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The GEOTRACES Intermediate Data Product 2014

The GEOTRACES Group

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ABSTRACT

The GEOTRACES Intermediate Data Product 2014 (IDP2014) is the first publicly available data product of the international GEOTRACES programme, and contains data measured and quality controlled before the end of 2013. It consists of two parts: (1) a compilation of digital data for more than 200 trace elements and isotopes (TEIs) as well as classical hydrographic parameters, and (2) the *eGEOTRACES Electronic Atlas* providing a strongly inter-linked on-line atlas including more than 300 section plots and 90 animated 3D scenes. The IDP2014 covers the Atlantic, Arctic, and Indian oceans, exhibiting highest data density in the Atlantic. The TEI data in the IDP2014 are quality controlled by careful assessment of intercalibration results and multi-laboratory data comparisons at cross-over stations. The digital data are provided in several formats, including ASCII spreadsheet, Excel spreadsheet, netCDF, and Ocean Data View collection. In addition to the actual data values the IDP2014 also contains data quality flags and 1-σ data error values where available. Quality flags and error values are useful for data filtering. Metadata about data originators, analytical methods and original publications related to the data are linked to the data in an easily accessible way. The *eGEOTRACES Electronic Atlas* is the visual representation of the IDP2014 data providing section plots and a new kind of animated 3D scenes. The basin-wide 3D scenes allow for viewing of data from many cruises at the same time, thereby providing quick overviews of large-scale tracer distributions. In addition, the 3D scenes provide geographical and bathymetric context that is crucial for the interpretation and assessment of observed tracer plumes, as well as for making inferences about controlling processes.

1. Introduction

GEOTRACES is an international study of the marine biogeochemical cycles of trace elements and their isotopes (TEIs), designed by marine geochemists to accelerate TEI research under a global program. Combining ocean sections, process studies, data synthesis, and modelling, GEOTRACES will identify and quantify the processes that supply TEIs at ocean boundaries as well as the physical and biological processes that redistribute TEIs within and between ocean basins (Anderson et al., 2014; SCOR Working Group, 2007; GEOTRACES, 2006; Anderson and Henderson, 2005; Frank et al., 2003; http://www.geotraces.org/).

GEOTRACES decided in 2011 to create and release the *GEOTRACES Intermediate Data Product 2014* (IDP2014). The main motivation was to not wait until the end of the programme to issue a final data product, but instead to create and release a first intermediate data product at a time when the programme is very active and still expanding, both in terms of observational activities as well as the scientific analysis of the data produced so far. By releasing and sharing the data at an early stage, GEOTRACES intends not only to strengthen and intensify collaboration within the geochemical community itself, but also to attract and invite colleagues from other communities, such as physical and biological oceanography, as well as modelling, to apply their unique knowledge and skills to marine geochemical problems.

Realising that building-up and strengthening multi-disciplinary collaboration takes time, GEOTRACES from its beginning has stimulated cross-disciplinary collaboration by organising a series of data/model synergy workshops (6–8 September 2007, Hanse Wissenschaftskolleg, Delmenhorst, Germany; 7–10 December 2009, École Normale Supérieure, Paris, France; 14–17 November 2011, Universitat Autònoma de Barcelona, Spain). The release of the IDP2014 now provides the extensive and high-quality observational dataset needed for conducting the many new collaborative projects and modelling studies initially discussed at these workshops and aimed at improving our understanding of the cycling of TEIs in the ocean and quantifying respective sources and sinks (GEOTRACES, 2006).

The IDP2014 is the result of a community effort and would not exist without the successful collaboration of a large part of the marine geochemical community within GEOTRACES and the willingness of participating scientists to release their published and even unpublished data as part of this product. In a field where sampling, measurement and calibration of the various tracers involve highly specialised skills and can only be achieved by few laboratories world-wide, this degree of collaboration, openness and sharing of data is exceptional.

The IDP2014 consists of two parts: (1) the digital data compilation of trace elements and isotopes (TEIs) as well as classic hydrographic parameters and (2) the *eGEOTRACES Electronic Atlas* providing section plots and animated 3D scenes of the data.

