World Ocean Circulation

Product User Manual

WOC-L4-CUR-NATL2D_REP-1D, WOC-L4-CUR-NATL3D_REP-1D

(Theme 2)

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Contents

1 Introduction

1.1 Purpose of the document

The present document is the Product User Manual dedicated to the content and format description of the products WOC-L4-CUR-NATL2D_REP-1D and WOC-L4-CUR-NATL3D_REP-1D. WOC-L4-CUR-NATL2D_REP-1D provides a level 4 (L4) gap free reconstruction of 2D ocean surface currents obtained through the combination of altimeter-derived geostrophic currents and satellite-derived sea surface temperature (SST) L4 data.

The second product (WOC-L4-CUR-NATL3D_REP-1D) provides a 3D reconstruction of the horizontal and vertical currents, as well as of temperature and salinity, over 75 unevenly spaced vertical levels (denser close to the surface), between the surface and 1500 m depth.

Both products are computed on a 1/10°x1/10° horizontal resolution grid, with a daily resolution, covering the 2010-2019 period, over a wide portion of the North Atlantic Ocean (20°N-50°N, 76°W-6°W).

This is the primary document that users should read before handling the products. It provides an overview of processing algorithms, technical product content and format and main validation results.

1.2 Document structure

In addition to this introduction, this document includes the following chapters:

- Chapter 2 describes the methodology and validation results for the WOC-L4-CUR-NATL2D_REP-1D product. The details on the product format, nomenclature and content are also provided.
- Chapter 3 describes the methodology and validation results for the WOC-L4-CUR-NATL3D_REP-1D product. The details on the product format, nomenclature and content are also provided.

1.3 Applicable & Reference documents

- [RD-1] ESA WOC2019: http://woc2019.esa.int/index.php
- [RD-2] Synthesis of the WOC2019 User Consultation Meeting recommendations http://woc2019.esa.int/files/WOC2019_summary_synthesis.pdf

- [RD-3] Algorithm Theoretical Basis Document for North Atlantic data-driven 2D currents and 3D currents and tracers products: WOC-L4-CUR-NATL2D_REP-1D, WOC-L4-CUR-NATL3D_REP-1D (THEME 2), Doc. Ref. WOC-ESA-ODL-NR-009_T2_WOC-L4-CUR-NATL2D_3D_REP-1D_V2.0

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- [RD-5] Rio, M.H.; Santoleri, R. Improved global surface currents from the merging of altimetry and Sea Surface Temperature data. *Remote. Sens. Environ.* 2018

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- [RD-13] Droghei, R.; Buongiorno Nardelli, B.; Santoleri, R. Combining in-situ and satellite observations to retrieve salinity and density at the ocean surface. J. Atmos. Ocean. Technol. 2016, 33, 1211–1223, doi:10.1175/JTECH-D-15-0194.1.

- [RD-14] Szekely, T.; Gourrion, J.; Pouliquen, S.; Reverdin, G. The CORA 5.2 dataset for global in situ temperature and salinity measurements: Data description and validation. Ocean Sci. 2019, 15, 1601–1614, doi:10.5194/os-15-1601-2019.

- [RD-15] Droghei, R., Buongiorno Nardelli, B. and Santoleri, R.: A New Global Sea Surface Salinity and Density Dataset From Multivariate Observations (1993–2016), Front. Mar. Sci., 5(March), 1–13, doi:10.3389/fmars.2018.00084, 2018.

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1.4 Terminology

ACCUA	Analisi della dinamica della Corrente CircUmpolare Antartica
ACCD	Attribute Convention for Data Discovery
AMSR2	Advanced Microwave Scanning Radiometer 2
ADT	Absolute Dynamic Topography
AI	Artificial Intelligence
AIL	Action Items List
AIS	Automatic Identification System
ASAR	Advanced Synthetic Aperture Radar
ASCAT	Advanced SCATterometer
ATBD	Algorithm Theoretical Basis Document
AVHRR	Advanced Very High Resolution Radiometer
CCD	Contract Closure Document
CCI	Climate Change Initiative
CCMP	Cross-Calibrated Multi-Platform
CFOSAT	Chinese-French Oceanography Satellite
CIESM	Mediterranean Science Commission
CMEMS	Copernicus Marine Environment Monitoring Service
CNES	Centre National d'Etudes Spatiales
CNR	Consiglio Nazionale delle Ricerche
CTD	Conductivity, Temperature and Depth
DP	Data Pool
DTU	Danmarks Tekniske Universitet
DUACS	Data Unification and Altimeter Combination System
EBUS	Eastern Boundary Upwelling System
ECCO	Estimating the Circulation & Climate of the Ocean
ECMWF	European Centre for Medium-Range Weather Forecasts
EFARO	European Fisheries and Aquaculture Research Organisations
EMB	European Marine Board
ENVISAT	Environmental Satellite
EO	Earth Observation
EPB	European Polar Board
EOEP-5	5th Earth Observation Envelope Programme (2017-2021)
ERA	ECMWF Reanalysis
ESA	European Space Agency
ESF	European Science Foundation
EU	European Union
EuroGOOS	European Global Ocean Observing System
FAO	Food and Agriculture Organization of the United Nations

