Scattered Dataset of Global Ocean Temperature and Salinity Profiles from the International Argo Program

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Abstract: By the end of 2020, the International Argo Program had collected more than 2.3 million temperature and salinity (TS) profiles throughout the global ocean. Although the Argo Data Assembly Centers (DACs) of various countries conduct quality controls on each TS profile, the data quality that DACs submit is uneven because of differences in decoding software, float technical faults and selected thresholds in the quality control procedures. In addition, Argo datasets are becoming increasingly complicated, which introduces difficulty when users read and make use of them. To facilitate the usage of Argo datasets, the China Argo Real-Time Data Center (CARDC) has started to reconstruct TS data through the use of strict post-quality control measures. The dataset is archived in .dat format and comprises 2,244,712 data files with a data size of 41.1 GB (compressed to 18 files of 7.56 GB).

Keywords: Argo; temperature; salinity; global ocean

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Dataset Availability Statement:

The dataset supporting this paper was published and is accessible through the *Digital Journal of Global Change Data Repository* at: https://doi.org/10.3974/geodb.2021.06.05.V1 or CSTR:20146.11.2021.06.05.V1.

1 Introduction

Ocean and atmospheric scientists from the United States, Australia, France and Japan formally proposed the "Array for Real-time Geostrophic Oceanography (Argo)", or the International Argo $Program^{[1-3]}$ in 1998, with the aim to build an observation network

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comprising 3,000 autonomous profiling floats in the ice-free regions of the world ocean within 5-7 yrs. With this network, temperature and salinity profiles in the global ocean (0 to 2,000 m water depth) were collected with the intention to improve the accuracy of climate forecasts and more effectively mitigate against hazards caused by global climate change, such as hurricanes, tornadoes, floods and droughts. Many coastal countries quickly responded to the program since its release. The United States and Australia first deployed two batches of autonomous profiling floats in 2000 in the Atlantic Ocean, southeastern Pacific Ocean and the eastern Indian Ocean, marking the comprehensive initiation of the global Argo network. As of November 2007, an observation network comprising 3,000 floats, known as "core Argo," that records seawater temperature and conductivity/salinity only had been officially established under the combined efforts of nearly 30 countries. Furthermore, about 800–1,000 floats were planned for deployment every year to maintain the normal operation of the observation network. As an important component of the Global Ocean Observing System (GOOS), the Argo network is a revolution in oceanographic observations because it is the most effective method for obtaining temperature and salinity profiles in the middle and upper layers of the global ocean^[4-5].</sup>

Autonomous profiling floats were used as observation equipment in the global Argo network, termed "Argo profiling floats". In general, an Argo float can dive to 1,000 m by changing its own buoyancy after being deployed by a ship or aircraft, and drift freely with the ocean current at this depth for about 9 days. Then, the float dives another 1,000 m. After reaching 2,000 m, the float ascends to the surface at a speed of about 10 cm/s. During the ascent, temperature, conductivity (automatically converted to salinity) and pressure (10^4 Pa) is roughly equal to 1 m in shallow water) are measured by a mounted conductivitytemperature-depth (CTD) sensor. When the float reaches the sea surface, the top-mounted satellite antenna obtains positioning information and then transmits the observation data and float technical information. After all of the data are sent, the float dives again to start the next mission cvcle^[2,3,6,7]. The International Argo Program collected one million temperature and salinity profiles over the global ocean in 14 yrs (1999 to 2013). As of September 2018, up to two million temperatures and salinity profiles had been collected, which far exceeds the volume of data obtained through ship-borne CTD, expendable bathythermograph (XBT) and moored buoys. Currently, the International Argo Program is expanding into the deep water, polar regions, marginal seas and various biogeochemical variables with the goal of building a truly global, full-depth and multi-disciplinary integrated ocean observation network comprising 4,700 floats, including 2,500 core Argo floats, 1,200 deep Argo floats and 1000 biogeochemical Argo floats^[8].

To ensure the quality of Argo float observation data, the International Argo Program developed real-time/delayed mode quality control methods and unified data storage specifications and formats at the initial stage of implementation. Additionally, it required the various Data Assembly Centers (DACs) from different countries to conform to those methods. Moreover, the Argo Data Management Team (ADMT) was also established to oversee any improvements in quality control methods and revision criteria^[9–12]. Two Global Argo DACs (GDACs), located in France and the United States, also conduct quality inspections on each temperature and salinity profile to aggregate the Argo data submitted by various countries. If problems are found, these GDACs send reminders to the affiliated data centers and ask that the quality control operators re-test the data. An individual Argo float is an expendable marine observation instrument that operates continuously at sea for about 3–5