2. IDP2014 digital data

The IDP2014 digital data package consists of two datasets: (1) the CTD sensor data and (2) the discrete sample dataset containing the TEI data. Both datasets include data from 15 cruises conducted in the 5-year period from 2007 to 2012 (Table 1). These cruises cover the Arctic, Atlantic and Indian oceans (Fig. 1). The best coverage and highest station density are found in the Atlantic. In addition to GEOTRACES Sections, GA02, GA03, GA10, GA11, and GI04, the IDP2014 also includes data from the GEOTRACES compliant cruise GAc01 (CoFeMUG) and five cruises GIPY2, GIPY4, GIPY5, GIPY6, and GIPY11, which were conducted as part of the International Polar Year (for an overview of IPY activities see: http://www.icsu.org/publications/reports-and-reviews/ipy-summary). Links to the cruise reports of all cruises are provided in Table 2.

The CTD sensor dataset contains temperature, salinity, oxygen, fluorescence, transmissometer, turbidity, and photosynthetically-active radiation (PAR) data at 1126 stations at 1 meter vertical resolution. The fluorescence and transmissometer data provide information on phytoplankton abundance and suspended particle concentrations and are thus important for the interpretation of TEI data. Where calibrated data were not available, raw values are provided. These uncalibrated data are still useful as they reveal the relative magnitude and vertical extent of phytoplankton and suspended particle features.

The IDP2014 discrete sample dataset contains data for 796 stations. Of these stations, 693 provide full-depth coverage of the water column. There are data for a total number of 237 parameters, including (1) classic hydrographic parameters and tracers such as temperature, salinity, oxygen, nutrients, CFCs, SF6, Tritium, and He-3, (2) dissolved and particulate trace elements such as Al, Ba, Cd, Cu, Fe, Mn, Mo, Ni, Pb, Zn and Rare Earth Elements (REEs), (3) stable isotopes such as H-2, C-13, N-15, O-18, Si-30, Fe-56, Cd-110, Cd-114, and Nd-143 as well as (4) - radioactive isotopes like Pb-210, Po-210, Th-230, Pa-231, Th-232, and Th-234.

Table 1
List of cruises included in the GEOTRACES Intermediate Data Product 2014. Suffixes (n), (s), (w), (e), and (c) indicate northern, southern, western, eastern or central parts of a section.

Section	Cruise	Chief scientist	Country	Start date	End date
GA02 (n)	PE319	Gerringa, Loes	Netherlands	28-Apr-2010	26-May-2010
GA02 (c)	PE321	Rijkenberg, Micha	Netherlands	11-Jun-2010	08-Jul-2010
GA02 (s)	JC057	Rijkenberg, Micha	Netherlands	01-Mar-2011	07-Apr-2011
GA03 (e)	KN199-4	Jenkins, William	USA	15-Oct-2010	04-Nov-2010
GA03 (w)	KN204-1	Boyle, Edward	USA	06-Nov-2011	11-Dec-2011
GA10 (e)	D357	Henderson, Gideon	UK	18-Oct-2010	22-Nov-2010
GA10 (w)	JC068	Henderson, Gideon	UK	24-Dec-2011	27-Jan-2012
GA11	M81_1	Frank, Martin	Germany	04-Feb-2010	08-Mar-2010
GAc01	KN192-5	Saito, Mak	USA	16-Nov-2007	13-Dec-2007
GI04	KH09-05	Gamo, Toshitaka	Japan	06-Nov-2009	10-Jan-2010
GIPY2	AU0703	Griffiths, Brian	Australia	21-Jan-2007	19-Feb-2007
GIPY4	MD166	Speich, Sabrina	France	08-Feb-2008	24-Mar-2008
GIPY5	ANTXXIV/3	Fahrbach, Eberhard	Germany	06-Feb-2008	16-Apr-2008
GIPY6	AU0806	Rintoul, Steve	Australia	22-Mar-2008	17-Apr-2008
GIPY11	ARKXXII/2	Schauer, Ursula	Germany	29-Jul-2007	07-Oct-2007