FR	Final Report
FSLE	Finite Size Lyapunov Exponent
GCM	Global Circulation Model
GHRSST	Group of High Resolution Sea Surface Temperature
GOCE	Gravity Field and Steady-State Ocean Circulation Explorer
GOOS	Global Ocean Observing System
GMI	Global precipitation monitoring Microwave Imager
GMM	Gaussian Mixture Models
HYCOM	Hybrid Coordinate Ocean Model
IAR	Impact Assessment Report
ICCAT	International Commission for the Conservation of Atlantic Tunas
ICSU	International Council for Science
IGPB	International Geosphere-Biosphere Programme
IUGG	International Union of Geodesy and Geophysics
IFREMER	Institut Français de Recherche pour l'Exploitation de la Mer
IOC	Intergovernmental Oceanographic Commission
ITCZ	InterTropical Convergence Zone
mEOF-r	Multivariate Empirical Orthogonal Functions reconstruction
MoM	Minutes of Meeting
NATL3D	North Atlantic 3D Ocean Currents
NEMO	Nucleus for European Modelling of the Ocean
NOAA	National Oceanic and Atmospheric Administration
NCC	Norwegian Coastal Current
NwAFC	Norwegian Atlantic Front Current
NwASC	Norwegian Atlantic Slope Current
OLCI	Ocean and Land Color Imager
OSSE	Observing System Simulation Experiment
OC	Ocean color
OSCAT	Oceansat-2 SCATterometer
PD	Product Delivery
PM	Project Manager
PMP	Project Management Plan
PUB	Publication
PUM	Product User Manual
QUID	Quality Information Document
RB	Requirement Baseline
REMSS	Remote Sensing Systems
ROMS	Regional Oceanic Modeling System
RTOFS	Real-Time Ocean Forecast System
S3	Sentinel 3

SAR	Synthetic Aperture Radar
SEVIRI	Spinning Enhanced Visible and InfraRed Imager
SCOR	Scientific Committee on Oceanic Research
SIED	Single Image Edge Detection
SKIM	Sea surface KInematics Multiscale monitoring
SLSTR	Sea & Land Surface Temperature Radiometer
SOCIB	Sistema d'observació i predicció costaner de les Illes Balears
SODA	Simple Ocean Data Assimilation Ocean/sea ice reanalysis
SSH	Sea Surface Height
SSS	Sea Surface Salinity
SST	Sea Surface Temperature
SVP	Surface Velocity Program
SoW	Statement of Work
TN	Technical Note
TOPAZ	Tracers of Phytoplankton with Allometric Zooplankton
TUOC	Total Upper Ocean Currents
UCL	Use Case Library
UCM	User Consultation Meeting
UCPC	Upper-layer ocean Circulation Processes e-Catalogue
UI	Upwelling Index
UN	United Nations
URD	User Requirement Document
VR	Validation Report
VT	Visualization Tool
WBS	Work Breakdown Structure
WOC	World Ocean Circulation

2 North Atlantic Merged SSH/SST 2D Currents (WOC-L4-CUR-NATL2D_REP-1D)

2.1 Overview

The WOC-L4-CUR-NATL2D_REP-1D product has been developed by CNR-ISMAR applying a methodology to optimally combine altimeter-derived geostrophic currents and sequences of L4 SSTs based on the results of [RD-4], [RD-5] and [RD-6]. This technique enables to reconstruct the ocean surface circulation from the altimeter-derived geostrophic currents and sequences of satellite L4 SST observations taking into account the source/sink terms for the SST evolution equation (related to the large scale interactions with the atmospheric boundary layer).
The idea behind the methodology is to infer the two components of the marine surface circulation using the geostrophic currents as a first guess estimate and inverting the SST evolution equation (1) to infer the correction factors to compute an optimized surface current estimate:

$$\frac{\partial SST}{\partial t} + u\frac{\partial SST}{\partial x} + v\frac{\partial SST}{\partial y} = F \qquad (1)$$

where (u,v) are respectively the zonal and meridional components of the ocean surface flow, (x,y) are the zonal and the meridional directions and F is the forcing term (here approximated as the low pass spatial filtering of the satellite SST temporal derivatives, choosing the 1000 km filtering scale).

This synergistic approach, applied to the CMEMS OSTIA L4 SST at global scale, allowed to improve the global sea surface currents estimates with respect to the altimeter system up to 30%. This was evaluated relying on in-situ measured currents provided by drogued SVP drifting buoys. The methodology exhibits best performances in the equatorial to mid-latitudes areas, and generally yields larger improvements for the meridional component of the surface currents [RD-5], [RD-6]. This is due to the intrinsic limitations of the altimeter system, providing less accurate surface currents estimates for the meridional flow and in proximity of the equator [RD-5], [RD-6] and [RD-7]. The validation of the WOC-L4-CUR-NATL2D_REP-1D product (still based on in-situ measured currents from SVP drifting buoys) yielded local improvements up to 20% and 25% for the zonal and meridional component of the surface currents, respectively [RD-3].

2.2 Algorithm

2.2.1 Retrieval methodology

The algorithm implementation requires the input fields listed below:

1. daily maps of gap-free (L4) satellite SST, obtained from CMEMS (CMEMS product ID: SST_GLO_SST_L4_REP_OBSERVATIONS_010_011);
2. daily maps of altimeter-derived L4 absolute geostrophic currents, obtained from CMEMS (CMEMS product ID: SEALEVEL_GLO_PHY_L4_REP_OBSERVATIONS_008_047);
3. daily maps of satellite SST temporal derivatives (∂_tSST, with the subscript t indicating derivative with respect to time) ;
4. daily maps of satellite SST spatial derivatives, (∂_xSST and ∂_ySST, with the subscripts x,y indicating derivative with respect to longitude and latitude, respectively);
5. a static map describing the uncertainty on the geostrophic currents, obtained via comparison with SVP drifting buoys in the 1993-2018 period);
6. a static map describing the uncertainty on the SST forcing (F in equation 1). (computed via comparison with SVP drifting buoys in the 1993-2018 period);

Relying on the input fields labelled with 1-6 one can optimally merge the daily altimeter-derived currents with the daily satellite SST through the equation provided below:

$$(U,V)_{OPC}=(U,V)_{GEO}+(U,V)_{CORR} \qquad (2)$$

where the variables U,V stand for zonal and meridional surface currents, respectively. Equation (2) indicates that the OPtimized Currents (OPC) are obtained by applying correction factors $(U,V)_{CORR}$ to the altimeter-derived geostrophic (GEO) currents, which are used as first guess. The correction factors are a function of the satellite SST spatial-temporal derivatives, and are also computed accounting for the uncertainties on the geostrophic currents as well as on the SST forcing term. In order to compute the correction factors $(U,V)_{CORR}$, we account for the aforementioned variables relying on the set equations reported in [RD-3]. More details on the methodology are accessible through [RD-3] to [RD-6].

