Climate Data Record (CDR) Program

Climate Algorithm Theoretical Basis Document (C-ATBD)

Ocean Heat Content CDR

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REVISION HISTORY

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1. Introduction

1.1 Purpose

The purpose of this document is to describe the algorithm submitted to the National Centers for Environmental Information (NCEI) by Tim Boyer, NCEI that will be used to create the Ocean Heat Content Climate Data Record (CDR). The actual algorithm is defined by the computer program (code) that accompanies this document, and thus the intent here is to provide a guide to understanding that algorithm, from both a scientific perspective and in order to assist a software engineer or end-user performing an evaluation of the code.

1.2 Definitions

OHCA= ocean heat content anomaly

WOD= world ocean database

Temperature anomaly = difference between in situ temperature measurement (interpolated to a standard depth level) and a long-term mean climatology.

First-guess field = a priori assumption of the structure of the geographic distribution of an ocean variable (in this case temperature anomaly).

1.3 Referencing this Document

This document should be referenced as follows:

Ocean Heat Content - Climate Algorithm Theoretical Basis Document, NOAA Climate Data Record Program CDRP-ATBD-0938 Rev. 0 (2017). Available at http://www.ncdc.noaa.gov/cdr/operationalcdrs.html

1.4 Document Maintenance

The algorithm will only evolve upon publication of a peer-reviewed paper describing any changes to the algorithm. In conjunction with publication of any such paper, this document will be updated by the first author of the paper and submitted to the CDR program for review and acceptance.

2. Observing Systems Overview

2.1 Products Generated

One of the critical environmental topics of the present day is climate change related to rising global surface temperatures. In order to understand present climate change and predict future climate change we need to understand the rate at which the Earth is warming and will warm. This requires a fundamental quantification of the amount of heat energy contained in the Earth's system from the top of the atmosphere to the bottom of the ocean (and even below). Earth's energy budget is currently imbalanced, with an estimated +0.5 W m-2 to +1.0 Wm-2 net top-of-the-atmosphere energy flux over the first decade of the 21st century (Trenberth et al. 2014). Oceans cover more than 70% of Earth's surface. Their extensive interface with the atmosphere, combined with their high heat capacity, low albedo, and great depth, has resulted in ocean sequestration of more than 90% of Earth's excess heat over recent years (Roemmich et al. 2015) and recent decades (Bindoff et al., 2007, Rhein et al. 2013). This net buildup of excess heat in the ocean mitigates surface warming, but it increases ocean temperature, contributing to sea ice melt (Liu and Curry 2010; Polyakov et al. 2010), melting at the marine terminations of ice sheets (Straneo and Heimbach 2013; Rignot et al. 2013), changes in atmospheric and oceanic circulations (e.g., Hoerling et al. 2001; Toggweiler and Russell 2008), and sea level rise (Church et al. 2011). So quantification of ocean heat content (OHC) change over time is imperative for understanding the Earth's energy budget and climate change.

The Ocean Climate Lab (OCL) at the National Centers for Environmental Information (NCEI) has developed a method for estimating OHC anomaly (OHCA), the difference of OHC at a given time step (3-month, yearly ,pentadal) from long-term mean OHC, from in situ subsurface oceanographic temperature profiles. The method and results have been published in the peer-reviewed literature (Levitus et al., 2000, Levitus et al., 2005, Levitus et al., 2009, Levitus et al., 2012). All steps in the method are executed by the OCL from aggregation of the in situ data into the World Ocean Database (WOD, Boyer et al. 2013) to calculation of long-term means (World Ocean Atlas, Locarnini et al., 2012 through global OHCA integration and posting for public access (http://www.nodc.noaa.gov/OC5/3M_HEAT_CONTENT/). All methods, necessary data and results are also posted for transparency