yrs after deployment. They can be affected by seawater corrosion, biological fouling and biocide leakage into the conductivity cells, which may lead to sensor drift in the conductivity sensor; once noted, this needs to be corrected to prevent systematic errors in the conductivity/salinity observation profiles^[13]. Therefore, ADMT organized technicians to develop a delayed-mode quality control method for float observation data. Specifically, float salinity is corrected with a historical high-quality shipboard CTD dataset near the float as a reference^[14]. In general, the first delayed-mode quality control is carried out within 6-12 months after a float deployment. Nevertheless, conducting this on profiling data from the global ocean is time-consuming and laborious and requires judgments from skilled personnel. Further, the different human resources invested by DACs lead to different progress in delayed-mode quality control. Hence, quality problems can still be found in the global ocean Argo dataset, and it is suggested that users conduct careful post-quality control for ensuring high-quality data. The China Argo Real-Time Data Center (CARDC) developed a set of Argo temperature and salinity post-quality control methods in 2019 that are operated automatically. They can quickly detect data problems such as sensor drift or offset, satisfying the needs of users in pursuit of high-quality Argo data.

2 Metadata of the Dataset

The metadata of the "Scattered dataset of global ocean temperature and salinity profiles from the International Argo Program" is summarized in Table 1. It includes the dataset full name, short name, authors, year of the dataset, temporal resolution, spatial resolution, data format, data size, data files, data publisher, and data sharing policy, etc.^[15].

3 Data Coverage and Composition

3.1 Spatio-temporal data coverage

The float observation profiles collected by the global ocean Argo temperature and salinity profiling scattered dataset cover from July 1997 to December 2020. The spatial range was 90 S-90 N to 180 W-180 E and incorporated the Pacific, Indian, Atlantic and Arctic oceans and major marginal seas. Data coverage and density are shown in Figure 1.

3.2 Data composition

Each Argo temperature–salinity profile was saved as a data file (.dat). The whole dataset comprises 2,244,712 data files, and each set of data files comprises header information and observational data. More precisely, the header information includes the World Meteorological Organization (WMO) number of the float, cycle number, affiliated project, principal investigator (PI), float model, float serial number, communication system, positioning system, sampling direction, data mode, observation time and satellite positioning information. The observation data contains pressure (10^4 Pa), corrected pressure (10^4 Pa), temperature ($^{\circ}$ C), corrected temperature ($^{\circ}$ C), salinity (psu), corrected salinity (psu) and the quality control flags of three elements (Table 2). The file is named XXXXXXX_NNN.dat. In this, XXXXXXX refers to the WMO number (unique identification code) of the float, and NNN is the cycle number of the float.

Itoma	Descriptions
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Dataset name	Scattered dataset of global ocean temperature and samily profiles from the international Argo Program
Dataset Short name	Global_Argo_TS_dataset_1997-2020
Authors	Liu, Z. H. M-9975-2015, Second Institute of Oceanography, Ministry of Natural Resources, liuzenghong@139.com
	Li, Z. Q. AAJ-4021-2021, Second Institute of Oceanography, Ministry of Natural Resources, lizbaogin@sio.org.cn
	Lu, S. L. AAJ-7419-2021, Second Institute of Oceanography, Ministry of Natural Resources, 13224004@163.com
	Wu, X. F. J-2546-2016, Second Institute of Oceanography, Ministry of Natural Resources, wuxiaofen 3° 0163 com
	Sun, C. H. AAK-6331-2021, Second Institute of Oceanography, Ministry of Natural Resources, siosun@163.com
Geographic area	Xu, J. P., Second Institute of Oceanography, Ministry of Natural Resources, sioxjp@139.com Oceans (including marginal seas such as the Gulf of Mexico, Japan Sea, Bering Sea,
Year	Mediterranean Sea, South China Sea, Red Sea, and Black Sea, etc.) in the globe 1997–2020
Data format	.dat
Data size	7.56 GB (compressed)
Dataset composition	Global ocean Argo temperature and salinity profile data
Foundations	Program of Ministry of Science and Technology (2012FY112300); Scientific Research Fund of the Second Institute of Oceanography, MNR (JG1709, JG1812); Zhejiang Natural Science Foundation (LQY18D060001); National Natural Science Foundation of China (U1811464)
Data Computing Environment	Linux version 3.10.0-693.el7.x86_64, MATLAB R2018b 64bit
Data publisher	Global Change Research Data Publishing & Repository, http://www.geodoi.ac.cn
Address	No. 11A, Datun Road, Chaoyang District, Beijing 100101, China
Address	Institute of Geographic Sciences and Natural Resources Research, Chinese Academy of Sciences, Jia No. 11, Datun Road, Chaoyang District, Beijing 100101, China
Data sharing policy	Data from the Global Change Research Data Publishing & Repository includes metadata, datasets (in the <i>Digital Journal of Global Change Data Repository</i>), and publications (in the <i>Journal of Global Change Data & Discovery</i>). Data sharing policy includes: (1) Data are openly available and can be free downloaded via the Internet; (2) End users are encouraged to use Data subject to citation; (3) Users, who are by definition also value-added service providers, are welcome to redistribute Data subject to written permission from the GCdataPR Editorial Office and the issuance of a Data redistribution license; and (4) If Data are used to compile new datasets, the 'ten per cent principal' should be followed such that Data records utilized should not surpass 10% of the new dataset contents, while sources should be clearly noted in suitable places in the new dataset ^[16]
Communication and searchable system	DOI, CSTR, Crossref, DCI, CSCD, CNKI, SciEngine, WDS/ISC, GEOSS