2.2.2 Limitations

By construction, the WOC-L4-CUR-NATL2D_REP-1D product cannot be derived in areas where the spatial SST gradient magnitude equals zero, see e.g. (2) and (3) in [RD-5]. Moreover, it was demonstrated that the methodology behind the WOC-L4-CUR-NATL2D_REP-1D does not bring improvement in low SST gradient areas (i.e. $\leq 10^{-5}$ °C $\cdot m^{-1}$) [RD-5] and [RD-6]. In such areas, the WOC-L4-CUR-NATL2D_REP-1D does not add information with respect to the CMEMS altimeter-derived geostrophic currents and the two products have to be considered equivalent (CMEMS product ID: SEALEVEL_GLO_PHY_L4_REP_OBSERVATIONS_008_047).

The WOC-L4-CUR-NATL2D_REP-1D validation (detailed in [RD-3]) also suggests that the synergy between the altimeter-derived currents and the satellite SST brings larger improvements for the meridional component of the surface circulation, up to 25% with respect to the altimeter system. The maximum improvements are less intense for the zonal currents, being around 20%. Occasional degradations around 5% may also occur.

2.2.3 Differences with previous version (if relevant, phase 2)

Updated references and product temporal coverage.

2.3 Product Description

2.3.1 spatial information

Product Specification Customer Name	WOC-L4-CUR-NATL2D_REP_1D
Geographical coverage	Central/North Atlantic Ocean (20°N-50°N, 76°W-6°W).
Horizontal resolution	1/10° on a regular grid

2.3.2 temporal information

Product Specification Customer Name	WOC-L4-CUR-NATL2D_REP_1D
Available time series	Version2 = 2010-2019
Temporal resolution	daily

2.3.3 product content

PRODUCT	variables name in the NetCDF file and Unit; long_name standard_name
WOC-L4-CUR-NATL2D_REP_1D	**uo** (meter per second) eastward velocity eastward_sea_water_velocity; **vo** (meter per second) northward velocity northward_sea_water_velocity
scale_factor/add_offset/missing_value/land mask	Land mask are equal to "_FillValue" (see variable attribute in NetCDF file).

2.3.4 file name convention

Filename and format have been chosen to match the conventions adopted by ESA CCI, CMEMS, GlobCurrent, GHRSST (all complying to the more general Climate & Forecast and ACDD conventions). Following these conventions, the filename is:

<Indicative Date-*yyyymmdd*><Indicative Time-*hhmmss*>-WOC-<Processing Level>-<Parameter>-<Product String>-v< ProductVersion>-fv<File Version>.<File Type>

2.3.5 file format

The products are stored using the NetCDF format.

NetCDF (Network Common Data Form) is an interface for array-oriented data access and a library that provides an implementation of the interface. The netCDF library also defines a machine-independent format for representing scientific data. Together, the interface, library, and format support the creation, access, and sharing of scientific data. The netCDF software was developed at the Unidata Program Center in Boulder, Colorado.

Please see Unidata netCDF pages for more information, and to retrieve netCDF software package.

NetCDF data is:

* Self-Describing. A netCDF file includes information about the data it contains.

* Architecture-independent. A netCDF file is represented in a form that can be accessed by computers with different ways of storing integers, characters, and floating-point numbers.

* Direct-access. A small subset of a large dataset may be accessed efficiently, without first reading through all the preceding data.

* Appendable. Data can be appended to a netCDF dataset along one dimension without copying the dataset or redefining its structure. The structure of a netCDF dataset can be changed, though this sometimes causes the dataset to be copied.

* Shareable. One writer and multiple readers may simultaneously access the same netCDF file.

2.3.6 metadata

```
netcdf file:20180101120000_WOC-L4-CUR-NATL2D_REP-1D-v1.0-fv1.0.nc {
dimensions:
   depth = 1;
   lat = 300;
   lon = 700;
   time = UNLIMITED;   // (1 currently)
 variables:
   float uo(time=1, depth=1, lat=300, lon=700);
     :long_name = "eastward velocity";
     :standard_name = "eastward_sea_water_velocity";
     :units = "m s-1";
     :_ChunkSizes = 1, 1, 300, 700; // int

   float vo(time=1, depth=1, lat=300, lon=700);
     :long_name = "northward velocity";
     :standard_name = "northward_sea_water_velocity";
     :units = "m s-1";
     :_ChunkSizes = 1, 1, 300, 700; // int

   float depth(depth=1);
     :standard_name = "depth";
     :units = "m";
     :axis = "Z";
     :positive = "down";
     :_CoordinateAxisType = "Height";
     :_CoordinateZisPositive = "down";

   float lat(lat=300);
     :units = "degrees north";
```

```
      :axis = "Y";
      :standard_name = "latitude";
      :_CoordinateAxisType = "Lat";

    float lon(lon=700);
      :units = "degrees east";
      :axis = "X";
      :standard_name = "longitude";
      :_CoordinateAxisType = "Lon";

    int time(time=1);
      :units = "hours since 1981-01-01 00:00:00";
      :long_name = "time";
      :standard_name = "time";
      :calendar = "gregorian";
      :axis = "T";
      :_ChunkSizes = 1024; // int
      :_CoordinateAxisType = "Time";

  // global attributes:
  :Conventions = "CF-1.7, ACDD-1.3, ISO 8601";
  :Metadata_Conventions = "Climate and Forecast (CF) 1.7, Attribute Convention for Data Discovery (ACDD) 1.3";
  :standard_name_vocabulary = "NetCDF Climate and Forecast (CF) Metadata Convention version 1.8";
  :title = "North Atlantic Merged SSH-SST Surface Currents (NATL2D)";
  :summary = "This is a surface current product combining altimeter-derived geostrophic currents and satellite L4 SSTs. It was developed in the framework of the European Space Agency World Ocean Circulation Project";
  :id = "WOC-L4-CUR-NATL2D_REP-1D";
  :product_version = "1.0";
  :references = "Rio, M. H., & Santoleri, R. (2018). Improved global surface currents from the merging of altimetry and sea surface temperature data. Remote sensing of Environment, 216, 770-785, https://doi.org/10.1016/j.rse.2018.06.003.  Ciani, D., Rio, M. H., Nardelli, B. B., Etienne, H., & Santoleri, R. (2020). Improving the altimeter-derived surface currents using sea surface temperature (SST) data: A sensitivity study to SST products. Remote Sensing, 12(10), 1601, https://doi.org/10.3390/rs12101601";
  :creator_name = "Daniele Ciani";
  :creator_url = "www.ismar.cnr.it";
  :creator_email = "daniele.ciani@cnr.it";
  :creator_institution = "Consiglio Nazionale delle Ricerche-Istituto di Scienze Marine";
```

