)

228Ra (dpm m-3) - Charrette et al., 2015 (available in dataset https://www.bco-dmo.org/dataset/3847)

228Thd,p (dpm m-3) - unpublished (available on BCO-DMO dataset page: http://lod.bco-dmo.org/id/dataset/3846, Charrette et al., 2014)

Particle concentration (mg m-3) - Lam et al., 2015 (available in dataset https://www.bco-dmo.org/dataset/3871)

The depths at which the radiochemical and particle data are available do not generally coincide. Hence, at each station, an objective interpolation procedure was used to interpolate the data onto an irregular grid (the grid varies with each station and the range of the grid is the same as the "depth range"). This procedure is described in detail in section 2.4 of Lerner et al., 2016.

Inverse Method: The algorithm used to fit the model (eqs. 1-3 available in the model manual) to the radionuclide and particle data is a nonlinear programming technique as implemented in Matlab's FMINCON (Matlab R2016b), a constrained optimization routine used to solve nonlinear problems. This algorithm takes as its argument a vector $\boldsymbol{x}0$ containing radionuclide activities, particle concentration, and prior estimates of the rate parameters (parameters listed in "Parameter names…" section, all at different depths of the model grid, as well as an error covariance matrix, **C0**, whose diagonal elements are the variances in $\boldsymbol{x}0$ and whose off-diagonal elements are the error covariances in $\boldsymbol{x}0$. FMINCON seeks a vector $\boldsymbol{x}$ which both perfectly satisfies the model (that is, the rhs of equations (1-3) equal 0 when a solution is found), and fits radionuclide and particle concentration data, as well as prior estimates of rate parameters, in a least squares sense, with due consideration for the errors in the data and in the estimates (see equation Further details on the procedure used by FMINCON are reported in Byrd et al. (2000) and Waltz et al. (2005).

For more detail see the model manual "Manual of Matlab Code: Nonlinear Inversion of Thorium and Particle Data."

Data Processing Description

Problem report: Beyond issue with gaps in previously reported radionuclide and particle measurements, there are no known issues with rate parameters and routine provided.

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Data Files

File	
Lerner_Th_P_model_parameters.csv	(Comma Separated Values (.csv), 47.04 KB) MD5:255db65cd9ef4f3727649edee86d8f2a
Primary data file for dataset ID 721940	

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Related Publications

Byrd, R. H., Gilbert, J. C., & Nocedal, J. (2000). A trust region method based on interior point techniques for nonlinear programming. Mathematical Programming, 89(1), 149–185. doi:10.1007/pl00011391 https://doi.org/10.1007/PL00011391
Methods

Charette, M. A., Morris, P. J., Henderson, P. B., & Moore, W. S. (2015). Radium isotope distributions during the US GEOTRACES North Atlantic cruises. Marine Chemistry, 177, 184–195. doi:10.1016/j.marchem.2015.01.001
Results

Hayes, C. T., Anderson, R. F., Fleisher, M. Q., Huang, K.-F., Robinson, L. F., Lu, Y., … Moran, S. B. (2015a). 230Th and 231Pa on GEOTRACES GA03, the U.S. GEOTRACES North Atlantic transect, and implications for modern and paleoceanographic chemical fluxes. Deep Sea Research Part II: Topical Studies in Oceanography, 116, 29–41. doi:10.1016/j.dsr2.2014.07.007
Results

Hayes, C. T., Anderson, R. F., Fleisher, M. Q., Vivancos, S. M., Lam, P. J., Ohnemus, D. C., … Moran, S. B. (2015). Intensity of Th and Pa scavenging partitioned by particle chemistry in the North Atlantic Ocean. Marine Chemistry, 170, 49–60. doi:10.1016/j.marchem.2015.01.006
Results

Lam, P. J., Ohnemus, D. C., & Auro, M. E. (2015). Size-fractionated major particle composition and concentrations from the US GEOTRACES North Atlantic Zonal Transect. Deep Sea Research Part II: Topical Studies in Oceanography, 116, 303–320. doi:10.1016/j.dsr2.2014.11.020
Results