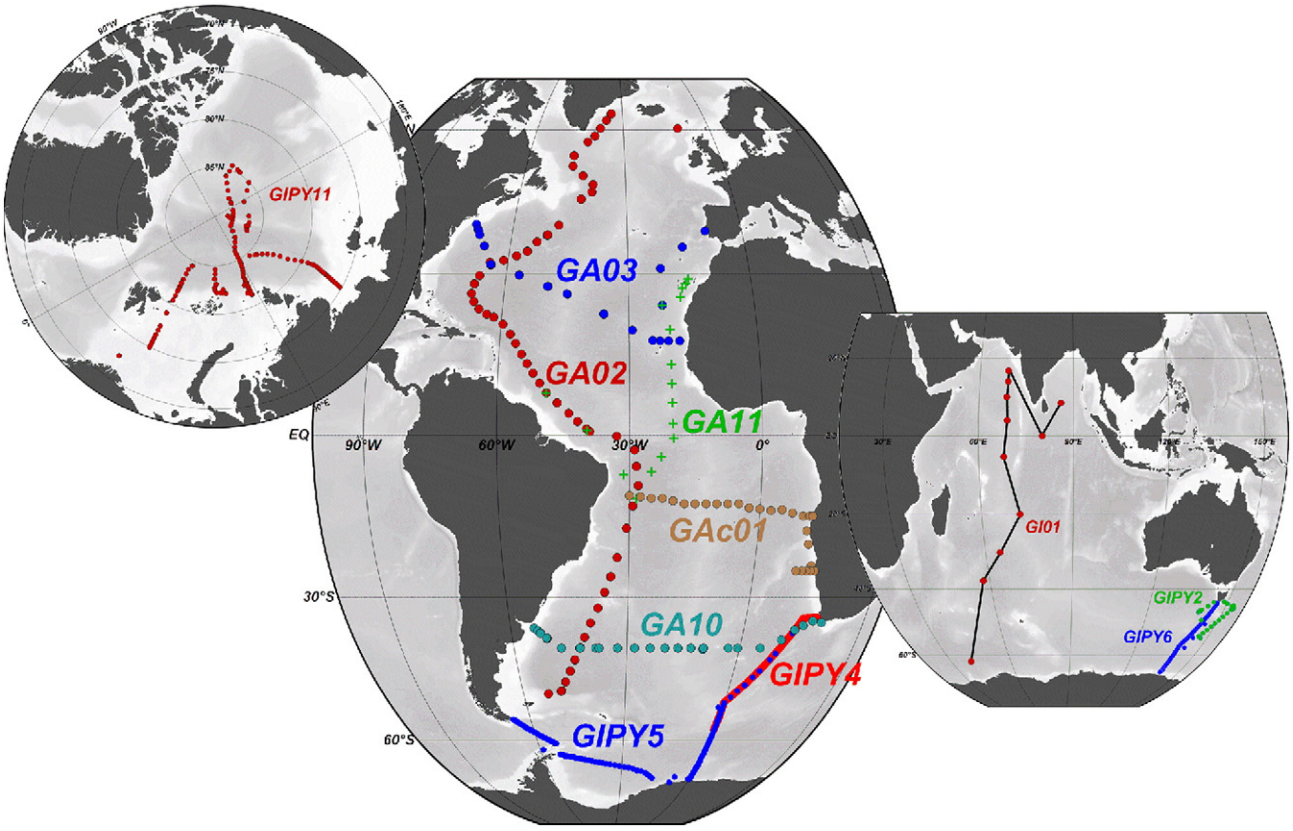


Fig. 1. Map of stations included in the GEOTRACES Intermediate Data Product 2014.

The 796 stations include a total number of 27,366 discrete samples. The average number of depths sampled at each station is 34 but reached up to 182 depths at heavily sampled "super" stations. Table 3 summarises the number of observations for GEOTRACES key parameters, including micronutrients essential to life in the ocean (e.g., Fe, Zn, Cd, Cu), tracers of modern processes in the ocean (e.g., Al, Mn, N-15), tracers significantly perturbed by human activities (e.g., Pb), and tracers used as proxies to reconstruct the past (e.g., Th-230, Pa-231, Nd isotopes). Data for micronutrients are most abundant, with the total number of Fe measurements amounting to 6715, 4840 of which are for dissolved Fe alone. There are almost 2500 data values for the radioactive isotope Th-234 and almost 1000 values for Th-230 and Pa-231.

This is, however, an "intermediate" product, and there is clearly a significant amount of further data to come from GEOTRACES cruises, both those represented in the IDP2014, and those more recently completed or planned. The IDP2014 contains only those data that were completed and submitted before the cut-off date of December 2013. Further data will be included in subsequent intermediate products (as detailed below) and will significantly augment the data coverage represented in IDP2014.

The GEOTRACES Standards and Intercalibration Committee reviewed all key GEOTRACES TEI data for the IDP2014 following procedures developed as part of the 2008–2010 Intercalibration programme (Cutter, 2013) and the results from the GEOTRACES Intercalibration programme can be found in a special issue of Limnology & Oceanography Methods http://www.aslo.org/lomethods/si/intercal2012.html, which outlines procedures for all TEI's. The intercalibration procedures used for the IDP can be found at http://www.geotraces.org/science/intercalibration/945-intercalibration-procedures. In brief, at common stations occupied by two GEOTRACES cruises – crossover stations –

Table 2
Links to cruise reports of cruises included in the GEOTRACES Intermediate Data Product 2014.