:institution = "Consiglio Nazionale delle Ricerche, Institut Francais de Recherche pour l\'Exploitation de la mer / CERSAT, European Space Agency";
:institution_abbreviation = "CNR, Ifremer/CERSAT, ESA";
:keywords_vocabulary = "NASA Global Change Master Directory (GCMD) Science Keywords";
:comment = "These data were produced at CNR as part of the ESA WOC project.";
:publisher_name = "CERSAT";
:publisher_url = "cersat.ifremer.fr";
:publisher_email = "cersat@ifremer.fr";
:naming_authority = "fr.ifremer.cersat";
:publisher_institution = "Ifremer/CERSAT";
:scientific_support_contact = "daniele.ciani@cnr.it";
:technical_support_contact = "cersat@ifremer.fr";
:key_variables = "eastward_current_velocity, westward_current_velocity”;
:source = "WOC2D Processor V1.0";
:source_version = "1.0";
:processing_software = "WOC2D";
:format_version = "WOC v1.0";
:netcdf_version_id = "4.4.1 of Aug 10 2016 17:24:31 ";
:date_created = "2021-06-15T13:39:08Z";
:date_modified = "2021-06-15T13:39:08Z";
:track_id = "86a3b6f5-888a-477b-b6ac-bed2ef230cf9";
:grid_resolution = "0.1 degrees";
:software_version = "WOC2D Processor V1.0";
:processing_level = "L4";
:cdm_data_type = "grid";
:time_coverage_start = "2018-1-2T12:00:00Z";
:time_coverage_end = "2018-1-2T12:00:00Z";
:geospatial_lon_min = "-75.975";
:geospatial_lon_max = "-6.075";
:geospatial_lat_min = "20.025";
:geospatial_lat_max = "49.925";
:geospatial_lat_units = "degree_north";
:geospatial_lon_units = "degree_east";
:spatial_resolution = "0.1 degree";
:Scaling_Equation = "(scale_factor*data) + add_offset";
:project = "World Ocean Circulation (WOC) - European Space Agency";
:method = "Correction of altimeter-derived geostrophic currents with constraints provided by the spatial-temporal SST derivatives";
:history = "2021-06-15T13:39:08Z - Creation";
:acknowledgement = "Please acknowledge the use of these data with the following statement: these data were obtained from the ESA WOC project";

```
  :license = "ESA WOC Data Policy: free and open access";
  :_CoordSysBuilder = "ucar.nc2.dataset.conv.CF1Convention";
}
```

3 North Atlantic data-driven 3D Currents and Tracers (WOC-L4-CUR-NATL3D_REP-1D)

3.1 Overview

The WOC-L4-CUR-NATL3D_REP-1D product has been developed by CNR starting from the Omega diagnostic model initially set-up during the ACCUA (Analisi della dinamica della Corrente CircUmpolare Antartica) project [RD-9], that has been successively implemented over the global oceans within the Copernicus Marine Environment Monitoring Service (CMEMS) at 1/4°x1/4°, weekly resolution (OMEGA3D, CMEMS product ID: MULTIOBS_GLO_PHY_W_REP_015_007, [RD-11]).
The WOC Omega diagnostic tool takes in input 3D fields of density and geostrophic and empirical horizontal Ekman currents, as well as momentum and heat fluxes at the air-sea interface.
The 3D fields of density are obtained through a deep learning technique based on a Long-Short Term Memory network (LSTM3D), tuned to optimize the reconstruction of 3D temperature and salinity fields (from which density is obtained through standard UNESCO formula) in the study area. The LSTM3D reconstruction allows to combine remotely sensed surface measurements of sea surface temperature (SST), salinity (SSS), absolute dynamic topography and in situ profiles of temperature (T) and salinity (S).
Within WOC, the input surface fields have been taken from existing or specific newly-developed high resolution data (1/10°, daily).
With respect to CMEMS processing, the Omega algorithm has been adapted to the new input data and NATL3D output grid. Moreover, it has been modified to improve the reconstruction of the diabatic components of the ageostrophic motion in the surface layer, by taking advantage of the modelled horizontal Ekman currents developed during ESA-Globcurrent project and operationally provided by CMEMS (product ID: MULTIOBS_GLO_PHY_REP_015_004,[RD-12]) and including the atmospheric forcings derived from the ERA5 reanalysis.

3.2 Algorithm

3.2.1 Retrieval methodology

The NATL3D retrieval algorithm is made up of 3 main steps/modules, which are briefly recalled in the next sections. Full details are given in the Algorithm Theoretical Basis Document, [RD-3]:

1) Step/module 1: Input data preparation
2) Step/module 2: 2D-to-3D projection
3) Step/module 3: 3D currents retrieval

3.2.1.1 Step 1: Input data preparation

The first step consists in the preparation of the input data to be used for the successive retrievals.