Lerner, P., Marchal, O., Lam, P. J., Anderson, R. F., Buesseler, K., Charette, M. A., … Solow, A. (2016). Testing models of thorium and particle cycling in the ocean using data from station GT11-22 of the U.S. GEOTRACES North Atlantic section. Deep Sea Research Part I: Oceanographic Research Papers, 113, 57–79. doi:10.1016/j.dsr.2016.03.008
Methods

Lerner, P., Marchal, O., Lam, P. J., Buesseler, K., & Charette, M. (2017). Kinetics of thorium and particle cycling along the U.S. GEOTRACES North Atlantic Transect. Deep Sea Research Part I: Oceanographic Research Papers, 125, 106–128. doi:10.1016/j.dsr.2017.05.003
Results
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Matlab (2016), Optimization Toolbox (r2016a), User's guide, The Mathworks, Inc., http://ww.mathworks.com/help/optim/, accessed: 22 July, 2016.
Software

Mawji, E., Schlitzer, R., Dodas, E. M., Abadie, C., Abouchami, W., Anderson, R. F., … Bates, N. R. (2015). The GEOTRACES Intermediate Data Product 2014. Marine Chemistry, 177, 1–8. doi:10.1016/j.marchem.2015.04.005
Results

Owens, S. A., Buesseler, K. O., & Sims, K. W. W. (2011). Re-evaluating the 238U-salinity relationship in seawater: Implications for the 238U–234Th disequilibrium method. Marine Chemistry, 127(1-4), 31–39. doi:10.1016/j.marchem.2011.07.005
Results

Owens, S. A., Pike, S., & Buesseler, K. O. (2015). Thorium-234 as a tracer of particle dynamics and upper ocean export in the Atlantic Ocean. Deep Sea Research Part II: Topical Studies in Oceanography, 116, 42–59. doi:10.1016/j.dsr2.2014.11.010
Results

Waltz, R. A., Morales, J. L., Nocedal, J., & Orban, D. (2005). An interior algorithm for nonlinear optimization that

combines line search and trust region steps. Mathematical Programming, 107(3), 391–408. doi:10.1007/s10107-004-0560-5
Methods

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Parameters

Parameter	Description	Units
CRUISE	Cruise identifier	unitless
Station_ID	Station identifier	unitless
STATION	Station number (same as station ID)	unitless
LAT	Latitude	decimal degrees
LONG	Longitude	decimal degrees
DEPTH	Water column depth	meters (m)
Th_absorp	Thorium adsorption rate	per year (yr -1)
Th_absorp_1sd	One standard deviation of the Thorium adsorption rate	per year (yr -1)
Th_desorp	Thorium desorption rate	per year (yr -1)
Th_desorp_1sd	One standard deviation of the Thorium desorption rate	per year (yr -1)
particle_degred	Particle degradation rate	per year (yr -1)
particle_degred_1sd	One standard deviation of the Particle degradation rate	per year (yr -1)
partile_sink_speed	Particle sinking speed	per year (yr -1)
particle_sink_speed_1sd	One standard deviation of the Particle sinking speed	meters per year (m/yr)

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Deployments

KN199-04

Website	https://www.bco-dmo.org/deployment/58066
Platform	R/V Knorr
Report	http://bcodata.whoi.edu/US_GEOTRACES/AtlanticSection/Cruise_Report_for_Knorr_199_Final_v3.pdf
Start Date	2010-10-15
End Date	2010-11-04
Description	This cruise constitutes the first survey section as part of the U.S. participation in an international program named GEOTRACES. Funding: NSF OCE award 0926423 Science Objectives: To obtain state of the art trace metal and isotope measurements on a suite of samples taken on a mid-latitude zonal transect of the North Atlantic. In particular, sampling targeted the oxygen minimum zone extending off the west African coast near Mauritania, the TAG hydrothermal field, and the western boundary current system along Line W. For additional information, please refer to the GEOTRACES program Web site (https://www.geotraces.org/) for overall program objectives and a summary of properties measured. Science Activities include seawater sampling via GoFLO and Niskin carousels, in situ pumping (and filtration), CTDO2 and transmissometer sensors, underway pumped sampling of surface waters, and collection of aerosols and rain. Hydrography, CTD and nutrient measurements were supported by the Ocean Data Facility (J. Swift) at Scripps Institution of Oceanography and funded through NSF Facilities. They provided an additional CTD rosette system along with nephelometer and LADCP. A trace metal clean Go-Flo Rosette and winch were provided by the group at Old Dominion University (G. Cutter) along with a towed underway pumping system. Additional cruise information is available from the Rolling Deck to Repository (R2R): https://www.rvdata.us/search/cruise/KN199-04 Other Relevant Links: List of cruise participants: [PDF] Cruise track: JPEG image (from Woods Hole Oceanographic Institution, vessel operator) ADCP data are available from the Currents ADCP group at the University of Hawaii: KN199-04 ADCP