The final product is a set of time series of OHCA from 1955 to present on a 3-monthly, yearly, and pentadal (five-yearly) time scale. OHCA is calculated from the surface to 700m and from the surface to 2000m. The 0-700m field is where the largest portion of heat sequestration occurs and coincides with the deepest depth of the expendable bathythermograph (XBT) the main component of the observing system for subsurface ocean temperatures 1967-2002. The 0-2000m field matches the domain of the Argo floats, the main observing system 2003-present. While there is contribution to OHCA from below 2000 m (Purkey and Johnson, 2010), the contribution is proportionally small and historic measurements are not abundant. The product includes time series of OHCA for the global ocean and each of the major basins (Atlantic, Pacific, and Indian). Time series for the global ocean and basins are also available divided by hemisphere (Northern, Southern). All base data (in situ temperature profiles) for the calculations are made available through the WOD. Baseline climatologies WOA 2009 (WOA09) are also publicly available, along with land/ocean bottom mask (derived from ETOPO1) and basin definition mask. Gridded temperature anomaly fields and OHCA fields are also publicly available. Data and accompanying graphics are all available at http://www.nodc.noaa.gov/OC5/3M_HEAT_CONTENT/.

2.2 Instrument Characteristics

OHCA calculations use in situ ocean profiles (depth vs. variable) of temperature. The source of these data is the World Ocean Database (WOD). The WOD is an NCEI product which aggregates historical and recent ocean profile data from all available sources, converts to one standard format, and performs documented quality control procedures (Boyer and Levitus, 1994) on the data. The database is fully described in Boyer et al. 2013 found at http://data.nodc.noaa.gov/woa/WOD/DOC/wod_intro.pdf. The WOD is released approximately every four years with full quality control. In order to calculate OHCA on a quarterly basis, the WOD is updated every three months with the most recent data.

The OHCA calculations depend entirely on the timely delivery of in situ data from the Argo program, the Global Temperature and Salinity Profile Program (GTSPP), and the three tropical moored buoy array programs (TAO/TRITON in the Pacific, PIRATA in the Atlantic, and RAMA in the Indian) through the Pacific Marine Environmental Laboratory (PMEL). All three data streams are gathered in the NCEI archive. These are the three main near-real time data streams which comprise the base dataset for OHCA calculations. Many other projects and programs contribute data in delayed-mode (> 48 hours after measurement) and these data are vital for augmenting and updating the OHCA time series. All of these data sets are aggregated in the WOD.

3. Algorithm Description

3.1 Algorithm Overview

The algorithm for calculating OHCA is fully described in a series of peer-reviewed publications (Levitus et al. 2001, Levitus et al. 2005, Levitus et al. 2012, Boyer et al. 2016). The basic premise is to subtract in situ temperature measurements from a long-term climatological mean, convert to units of energy, and integrate over the water column to a specified depth and over the geographic extent of the World's Ocean