Step 2, i.e. the reconstruction of 3D tracer fields from surface data, requires in input 2D fields of Sea Surface Temperature (SST), Sea Surface Salinity (SSS), Absolute Dynamic Topography (ADT) data, and vertical profiles of temperature and salinity from in situ sensors, as well as climatological 3D fields. The input data external sources for step 2 are:

1) SST: L4 multi-year reprocessed Operational Sea Surface Temperature and Sea Ice Analysis (OSTIA) developed by the U.K. Met Office and distributed by CMEMS (CMEMS product ID: SST_GLO_SST_L4_REP_OBSERVATIONS_010_011)
2) Vertical profiles: quality controlled Argo and CTD profiles produced by CMEMS CORA 5.2 (CMEMS product_id: INSITU_GLO_TS_REP_OBSERVATIONS_013_001_b)
3) 3D Climatology: monthly climatological fields computed by the World Ocean Atlas 2013.

Additional input data are built specifically for WOC NATL3D processing:

4) SSS: were obtained by adapting to the 1/10° North Atlantic grid the multidimensional optimal interpolation algorithm used within the CMEMS to retrieve the global SSS product (CMEMS product_id: MULTIOBS_GLO_PHY_S_SURFACE_MYNRT_015_013). This algorithm interpolates SMOS observations and in situ SSS observations using a space-time-thermal decorrelation function, which extracts information on water mass distribution from high-pass filtered daily SST data [RD-13]. Within WOC, we ingested as input data: the L3OS 2Q debiased daily valid ocean salinity values product from SMOS satellite, produced and disseminated by the Centre Aval de Traitement des Données SMOS (CATDS, 2017), the sub-sampled OSTIA SST data and CMEMS-CORA5.2 surface salinity values (CMEMS product_id: INSITU_GLO_TS_REP_OBSERVATIONS_013_001_b, doi: 10.17882/46219TS1, [RD-14]). CMEMS weekly SSS fields were used to build the background (linearly interpolating it in time between the two closest analysis dates, and upsizing to the 1/10° grid through a cubic spline). All other interpolation parameters have been set as in [RD-15].
5) ADT: WOC-L4-CUR-NATL2D_REP-1D data are used as input to the LSTM3D model, after additional processing is carried out to extract its steric component. The adjustment is carried out as in [RD-8], namely by regressing steric heights and co-located ADT data in the neighbourhood of each grid point, considering matchups within a temporal window of ± 10 days.

Step 3, i.e. the retrieval of 3D currents (including the vertical component), requires in input the 3D fields of density (temperature and salinity) and geostrophic fields obtained in the previous step, and additional data to estimate the Omega equation diabatic forcing term. Specifically these additional external data are:

1) Surface air-sea fluxes included in the ERA5 global atmospheric reanalysis by the European Centre For Medium-Range Weather Forecasts (ECMWF) [RD-16].
2) Modelled Ekman currents at 0 m and 15 m provided by CMEMS multi-year L4 at a 3h frequency over 1/4° regular grid (product ID: MULTIOBS_GLO_PHY_REP_015_004. These data are obtained by combining altimeter-derived geostrophic currents and Ekman currents estimated through the method developed by [RD-12].

3.2.1.2 Step 2: 2D-to-3D projection

The algorithm used to retrieve the 3D temperature and salinity from surface data is fully documented in [RD-11]. It is based on a Long Short-Term Memory Network (LSTM). LSTM networks are a particular type of Recurrent Neural Networks that is particularly fit to model ordered sequences of data. Here, the sequential information in input is provided by a multivariate output state vector comprising temperature, salinity and steric height anomaly profiles (all anomalies are computed with respect to WOA13 climatology). In practice, each LSTM cell in the sequence considers in input the same values (i.e., the anomalies of SST, SSS and adjusted ADT, plus latitude, longitude and cyclic day), but takes the output values at increasing depths (with depth "acting" as time in more standard applications of LSTM). All vectors are scaled within the 0–1 range before feeding the network. The best performance was obtained with a 2-layer stacked network, including 35 hidden units in each LSTM layer (hereafter, LSTM (35–35)). The LSTM code has been released under the terms of the GNU General Public Licence v3 and is available at the following address: https://github.com/bbuong/3Drec.

3.2.1.3 Step 3: 3D Currents retrieval

The reconstruction of the 3D horizontal and vertical currents is based on the solution of a diabatic Q-vector formulation of the QG Omega equation [RD-9, RD-10, RD-17].

$$\nabla^2{}_h(N^2 w) + f^2 \frac{\partial^2 w}{\partial z^2} = \nabla_h \cdot \boldsymbol{Q} \tag{3}$$

In Eq. (3), w represents the vertical velocity (positive upwards), N^2 is the Brunt–Väisälä frequency, f is the Coriolis parameter, h indicates the horizontal components, and the $\boldsymbol{Q}$ vector includes three components reflecting different processes (kinematic deformation, twg, turbulent buoyancy, th, and turbulent momentum, dm), as defined below:

$$\boldsymbol{Q} = 2\boldsymbol{Q_{twg}} + \boldsymbol{Q_{th}} + \boldsymbol{Q_{dm}}$$

$$\mathbf{Q}_{twg} = \frac{g}{\rho_0}\left(\frac{\partial u_g}{\partial x}\frac{\partial \rho}{\partial x} + \frac{\partial v_g}{\partial x}\frac{\partial \rho}{\partial y}, \frac{\partial u_g}{\partial y}\frac{\partial \rho}{\partial x} + \frac{\partial v_g}{\partial y}\frac{\partial \rho}{\partial y}\right)$$