KN204-01

Website	https://www.bco-dmo.org/deployment/58786
Platform	R/V Knorr
Report	http://bcodata.whoi.edu/US_GEOTRACES/AtlanticSection/STS_Prelim_GT11_Doc.pdf
Start Date	2011-11-06
End Date	2011-12-11
Description	The US GEOTRACES North Atlantic cruise aboard the R/V Knorr completed the section between Lisbon and Woods Hole that began in October 2010 but was rescheduled for November-December 2011. The R/V Knorr made a brief stop in Bermuda to exchange samples and personnel before continuing across the basin. Scientists disembarked in Praia, Cape Verde, on 11 December. The cruise was identified as KN204-01A (first part before Bermuda) and KN204-01B (after the Bermuda stop). However, the official deployment name for this cruise is KN204-01 and includes both part A and B. Science activities included: ODF 30 liter rosette CTD casts, ODU Trace metal rosette CTD casts, McLane particulate pump casts, underway sampling with towed fish and sampling from the shipboard "uncontaminated" flow-through system. Full depth stations are shown in the accompanying figure (see below). Additional stations to sample for selected trace metals to a depth of 1000 m are not shown. Standard stations are shown in red (as are the ports) and "super" stations, with extra casts to provide large-volume samples for selected parameters, are shown in green. Station spacing is concentrated along the western margin to evaluate the transport of trace elements and isotopes by western boundary currents. Stations across the gyre will allow scientists to examine trace element supply by Saharan dust, while also contrasting trace element and isotope distributions in the oligotrophic gyre with conditions near biologically productive ocean margins, both in the west, to be sampled now, and within the eastern boundary upwelling system off Mauritania, sampled last year. Funding: The cruise was funded by NSF OCE awards 0926204, 0926433 and 0926659. Additional cruise information is available from the Rolling Deck to Repository (R2R): https://www.rvdata.us/search/cruise/KN204-01 Other Relevant Links: ADCP data are available from the Currents ADCP group at the University of Hawaii at the links below: KN204-01A (part 1 of 2011 cruise; Woods Hole, MA to Bermuda) KN204-01B (part 2 of 2011 cruise; Bermuda to Cape Verde)

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Project Information

Selecting and Applying an Inverse Method to Infer Particle Dynamics from GEOTRACES Data (GEOTRACES Particle Dynamics)

NSF abstract:

Processes affecting ocean particles have important consequences for the marine biogeochemical cycles of trace elements; however, our present understanding of these processes is incomplete, as shown by the very large uncertainties (spanning orders of magnitude) of current estimates of particle cycling rates in the ocean. The extensive trace element dataset being generated as part of the GEOTRACES program provides an opportunity to enhance our knowledge of particle processes in a variety of oceanic environments. A scientist from Woods Hole Oceanographic Institution plans to determine the adequacy of different inverse methods to constrain particle processes such as solid-solution exchange and particle processes in the water column from measurements of thorium isotope activity, particle composition, and particle concentration in different size fractions. To attain this goal, the researcher would first assess the adequacy of different inverse methods to infer, from such an eclectic dataset, rate constants of sorption reactions (adsorption and desorption) and particle dynamics (aggregation, disaggregation, sinking, and remineralization). The second step would involve applying the selected method to estimate these constants and their uncertainties at the "superstations" of the GEOTRACES North Atlantic Zonal Section. Once the model is in place, the scientist would test the hypotheses that the rate constants varied (1) vertically within the mesopelagic layer and the deeper layers at these stations and (2) horizontally across the diverse environments sampled along the section.

Broader Impacts: The software to be developed would be archived with the Biological and Chemical

Oceanography Data Management Office with instructions so other scientist can use it. One graduate student would be trained on the use of inverse methods in data analyses.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1232578

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