3.2 Processing Outline

A diagram of the process for calculating OHCA is found in Figure 1. In situ temperature profiles from the last three months are used as input. These data are aggregated in the WOD. Please see Boyer et al., 2013 for details on input instruments and sensors, as well as applied quality control. As part of the WOD processing, standard levels are selected, or interpolated when necessary. The set of standard levels can be found in Johnson et al. 2013, appendix 9. [Note that based on Levitus et al., 2012, the standard depths in use are a subset of appendix 9, as listed in ftp://ftp.nodc.noaa.gov/pub/WOA09/DOC/woa09documentation.pdf, table 2. Temperature values at standard levels are then subtracted from a long-term climatological monthly mean. The climatological monthly mean set used is the World Ocean Atlas 2009 (WOA09, Locarnini et al., 2010). This climatological mean field is a long-term mean over the time period 1955-2006. Means of the resultant temperature anomalies at each depth are calculated for each one-degree latitude/longitude grid box over the World's Ocean. The in situ data are irregular in space, so an objective analysis procedure is executed on the temperature anomaly mean fields at each depth to create a temperature anomaly field without any geographic gaps (one-degree grid boxes without a value). The objective analysis technique is described in Locarnini, 2010. Now OHCA is calculated for each depth interval for each one-degree grid box. Each temperature anomaly at each standard depth represents a volume of ocean which consists of the area of the one-degree box multiplied by half the distance between adjacent standard levels (both above and below, excepting surface which has no level above and the last level, which has no level below). The volume of water multiplied by the temperature anomaly multiplied by the specific heat of sea water multiplied by the density of sea water gives the OHCA value for the depth interval for each one-degree box. The density used is from a climatological mean field of density calculated from in situ measurements of temperature and salinity found in the WOD. At this point, the OHCA fields (and if necessary, the gridded temperature anomaly fields) are scientifically quality controlled through a visual inspection by an expert. This is necessary, since, no matter the efficacy of the automatic quality control procedures for the WOD, there are many in situ measurements which represent perfectly legitimate oceanic conditions, but which are on such a small time/space scale as not to be representative of the given area of the ocean over the three month period of OHCA calculation. If such anomalous anomalies are encountered, the scientist will investigate all in situ measurements incorporated in the mean value and flag any that are not deemed within the norm for anomalies over the three month period. If this occurs, the flag information is fed back into the WOD and the OHCA gridded fields are recalculated from that point. Once a field free of anomalous anomalies is produced, the final step is to integrate (sum) the OHCA over depth for each one-degree box, and geographically over all one-degree boxes to get a OHCA for the World's Ocean.

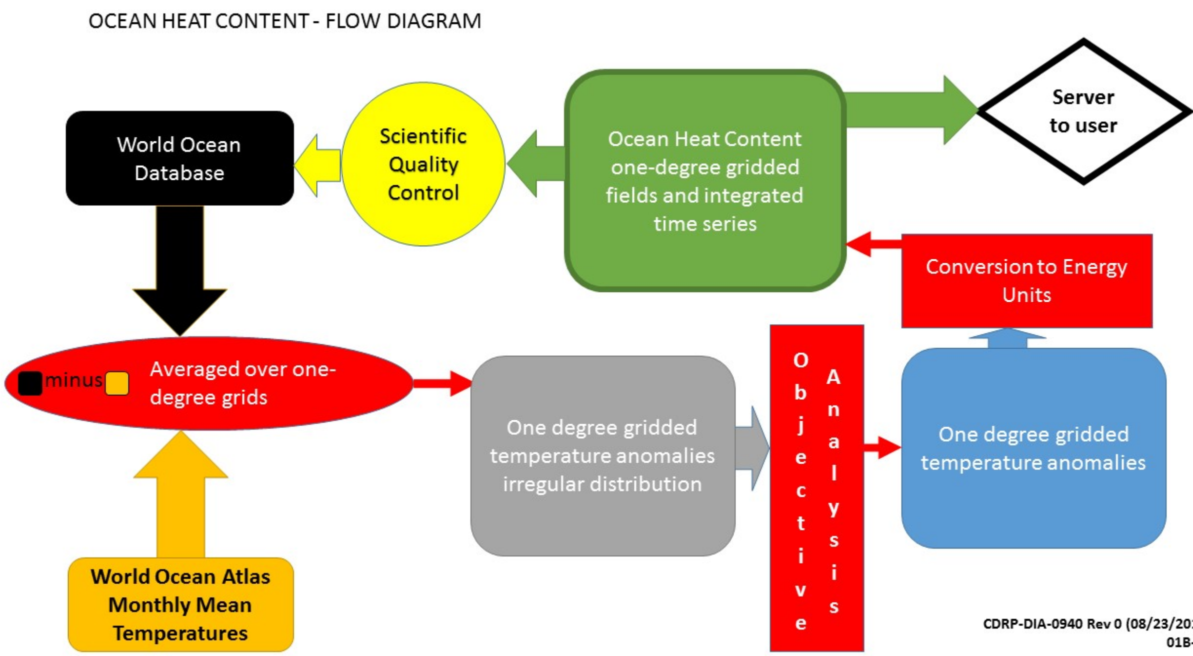

Figure 1: Diagram of OHCA calculation procedure

3.3 Algorithm Input

3.3.1 Primary Sensor Data

Raw sensor data are ocean profiles of temperature aggregated within the WOD. Details on the different sensors/instruments/platforms are found in Boyer et al., 2013.