$$\mathbf{Q}_{dm\_woc} = \frac{f}{\rho_0}\left(\frac{\partial^2}{\partial z^2}\left[\rho K_m\left(\frac{\partial v_g}{\partial z} + \frac{\partial v_{Ekman}}{\partial z}\right)\right], -\frac{\partial^2}{\partial z^2}\left[\rho K_m\left(\frac{\partial u_g}{\partial z} + \frac{\partial u_{Ekman}}{\partial z}\right)\right]\right)$$

$$\mathbf{Q}_{th} = -\frac{g}{\rho_0}\nabla_h\left(\frac{\partial}{\partial z}\left[K_\rho\left(\frac{\partial \rho}{\partial z} - \gamma_\rho\right)\right]\right) = \nabla_h\left(\frac{\partial}{\partial z}\left[K_\rho\left(N^2 + \frac{g}{\rho_0}\gamma_\rho\right)\right]\right)$$

In the above definitions, ρ indicates the potential density, g is the gravitational acceleration, (u_g, v_g) and (u_a, v_a) represent the geostrophic and ageostrophic horizontal velocities, while turbulent terms are defined through classical non-local effective gradient, γ_ρ, and viscosity/diffusivity, K_x.

Once the equation is solved for w, horizontal ageostrophic components can be estimated by integrating two expressions that are obtained during the analytical derivation of the omega equation:

$$u_a(z) = \int_{REF}^{z} \frac{\partial u_a}{\partial z} dz = \frac{1}{f^2} \int_{REF}^{z} \left(\frac{\partial}{\partial x}(N^2 w) - \frac{f}{\rho_0}\frac{\partial}{\partial z}\left(\frac{\partial \tau_{yz}}{\partial z}\right) - 2\frac{g}{\rho_0}\left(\frac{\partial u_g}{\partial x}\frac{\partial \rho}{\partial x} + \frac{\partial v_g}{\partial x}\frac{\partial \rho}{\partial y}\right) - \frac{g}{\rho_0}\frac{\partial}{\partial x}\left(\frac{\partial \mathrm{F}_{\rho z}}{\partial z}\right)\right) dz$$

$$v_a(z) = \int_{REF}^{z} \frac{\partial v_a}{\partial z} dz = \frac{1}{f^2} \int_{REF}^{z} \left(\frac{\partial}{\partial y}(N^2 w) + \frac{f}{\rho_0}\frac{\partial}{\partial z}\left(\frac{\partial \tau_{xz}}{\partial z}\right) - 2\frac{g}{\rho_0}\left(\frac{\partial u_g}{\partial y}\frac{\partial \rho}{\partial x} + \frac{\partial v_g}{\partial y}\frac{\partial \rho}{\partial y}\right) - \frac{g}{\rho_0}\frac{\partial}{\partial y}\left(\frac{\partial \mathrm{F}_{\rho z}}{\partial z}\right)\right) dz$$

where we have defined:

$$\tau_{xz} = \rho K_m \left(\frac{\partial u}{\partial z}\right)$$

$$\tau_{yz} = \rho K_m \left(\frac{\partial v}{\partial z}\right)$$

$$\mathrm{F}_{\rho z} = K_\rho \left(\frac{\partial \rho}{\partial z} - \gamma_\rho\right)$$

and assumed that the ageostrophic velocities can be neglected at the reference layer considered in the integral (here taken as the deepest level).

The function used to estimate the baseline vertical mixing coefficients is taken from the modified version of the K-Profile Parameterization (KPP) proposed by [RD-18], which originally includes an amplification of classical KPP turbulent velocity scales to account for Langmuir cells mixing, a nonlocal momentum flux term and a parameterization of Stokes drift effects. Here, we removed the nonlocal flux of momentum from the formulation of the upper layer mixing parameterization and further constrained the viscosity values not to exceed a consistent empirical estimate. Specifically, we assumed that the background Ekman velocity can be approximated through an analytical fit of the ageostrophic currents (provided at 0 m and 15 m by the empirical reconstruction) to a compressed Ekman spiral:

$$u_{Ekman}(z) = e^{\frac{z}{D_{amp}}}[\, u_0 \cos(z/D_{rot}) - \; v_0 \sin(z/D_{rot})]$$

$$v_{Ekman}(z) = e^{\frac{z}{D_{amp}}}[\, u_0 \sin(z/D_{rot}) + \; v_0 \cos(z/D_{rot})]$$

where (u_0,v_0) are the components of the empirical Ekman current at 0 m, and D_{amp} *and* D_{rot} are the Ekman depth estimates obtained from the amplitude decay and vector rotation between 0 m and 15 m depth, respectively (see also [RD-19]).

The maximum viscosity, K_{max}, allowed within the Ekman layer was then derived from the local Ekman amplitude decay scale:

$$K_{max} = \frac{f D_{amp}^2}{2}$$

imposing an analytical profile within the boundary layer, chosen as in [RD-20]:

$$K_m(z) = K_{max}\left[1 + \tanh\left(\frac{z - D_{amp}}{\delta}\right)\right]$$

where δ represents the thickness of the transition layer (here set to 40 m, as in [RD-20]).

All equations used for the NATL3D retrieval are solved numerically as in [RD-9-11].

3.2.2 Limitations

The LSTM3D reconstruction of the temperature and salinity significantly improves with respect to climatological data and other reference reconstruction tools all along the water column. The LSTM temperature RMSD (estimated vs independent CTD profiles) never exceeds 1 °C, and attains below 0.75 °C already at a 200 m depth, and the LSTM salinity reduces the RMSD to almost one half with respect to the climatology, further improving in the 200–800 m layer.