Cruise	Cruise report
PE319	http://www.bodc.ac.uk/data/information_and_inventories/cruise_inventory/report/pe319.pdf
PE321	http://www.bodc.ac.uk/data/information_and_inventories/cruise_inventory/report/pe321.pdf
JC057	http://www.bodc.ac.uk/data/information_and_inventories/cruise_inventory/report/jc057.pdf
KN199-4	http://www.bodc.ac.uk/data/information_and_inventories/cruise_inventory/report/kn199-4.pdf
KN204-1	http://www.bodc.ac.uk/data/information_and_inventories/cruise_inventory/report/knorr_kn204_1.pdf
D357	http://www.bodc.ac.uk/data/information_and_inventories/cruise_inventory/report/d357.pdf
JC068	http://www.bodc.ac.uk/data/information_and_inventories/cruise_inventory/report/jc068.pdf
M81_1	http://www.bodc.ac.uk/data/information_and_inventories/cruise_inventory/report/meteor81_1.pdf
KN192-5	http://www.bodc.ac.uk/data/information_and_inventories/cruise_inventory/report/kn192-5.pdf
KH09-05	http://www.bodc.ac.uk/data/information_and_inventories/cruise_inventory/report/hakuhomaru_kh-09-5.pdf
AU0703	http://www.bodc.ac.uk/data/information_and_inventories/cruise_inventory/report/auroraaustralis0703.pdf
MD166	http://www.bodc.ac.uk/data/information_and_inventories/cruise_inventory/report/mariondufresne166.pdf
ANTXXIV/3	http://www.bodc.ac.uk/data/information_and_inventories/cruise_inventory/report/polarstern_antxxiv3.pdf
AU0806	http://www.bodc.ac.uk/data/information_and_inventories/cruise_inventory/report/auroraaustralis0806.pdf
ARKXXII/2	http://www.bodc.ac.uk/data/information_and_inventories/cruise_inventory/report/polarstern_arkxxii2_07.pdf

Table 3
Number of discrete measurements of GEOTRACES key parameters in the IDP2014 and percentage contributions to the total number of discrete samples (27,366) in parentheses.

Key parameter	Number of observations
Trace elements	
Fe	All forms: 6715 (24.5%); dissolved: 4840 (17.7%)
Mn	All forms: 5444 (19.9%); dissolved: 4420 (16.2%)
Al	All forms: 4278 (15.6%); dissolved: 3539 (12.9%)
Zn	All forms: 3387 (12.4); dissolved: 3299 (12.1%)
Cd	All forms: 3865 (14.1%); dissolved: 2865 (10.5%)
Pb	All forms: 3035 (11.1%); dissolved: 2315 (8.5%)
Cu	All forms: 2214 (8.1%); dissolved: 1472 (5.4%)
Stable isotopes	
Si-30	All forms: 294 (1.1%); silicate: 266 (1.0%)
O-18	All forms: 2384 (8.7%); water: 1926 (7.0%)
N-15	All forms: 1226 (4.5%); nitrate: 768 (2.8%)
C-13	All forms: 846 (3.1%); DIC: 644 (2.4%)
Radioactive isotopes	
Th-234	All forms: 2459 (9.0%); dissolved: 1431 (5.2%)
Th-230	All forms: 924 (3.4%); dissolved: 752 (2.7%)
Pa-231	All forms: 921 (3.4%); dissolved: 751 (2.7%)
Pb-210	All forms: 606 (2.2%); dissolved: 311 (1.1%)
Radiogenic isotopes	
Nd-143	All forms: 237 (0.9%); dissolved: 237 (0.9%)

TEI data from both cruises were evaluated to see if they met criteria established by the larger TEI community (e.g., concentrations within 10% for Cd) and proper calibration and verification (e.g., analysing certified reference materials) procedures were followed. The distinct advantage of comparing crossover data was that it included the factors affecting accuracy due to sampling and sample handling procedures as well as from analytical methods. For cruises not having crossover stations to date (e.g., Indian Ocean), replicate sampling at multiple depths and having multiple labs analyse these samples allowed for examinations of accuracy for at least the sample handling through analytical steps.

In addition to the actual data values the IDP2014 also contains data quality flags and 1-σ data error values where available. Quality flags and error values are useful for data filtering. Quality flags are single character codes reflecting the quality of the respective data value. The IDP2014 uses the IODE quality flag set that was recently recommended as standard flagging scheme for the exchange of oceanographic and marine meteorological data (www.iode.org/mg54_3). The IODE flagging scheme is generic and simple, only containing the five flags listed in Table 4.