3.3.2 Ancillary Data

Ancillary data sets used in the objective analysis procedure can be found on https://www.nodc.noaa.gov/OC5/WOA09/masks09.html These consist of a land/sea bottom mask derived from the ETOP02 product https://www.ngdc.noaa.gov/mgg/global/etopo2.html The means of using the two minute mask to estimate a bottom depth and land/sea boundaries are detailed in Locarnini et al., 2010. The other two masks are for defining different oceanic regimes which may or may not mix within the objective analysis procedure. Use of the masks is described in Locarnini et al., 2010.

3.3.3 Derived Data

Quality control flags and interpolation to standard depth levels are described in Boyer et al., 2013. These procedures are performed in the assembly of the WOD. A bias correction is applied to the Expendable Baththermograph (XBT) instrument type. This correction is applied at the interpolation step in WOD and is described in Boyer et al., 2013, Levitus et al., 2012, and Boyer et al., 2016.

3.3.4 Forward Models

Not applicable

3.4 Theoretical Description

The code is written in FORTRAN with underlying C routines for read/write. The OHCA is integrated (summed) over all depths and all one-degree latitude longitude grid boxes to get a global OHCA. The specific heat of seawater and the density of seawater are used to transform a temperature anomaly into units of energy (OHCA). The temperature anomaly is calculated by subtracting in situ measurements interpolated to standard levels from a long-term climatological mean from 1955-2006, then averaging all such values over a one-degree latitude/longitude box.

3.4.1 Physical and Mathematical Description

For each one-degree grid box:

$$\mathbf{A}\int_{z1}^{z2} \rho \, C_p \Delta \mathrm{T} \, \mathrm{dz}$$

A = area of one-degree lat x one-degree lon square)

ρ = density of seawater

C_p = specific heat of seawater

ΔT = temperature anomaly

dz = thickness of the vertical layer of integration

Then sum (integrate) over all one-degree boxes.

3.4.2 Data Merging Strategy

In situ measurements from the WOD are used. For a full description of the WOD, please see Boyer et al.,, 2013.

3.4.3 Numerical Strategy

Objective analysis is a commonly used algorithm to create a full regular gridded data set from irregularly spaced data. Basically, for all one-degree grid boxes, a radius of influence is drawn from the center. A weighted mean of all one-degree boxes with data within that radius of influence minus a first-guess field for that box is calculated for the one-degree box at the center of the radius of influence. The first guess field for the temperature anomalies is set to 0.0˚C denoting the assumption that the ocean temperature field is static in the long-term. The procedure is described in full in Locarnini et al., 2010.

3.4.4 Calculations

Program finalsd.f calculates mean and standard deviation for one-degree temperature anomalies. Subroutine preparesddata.f implements XBT bias correction and compiles submeans for measurement sets which oversample a region (such as moored buoys which sample every hour or every day). Submean time step is one month. calconedegreestats.f calculates the actual statistics.

Program analysis_max.f runs the objective analysis as detailed in section 3.4.3. The main calculation steps in the program are in subroutine analyzepoint.f which performs the weighted averaging of the difference between the observed mean and the first guess field for all grid boxes within the radius of influence of a given grid box. Subroutine thesmoothers.f provides additional 3 and 5 point smoothing. Subroutine weights.f calculates weights for all grid boxes within a radius of influence.

Program layer_field_10ann_climatology_tmod.f calculates OHCA from temperature anomalies within a given depth range. All the calculations are in the main program: calculation of given volume of water, multiplication by specific heat of seawater, by density of sea water, and by temperature anomaly.