The 3D current velocity accuracy depends on both the input data and on the theoretical limits of the diagnostic models and parameterizations used. Overall, the Root Mean Square Differences (RMSD) of the total horizontal velocities vs independent measurements provided by colocated SVP velocities are 0.122±0.001 m/s at 0 m and 0.103±0.001 m/s at 15 m depth, respectively. They show a slight improvement with respect to simple geostrophic estimates, which show a RMSD of 0.148±0.001 m/s at 0 m and 0.107±0.001 m/s at 15 m depth. The number of matchups used to compute the statistics is 33515 for undrogued SVP velocities (at 0) m and 31818 for drogued SVP data (at 15 m). Due to their small magnitude (around 1-100 md^{-1}), vertical velocities cannot be directly measured in the open ocean. As such, NATL3D vertical velocities cannot be directly validated (no reference dataset is available). However, the algorithm used to retrieve NATL3D horizontal velocities requires the vertical velocity in input, and improvements in quasi-geostrophic horizontal components with respect to standard geostrophic velocities would necessarily imply that vertical velocity is reliable.

Moreover, as Neumann conditions are applied at the bottom and lateral boundaries in the Omega solution, the model is not suited to model current topography interactions along the coasts. Moreover, the accuracy of the algorithm and input data used for the SSS retrieval are also optimized for offshore areas. As such, the NATL3D product is basically suited for open ocean applications only, and coastal data must be looked at with caution.

3.2.3 Differences with previous version (if relevant, phase 2)

This is the first version of the product.

3.3 Product Description

3.3.1 spatial information

Product Specification Customer Name	WOC-L4-CUR-NATL3D_REP_1D
Geographical coverage	Central/North Atlantic Ocean (20°N-50°N, 76°W-6°W).
Horizontal resolution	1/10° on a regular grid

Number of vertical levels	76 levels: [1.25, 2.50, 4.25, 6.50, 9.25, 12.50, 16.25, 20.50, 25.25, 30.50, 36.25, 42.50, 49.25, 56.50, 64.25, 72.50, 81.25, 90.50, 100.25, 110.50, 121.25, 132.50, 144.25, 156.50, 169.25, 182.50, 196.25, 210.50, 225.25, 240.50, 256.25, 272.50, 289.25, 306.50, 324.25, 342.50, 361.25, 380.50, 400.25, 420.50, 441.25, 462.50, 484.25, 506.50, 529.25, 552.50, 576.25, 600.50, 625.25, 650.50, 676.25, 702.50, 729.25, 756.50, 784.25, 812.50, 841.25, 870.50, 900.25, 930.50, 961.25, 992.50, 1024.25, 1056.50, 1089.25, 1122.50, 1156.25, 1190.50, 1225.25, 1260.50, 1296.25, 1332.50, 1369.25, 1406.50, 1444.25, 1482.50]

3.3.2 temporal information

Product Specification Customer Name	WOC-L4-CUR-NATL3D_REP_1D
Available time series	Version2 = 2010-2019
Temporal resolution	daily

3.3.3 product content

PRODUCT	variables name in the NetCDF file and Unit; long_name standard_name
WOC-L4-CUR-NATL3D_REP_1D	**uo** (meter per second) eastward velocity eastward_sea_water_velocity; **vo** (meter per second) northward velocity northward_sea_water_velocity **wo** (meter per day) vertical velocity upward_sea_water_velocity; **to** (Kelvin) temperature sea_water_temperature; **so** (practical salinity unit) salinity sea_water_salinity
scale_factor/add_offset/missing_value/land mask	Land mask are equal to "_FillValue" (see variable attribute in NetCDF file).

3.3.4 file name convention

Filename and format have been chosen to match the conventions adopted by ESA CCI, CMEMS, GlobCurrent, GHRSST (all complying to the more general Climate & Forecast and ACDD conventions). Following these conventions, the filename is:

<Indicative Date-*yyyymmdd*><Indicative Time-*hhmmss*>-WOC-<Processing Level>-<Parameter>-<Product String>-v< ProductVersion>-fv<File Version>.<File Type>

example :20180912120000-WOC-L4-CUR-NATL3D_REP_1D-v1.0-fv1.0.nc

3.3.5 file format

The products are stored using the NetCDF format.

NetCDF (Network Common Data Form) is an interface for array-oriented data access and a library that provides an implementation of the interface. The netCDF library also defines a machine-independent format for representing scientific data. Together, the interface, library, and format support the creation, access, and sharing of scientific data. The netCDF software was developed at the Unidata Program Center in Boulder, Colorado.

Please see Unidata netCDF pages for more information, and to retrieve netCDF software package.

NetCDF data is:

* Self-Describing. A netCDF file includes information about the data it contains.
* Architecture-independent. A netCDF file is represented in a form that can be accessed by computers with different ways of storing integers, characters, and floating-point numbers.
* Direct-access. A small subset of a large dataset may be accessed efficiently, without first reading through all the preceding data.
* Appendable. Data can be appended to a netCDF dataset along one dimension without copying the dataset or redefining its structure. The structure of a netCDF dataset can be changed, though this sometimes causes the dataset to be copied.
* Shareable. One writer and multiple readers may simultaneously access the same netCDF file.