The IDP2014 employs the following parameter naming scheme. Standard hydrographic parameters, such as pressure, depth, oxygen, and nutrients, use names as defined in the WOCE/CLIVAR naming conventions (http://cchdo.ucsd.edu/parameter_descriptions). Examples are CTDPRS, CTDTMP, CTDSAL and CTDOXY for pressure, temperature, salinity and oxygen from CTD sensors, respectively, and SALNTY, PHSPHT, NITRAT, SILCAT for salinity, phosphate, nitrate and silicate, respectively, measured on bottle samples.

All other trace elements and isotope names are composed of up to six separate tokens as follows:

Table 4
The IODE quality flagging scheme used for the IDP2014.

Value	Flag short name	Definition
1	Good	Passed required QC tests
2	Not evaluated, not available or unknown	Used for data when no QC test performed or the information on quality is not available
3	Questionable/suspect	Failed non-critical metric or subjective test(s)
4	Bad	Failed critical QC test(s) or as assigned by the data provider
9	Missing data	Used as place holder when data are missing

1	2	3	4	5	6
Element/Compound	[_Oxidation State]	[_Atomic Mass]	_Phase	_Data Type	_Sampling System

Tokens 2 and 3 are optional, while all other tokens are mandatory. Meaning and possible values of all the six tokens are described in Table 5. Example parameter names are given in Table 6.

The IDP2014 digital data compilation is available for download at http://www.bodc.ac.uk/geotraces/data/idp2014/. Users are required to register and agree to usage rules asking for proper citation of the relevant original papers associated with the particular data used, as well as citation of the IDP2014 data product itself (this paper). The data are available in various formats: (1) as ASCII text files suitable for usage in standard software, (2) as Excel spreadsheet files for Microsoft Excel or similar software, (3) as netCDF files suitable for access by models and netCDF readers, and (4) as ODV collections for use with the popular *Ocean Data View* software (http://odv.awi.de).

Cruise reports as well as the data info files provide information about data originator, original publications related to the data as well as analytical methods and are maintained for every parameter and every cruise and are delivered with all format options. Access to these metadata is particularly easy in ODV, where only two mouse clicks are required to obtain detailed information about the data producer and the analytical methods for any given data value. One more mouse click shows the references of the original publications associated with a given parameter and cruise. Proper linkage of originator and publication information is used throughout the IDP2014.

The publication links in the IDP2014 point to a reference database of original publications maintained at the GEOTRACES International Programme Office (IPO). This reference database is updated whenever

Table 5
Description of the IDP2014 parameter naming scheme.

#	Explanation	Example
1	Element or compound (mandatory)	Fe, Th, DIC, NO3, L1Fe
2	Oxidation state as roman numeral (optional)	_II, _IV
3	Atomic mass (optional; two entries for isotope ratios)	_56, _208_204
4	Phase on which element or compound was measured (mandatory)	_D (dissolved), _S (soluble), _C (colloidal), _TD (total dissolvable), _TP (total particulate), _SP (small particulate), _SPL (small particulate, labile fraction), _SPR (small particulate, refractory fraction), _SPT (small particulate, total (unleached)), _LP (large particulate), _LPT (large particulate, total (unleached)), _F (free (un-complexed)), _TPL (total particulate, labile fraction), _TPR (total particulate, refractory fraction)
5	Data type (mandatory)	_CONC, _DELTA, _EPSILON, _RATIO, _LogK
6	Sampling system (mandatory)	_BOTTLE, _PUMP, _FISH

Table 6
Example IDP2014 parameter names. The last 5 parameters are not included in the IDP2014 but are expected to be part of future data products.