Program basin-layer10ann_climatology_tmod.f calculates basin and global OHCA integrals.

3.4.5 Look-Up Table Description

File devfile.d contains all instructions for running the one-degree mean compilation.

XBT bias correction tables are publicly available on https://data.nodc.noaa.gov/woa/WOD/XBT_BIAS/antonov_xbtbias_2.dat Corrections for subsequent years are the same as the last year in the table

File anlyfile.d contains all instructions for running the objective analysis.

File layer_field_10ann_climatology_tmod.inf contains all necessary information for layer_field_10ann_climatology_tmod.f

File basin-layer10ann_climatology_tmod.f

File OCL_basin.dat contains a list of basins to include in the calculation for basin-layer10ann_climatology_tmod.f All basins are included in the global integral.

3.4.6 Parameterization

Density used is not in situ (due to lack of accompanying salinity measurements in some cases) but rather climatological mean density.

3.4.7 Algorithm Output

Algorithm outputs ASCII files of OHCA by year + standard error of the mean representing uncertainty of the calculation.

4. Test Datasets and Outputs

4.1 Test Input Datasets

The test input data set is the WOD.

4.2 Test Output Analysis

4.2.1 Reproducibility

Run through the algorithm steps as outlined above and compare the results to those found on https://www.nodc.noaa.gov/OC5/3M_HEAT_CONTENT/basin_data.html

4.2.2 Precision and Accuracy

The uncertainty of the OHCA calculation has been documented in Boyer et al. (2016). The uncertainty (for each year) is roughly 31 ZJ (zetajoules=10^{21} joules)

4.2.3 Error Budget

	Mapping Method	**XBT bias correction**	**Baseline Climatology**
DOM	16.5 (17.1) ZJ	16.7 (18.9) ZJ	11.8 (7.1) ZJ
LEV	16.5 (17.1) ZJ	11.1 (10.4) ZJ	3.5 (2.7) ZJ
PMEL_M	16.5 (17.1) ZJ	7.4 (11.5) ZJ	14.5 (4.7) ZJ
PMEL_R	16.5 (17.1) ZJ	12.1 (15.3) ZJ	6.6 (4.9) ZJ
ISH	16.5 (17.1) ZJ	9.5 (10.5) ZJ	8.6 (3.9) ZJ
EN	16.5 (17.1) ZJ	12.8 (15.1) ZJ	11.8 (5.6) ZJ
GOU	16.5 (17.1) ZJ	11.3 (15.2) ZJ	11.5 (9.8) ZJ
WIL*	*(17.1) ZJ	* (12.8) ZJ	* (3.1) ZJ
Average	16.5 (17.1)	11.6 (12.2)	9.8 (5.2)

Table 1: Time-mean standard deviations of global OHCA associated with variations in XBT bias corrections and baseline climatologies for different mapping methods for 1970–2008 and 1993–2008 (in parentheses).

* WIL method can only be calculated from 1993–2008. XBT bias correction standard deviation only through 2004, since XBT were not used in this experiment beyond that year. XBT bias correction standard deviations also exclude years 1999–2001 due to obvious outliers in the W08 method for those years.

The above table is reproduced from Boyer et al. (2016) and is a breakdown of uncertainty in the OHCA calculation for eight different methods of calculation including the present (LEV).

5. Practical Considerations

5.1 Numerical Computation Considerations

Algorithm is run sequentially in the programs as listed above.

5.2 Programming and Procedural Considerations

None, except the need to run within the WOD database system. The WOD database system is a set of FORTRAN and C routines plus bash scripting. The FORTRAN and C compiler is GNU freeware (gfortran, gcc).

5.3 Quality Assessment and Diagnostics

As described above, one-degree fields are inspected visually and any 'anomalous anomaly' tracked down to source in situ data and flagged before rerunning fields. Overall quality assessment of procedure is carried out in the peer-reviewed literature (e.g. Boyer et al., 2016).

in situ profile data are converted to a single format for inclusion in the WOD. This in itself is a quality control step, insuring adherence to documented format. Once in the WOD automated quality control steps (Boyer et al., 1994, Johnson et al., 2013) are performed and any prevalent problems investigated.