3.3.6 metadata

The structure and semantic of netCDF files is shown in the following:

```
netcdf file:20180912120000_WOC-L4-CUR-NATL3D_REP-1D-v1.0-fv1.0.nc {
 dimensions:
   depth = 76;
   lat = 300;
   lon = 700;
   time = UNLIMITED;   // (1 currently)
```

```
variables:
  float depth(depth=76);
    :standard_name = "depth";
    :units = "m";
    :axis = "Z";
    :positive = "down";

  float lat(lat=300);
    :units = "degrees north";
    :axis = "Y";
    :standard_name = "latitude";

  float lon(lon=700);
    :units = "degrees east";
    :axis = "X";
    :standard_name = "longitude";

  int time(time=1);
    :units = "hours since 1981-01-01 00:00:00";
    :long_name = "time";
    :standard_name = "time";
    :calendar = "gregorian";
    :axis = "T";
    :_ChunkSizes = 1024U; // uint

  float wo(time=1, depth=76, lat=300, lon=700);
    :_FillValue = -32767.0f; // float
    :long_name = "vertical velocity";
    :standard_name = "upward_sea_water_velocity";
    :units = "m s-1";
    :add_offset = 0.0f; // float
    :scale_factor = 1.0f; // float
    :_ChunkSizes = 1U, 26U, 100U, 234U; // uint

  float uo(time=1, depth=76, lat=300, lon=700);
    :_FillValue = -32767.0f; // float
    :long_name = "eastward velocity";
    :standard_name = "eastward_sea_water_velocity";
    :units = "m s-1";
    :add_offset = 0.0f; // float
```

```
      :scale_factor = 1.0f; // float
      :_ChunkSizes = 1U, 26U, 100U, 234U; // uint

    float vo(time=1, depth=76, lat=300, lon=700);
      :_FillValue = -32767.0f; // float
      :long_name = "northward velocity";
      :standard_name = "northward_sea_water_velocity";
      :units = "m s-1";
      :add_offset = 0.0f; // float
      :scale_factor = 1.0f; // float
      :_ChunkSizes = 1U, 26U, 100U, 234U; // uint

    float to(time=1, depth=76, lat=300, lon=700);
      :_FillValue = -32767.0f; // float
      :long_name = "temperature";
      :standard_name = "sea_water_temperature";
      :units = "K";
      :unit_long = "Kelvin";
      :add_offset = 0.0f; // float
      :scale_factor = 1.0f; // float
      :_ChunkSizes = 1U, 26U, 100U, 234U; // uint

    float so(time=1, depth=76, lat=300, lon=700);
      :_FillValue = -32767.0f; // float
      :long_name = "salinity";
      :standard_name = "sea_water_salinity";
      :unit_long = "practical salinity unit";
      :units = "0.001";
      :add_offset = 0.0f; // float
      :scale_factor = 1.0f; // float
      :_ChunkSizes = 1U, 26U, 100U, 234U; // uint

// global attributes:
  :Conventions = "CF-1.7, ACDD-1.3, ISO 8601";
  :Metadata_Conventions = "Climate and Forecast (CF) 1.7, Attribute Convention for Data Discovery (ACDD) 1.3";
  :standard_name_vocabulary = "NetCDF Climate and Forecast (CF) Metadata Convention version 1.8";
  :title = "North Atlantic data-driven 3D Currents and Tracers (NATL3D)";
  :summary = "This is a data-driven reconstruction of the 3D Currents and Tracers in the North Atlantic obtained by applying artificial intelligence and dynamical diagnostic models to a
```

combination of in situ and satellite data. It was developed in the framework of the European Space Agency World Ocean Circulation Project";

:id = "WOC-L4-CUR-NATL3D_REP-1D";

:product_version = "1.0";

:references = "Buongiorno Nardelli, B. A Deep Learning Network to Retrieve Ocean Hydrographic Profiles from Combined Satellite and In Situ Measurements. Remote Sens. 2020, 12 (19), 3151. https://doi.org/10.3390/rs12193151; Buongiorno Nardelli, B. A Multi-Year Timeseries of Observation-Based 3D Horizontal and Vertical Quasi-Geostrophic Global Ocean Currents. Earth Syst. Sci. Data 2020, No. 12, 1711–1723. https://doi.org/10.5194/essd-12-1711-2020.";

:creator_name = "Bruno Buongiorno Nardelli";

:creator_url = "www.ismar.cnr.it";

:creator_email = "bruno.buongiornonardelli@cnr.it";

:creator_institution = "Consiglio Nazionale delle Ricerche-Istituto di Scienze Marine";

:institution = "Consiglio Nazionale delle Ricerche, Institut Francais de Recherche pour l\'Exploitation de la mer / CERSAT, European Space Agency";

:institution_abbreviation = "CNR, Ifremer/CERSAT, ESA";

:keywords_vocabulary = "NASA Global Change Master Directory (GCMD) Science Keywords";

:comment = "These data were produced at CNR as part of the ESA WOC project.";

:publisher_name = "CERSAT";

:publisher_url = "cersat.ifremer.fr";

:publisher_email = "cersat@ifremer.fr";

:naming_authority = "fr.ifremer.cersat";

:publisher_institution = "Ifremer/CERSAT";

:scientific_support_contact = "bruno.buongiornonardelli@cnr.it";

:technical_support_contact = "cersat@ifremer.fr";

:key_variables = "eastward_current_velocity, westward_current_velocity, upward_current_velocity";

:source = "WOC3D Processor V1.0";

:source_version = "1.0";

:processing_software = "WOC3D";

:format_version = "WOC v1.0";

:netcdf_version_id = "4.7.3 of Feb 19 2020 13:19:27 ";

:date_created = "2021-05-25T17:21:08Z";

:date_modified = "2021-05-25T17:21:08Z";

:track_id = "ec6add23-6c11-4709-9c26-c9182a20ba89";

:grid_resolution = "0.1 degrees";

:software_version = "WOC3D Processor V1.0";

:processing_level = "L4";

:cdm_data_type = "grid";

:time_coverage_start = "2018-09-12T12:00:00Z";

:time_coverage_end = "2018-09-12T12:00:00Z";

:geospatial_lon_min = "-75.975";
:geospatial_lon_max = "-6.075";
:geospatial_lat_min = "20.025";
:geospatial_lat_max = "49.925";
*:Scaling_Equation = "(scale_factor*data) + add_offset";*
:project = "World Ocean Circulation (WOC) - European Space Agency";
:method = "LSTM 3D reconstruction network/ Quasi-geostrophic Omega equation";
:history = "2021-05-25T17:21:08Z - Creation";
:acknowledgement = "Please acknowledge the use of these data with the following statement: these data were obtained from the ESA WOC project";
}