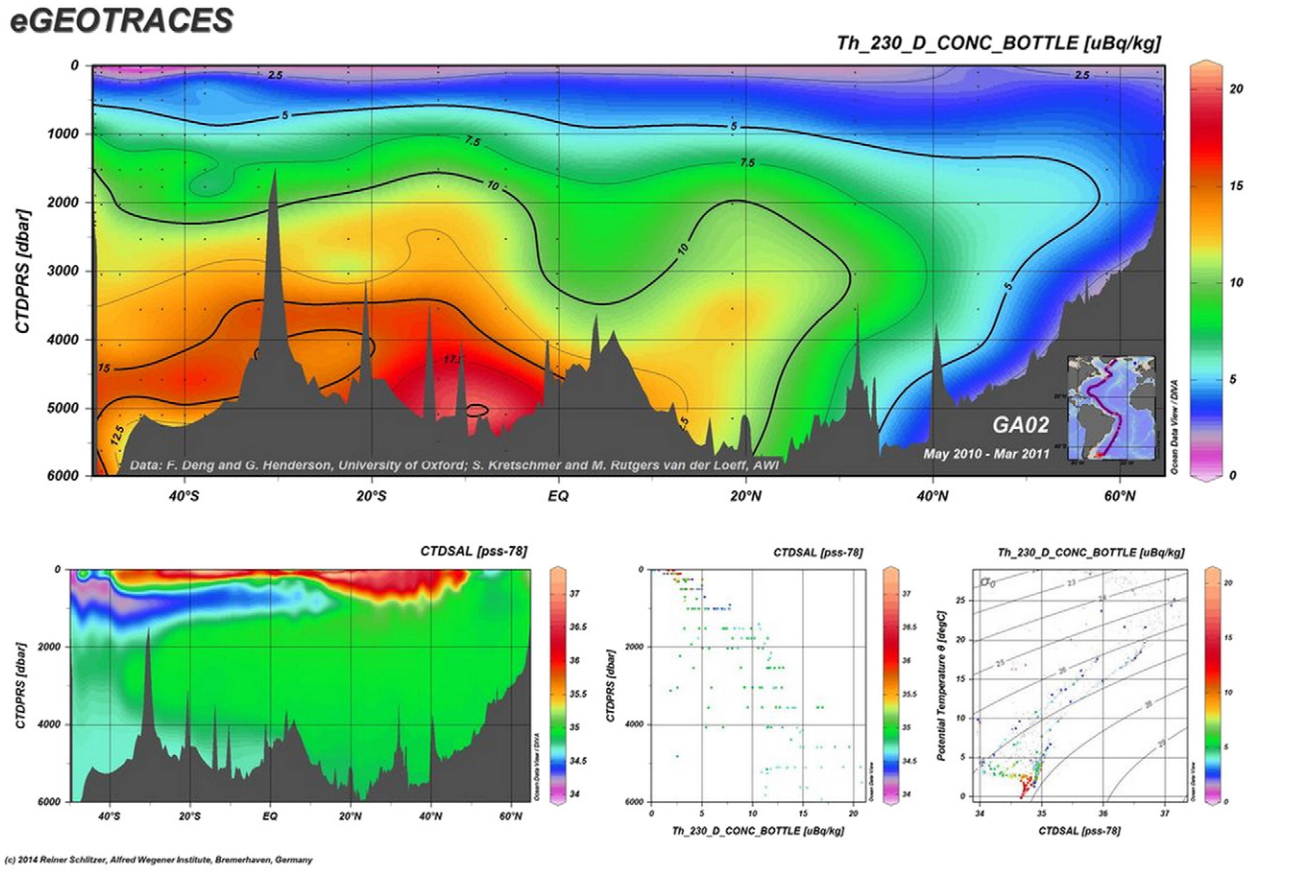
Parameter name	Explanation
Fe_D_CONC_BOTTLE	Concentration of dissolved Fe
Fe_II_D_CONC_BOTTLE	Concentration of dissolved Fe(II)
Fe_II_TP_CONC_BOTTLE	Concentration of total particulate Fe(II) determined by filtration from a water sampling bottle
Fe_TPL_CONC_BOTTLE	Concentration of labile particulate iron determined by filtration from a water sampling bottle
Nd_143_144_D_RATIO_BOTTLE	Atom ratio of given isotopes for dissolved Nd
Nd_143_D_EPSILON_BOTTLE	Atom ratio of dissolved Nd isotopes expressed in conventional EPSILON notation
DIC_13_D_DELTA_BOTTLE	δ13C of DIC
NO3_15_D_DELTA_BOTTLE	δ15N of nitrate
DIC_14_D_DELTA_BOTTLE	Δ14C of DIC
Cu_II_F_CONC_BOTTLE	Concentration of free Cu^{++}
Pb_206_204_D_RATIO_BOTTLE	Atom ratio of given isotopes for dissolved Pb
L1Fe_D_CONC_BOTTLE	Concentration of dissolved L1 Fe-binding ligand
L1Fe_D_LogK_BOTTLE	Log of the stability constant of L1 Fe

new papers are published. Clicking on a reference link in the IDP2014 will always show the up-to-date list of relevant publications in the reference database for a particular TEI. This mechanism was chosen to allow for dynamic inclusion of papers published after the release of the data product.