5.4 Exception Handling

Exception handling is performed in the compilation of the WOD where any suspect values are flagged. The software in this procedure will not produce exceptions based on non-flagged data from WOD.

5.5 Algorithm Validation

The algorithm has been extensively reviewed in the peer-reviewed literature. See Boyer et al., (2016) and citations therein for recent reviews.

5.6 Processing Environment and Resources

A standard processor running linux (any flavor should do, we run under both Red Hat 6.0 and Centos 7.0) with the bash shell, GNU gfortran and gcc compilers. No external libraries are necessary. However all routines are part of the WOD system. The WOD system is just a set of bash shells and FORTRAN/C programs/routines. One processor running for approximately six minutes will produce a quarterly OHCA to add to the existing time series. For the entire time series, 62 years * 4 quarters * 6 minues=a little more than 24 hours. Storage totals 56M per quarter or about 14G total.

6. Assumptions and Limitations

The algorithm is data limited in that ocean coverage below a certain level (usually estimated as about 40%) has an unacceptable uncertainty. This and the many assumptions leading to the OHCA algorithm (the present one and others extant) are covered in Boyer et al. (2016). The main assumption is the efficacy of the specific analysis used, in this case objective analysis and the proper first guess field to use. The first-guess field used for the temperature anomalies is 0.0˚C, the assumption of no change. This assumption is important mainly in areas of low data coverage (the main limitation of the algorithm). The assumption is also made that despite the change of instrumentation over the years, measurement errors (after WOD quality checks) are mainly random and cancel in the large-scale averaging performed as part of the algorithm.

6.1 Algorithm Performance

Again, Boyer et al. (2016) covers many aspects of algorithm performance and its relation to the limitations of data coverage.

6.2 Sensor Performance

The temperature sensors used in the algorithm are expected to be stable. However, the instrumentation and platforms used differ over the years in their accuracy and precision. As noted above, aside from specific bias correction, the instrument error is assumed to be random and cancel in the large-scale averaging performed here.

7. Future Enhancements

There is a wealth of peer-reviewed literature on possible improvements to the OHCA algorithm. One enhancement is the continued addition of historical and recent data to the WOD, mitigating the effects of data sparsity wherever and whenever possible. Other enhancements include a first-guess field which invokes the scientific consensus that the ocean is warming over time, and higher resolution in depth.

7.1 Enhancement 1

Cheng et al., 2017 discuss a first-guess field based on a large radius of influence, much larger than that used in the current algorithm. This larger radius of influence will be used to provide a mean first-guess field based on a much larger area, leaving many fewer areas (ultimately no area) without a measurement based first-guess field.

7.2 Enhancement 2

As shown in a number of peer-reviewed reports, including Levitus et al., 2012, most of the heating of the ocean occurs in the upper 700m and drops off significantly with depth. To better delineate this depth drop-off, we will be using the full set of depth levels from Johnson et al. (2013) rather than a subset as at present.

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Appendix A. Acronyms and Abbreviations

Acronym or Abbreviation	Definition
ANSI	American National Standards Institute
C-ATBD	Climate Algorithm Theoretical Basis Document
CDR	Climate Data Record
IEEE	Institute of Electrical and Electronic Engineers
ICD	Interface Control Document
IOC	Initial Operating Capability
FOC	Full Operating Capability
GTSPP	Global Temperature and Salinity Profile Program
NCEI	National Centers for Environmental Information
NOAA	National Oceanic and Atmospheric Administration
OAD	Operational Algorithm Description
OCL	Ocean Climate Laboratory
PMEL	Pacific Marine Environmental Laboratory
TAO	Tropical Atmosphere Ocean
WOD	World Ocean Database
XBT	Expendable Bathythermograph