3. *eGEOTRACES Electronic Atlas*

The *eGEOTRACES Electronic Atlas* (http://egeotraces.org/) is based on the digital data package described above and provides section plots (Fig. 2) and animated 3D scenes (Fig. 3) for many of the parameters. Users select tracers, cruise tracks and ocean basins using list-boxes and interactive maps. *eGEOTRACES* then presents tracer distributions along the selected sections, or animated 3D scenes showing tracer distributions along all available sections in the selected basin. Section plots and 3D animations contain the names of the scientists who produced or are responsible for the data.

Clicking on a section plot loads a high-resolution version of the image, which can be saved for use in publications and presentations.



References: Link to references asociated with these data

Other tracers along this section: Al dissolved | Ba dissolved | Fluorescence Chl-a | CTD Oxygen | CTD Salinity | CTD Potential Temperature | Transmissometer Beam Attenuation | Cd dissolved | Dissolved Inorganic Carbon | Dissolved Organic Carbon | Fe dissolved | delta O18 (H2O) | delta Deuterium (H2O) | La dissolved | Mn dissolved | Mo dissolved | Nitrate | Ni dissolved | Oxygen (Winkler or CTD) | Phosphate | Pa_231 dissolved | Pa_231/Th_230 dissolved Ratio | Pb dissolved | Salinity | Silicate | delta Si30 (SILCAT) | Total Alkalinity | Total Nitrogen | Total Organic Carbon | Potential Temperature | Th_232 total particulate (pump) | Th_234 dissolved | U dissolved | Y dissolved | Zn dissolved

Other sections with this tracer: GA03 | GA03_e | GIPY5_e | GIPY5_w

3D scenes with this tracer: Atlantic | North Atlantic | South Atlantic

Goto: Sections Home | 3D Scenes Home | eGEOTRACES Home

Fig. 2. Example of eGEOTRACES section page.

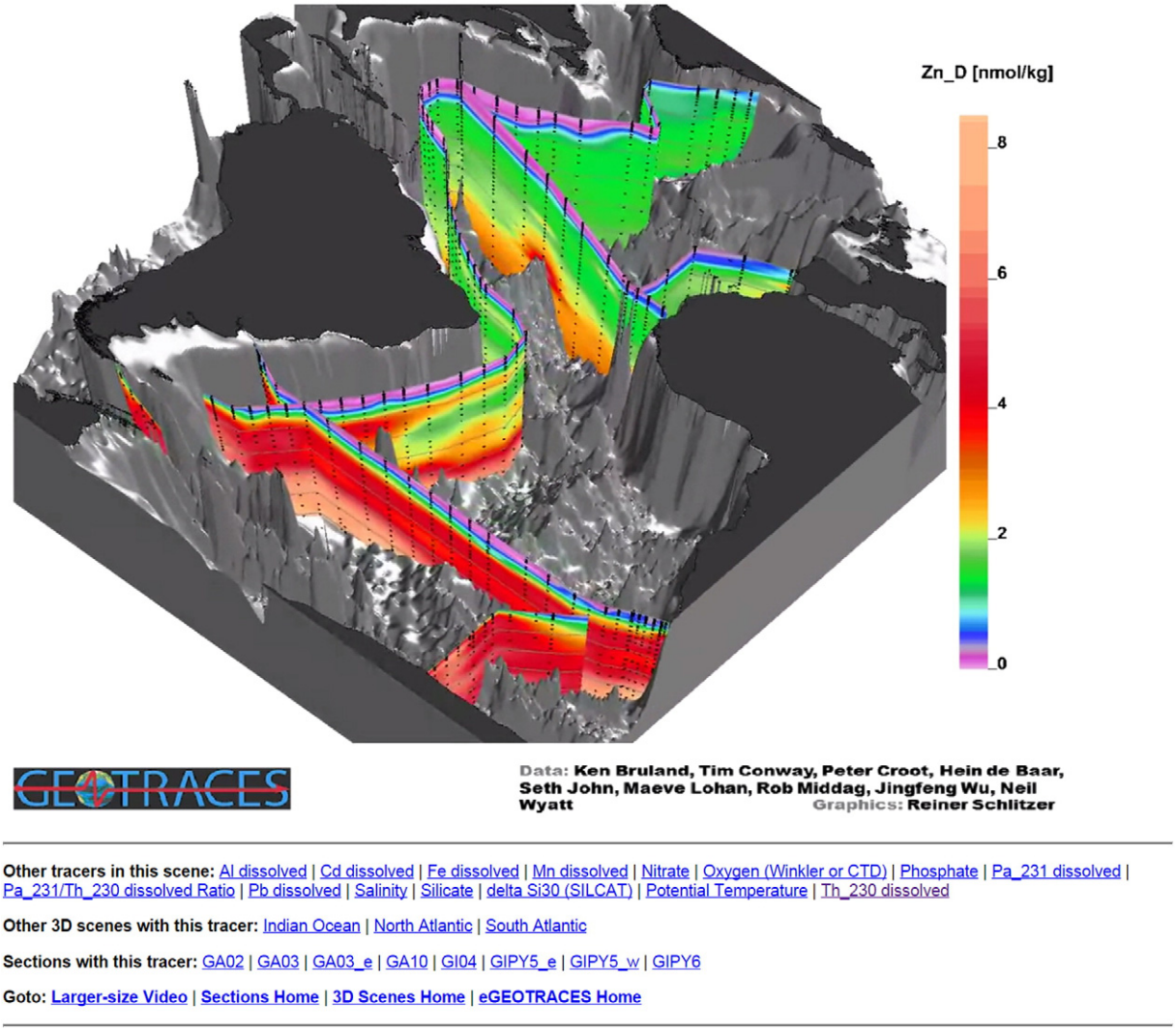


Fig. 3. Example of eGEOTRACES 3D scene.

You use the browser's "Back" button to return to the original section page. Clicking on a rotating 3D scene produces a blown-up version of the animation. Clicking on the blown-up animation returns it to the original size. An option bar appears when the mouse is over the animation. You can use the bar to stop the animation at arbitrary angles and quickly choose other viewing angles.

Section and 3D animation pages contain groups of links at the bottom of the page. These include (a) links to other tracers along this section or in this scene, (b) other sections or 3D scenes with this tracer, and (c) 3D scenes or sections with this tracer. These links greatly facilitate the switching between and comparing of different tracers, sections and 3D scenes. All section plots use the same window layout. Therefore section plots perfectly match when switching between tracers. The links under category (c) allow for easy transitions between section plots and 3D animations. Section pages also contain a link to the original publications associated with the given tracer and section. Clicking on this link shows the current list of publications from the dynamically updated reference database maintained at the IPO (see above).

eGEOTRACES provides quick overviews of the occurrence of geochemically relevant tracers. The 3D scenes provide geographical and bathymetric context crucial for correctly assessing the extent and origin of tracer plumes as well as for inferring processes acting on the tracers and shaping their distribution. The numerous links to other tracers, sections and basins found on section plots and 3D animations allow for quick switching between tracers and domains and facilitate comparative studies. In addition to the anticipated usage for marine research, *eGEOTRACES* and the contained visual material can help in teaching and outreach activities and can also facilitate conveying societally-relevant scientific results to interested non-scientists and policy makers.

Images from the *eGEOTRACES* Atlas are freely available for non-commercial purposes, such as in scientific publications, posters, presentations or teaching activities, if the source is cited as follows: *Schlitzer, R., eGEOTRACES - Electronic Atlas of GEOTRACES Sections and Animated 3D Scenes,* http://egeotraces.org, *2014*. Users must not remove the names of data producers and graphics creator. High-resolution images are available on request.

4. Summary

With the release of the IDP2014, GEOTRACES seeks to promote intensified collaboration within the marine geochemical community and beyond. The availability of a large integrated and quality controlled dataset, such as the IDP2014, will allow a much wider range of studies than would be possible with individual cruise data alone. Examples of such research include basin-wide tracer budgets and quantification

of sources and sinks on large scales. The new 3D visualisation techniques and the strong inter-linkage of sections and 3D scenes provided by the *eGEOTRACES Atlas* aids the scientific interpretation of TEI data, but also facilitates outreach to a wider community, including not only scientists from different disciplines but also the general public and policy makers.

In early 2015, the GEOTRACES Data Management Committee will formally seek feedback from the community on IDP2014, with an email sent out to those who provided data, those who have downloaded the product and also those on the GEOTRACES mailing list, directing them to an online survey.

The IDP2014 is the first in a series of intermediate data products planned to be produced at regular intervals with the next scheduled for release at the Goldschmidt Conference in 2017. These future data products will extend the geographical coverage by including data from new GEOTRACES cruises in the Mediterranean Sea, Pacific, Atlantic and Indian Oceans, as well as containing additional data from existing cruises for parameters that take longer to measure and complete. User feedback from the survey will help make the next IDP an even more useful product.

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