Table 1	Metadata profile of the "Scattered dataset of global ocean temperature and salinity profiles from
	the International Argo Program"



Figure 1 Profile density distribution of global Argo temperature and salinity data from 1997 to 2020

4 Methods for Data Quality Control

Argo temperature and salinity profiles from various floats over the global ocean were obtained from GDAC. Data might vary in quality for a number of reasons, although real-time quality control has been performed on all profiles according to the Argo real-time quality control manual with delayed-mode quality control also conducted on some data^[14]. To improve the dataset quality, the post-quality control method established by CARDC was adopted to perform rigorous

1	1 5 5
Quality control flags	Description
0	Without quality control
1	Good data
2	Possibly good data
3	Bad data that are correctable
4	Bad data
8	Interpolated data
9	Missing data

 Table 2
 Description of quality control symbols

screening and quality control over all profile data. Moreover, temperature and salinity observation data of various floats were mapped for manual review, thereby generating a set of high-quality global ocean Argo temperature and salinity profile scatter datasets^[15].

4.1 Post-quality Control Methods

Specifically, the post-quality control technical scheme for Argo temperature-salinity profile is composed of a real-time quality control manual specified by ADMT, and a set of special tests developed by CARC, which include steps such as observation time, positioning position, drift speed, abnormal temperature and salinity, density inversion and pressure anomaly, as well as the MEDD test developed by the Coriolis Data Center (France) and the climatology test developed by CARDC. In total, this can include up to 15 test steps:

(1) Observation time. Data files with a profile observation time prior to 1 January 1996 or later than the current date (i.e. date of data processing) were deleted.

(2) Longitude and latitude. When the longitude and latitude of the profile were outside of the ranges (-180, 180) and (-90, 90), respectively, the quality control flag of the position was marked as "4".

(3) Satellite positioning: The bathymetry was calculated from the Earth topography five minute grid (ETOPO5; http://iridl.ldeo.columbia.edu/SOURCES/.NOAA/.NGDC/.ETOPO5/ datasetdatafiles.html) based on the profile positioning information. If the bathymetry was greater than 0, the quality control flag of the position was marked as "4"; if the position was obtained after linear interpolation of the current profile, the position quality flag was marked as "8".

(4) Float drift speed. The float drift speed is calculated according to the latitude, longitude and time of the current and previous profiles. If the speed was greater than 2 m/s, it was judged as failing the test, marking the quality control flag of the position as "4".

(5) Global range test of variables. When the pressure was less than -2.5×10^4 Pa, the temperature was outside of -2.5-40.0 °C or the salinity was outside 2.00-41.00 psu, the quality control flags of pressure, temperature and salinity were marked as "4". Thus, when problems arose in the pressure range, the associated temperature and salinity were also marked.

(6) Specific area. When a profile originated in the Red or Mediterranean seas, the temperature and salinity ranges were 4.0–21.7 $^{\circ}$ C and 10.0–40.0 psu (Red Sea) and

2.00–41.00 $^{\circ}$ C and 2.00–41.00 psu (Mediterranean Sea). If the temperature or salinity was out of this range, the quality control flag was marked as "4".

(7) Increasing pressure. If the observed pressure does not increase uniformly, the corresponding pressure and its adjacent pressure were marked as "4", as were the associated temperature and salinity.

(8) Profile spike. The test first detected whether a spike was present in the temperature and salinity profile. If yes, the quality control flage was marked as "4".

Table 5	I freshold settings of the	e MEDD method
Pressure	Temperature (\mathcal{C})	Salinity (psu)
(MPa)	threshold	threshold

Tressure	Temperature (C)	Samily (psu)
(MPa)	threshold	threshold
<0.6	5.0	1.0
0.6-1.5	3.5	1.0
1.5-5	0.5	0.08
5-10	0.15	0.02
10-21	0.05	0.004
>21	0.004	0.000,2

(9) Profile gradient. Detection was performed according to the corresponding gradient thresholds of temperature and salinity in different pressure ranges. If the calculated gradient was greater than the corresponding threshold, the quality control flag was marked as "4".

(10) MEDD. This method was proposed by Dr. D. Dobler (Coriolis Data Center) at the 20th ADMT meeting (Villefranche-sur-Mer, France, 2019), and the relevant program scripts were distributed to DACs for shared application. The MEDD method first sets temperature and salinity change thresholds for different depths (see Table 3), obtains the vertical sliding median value and data boundary and finally calculates the distance between the observation value and the median value of the corresponding depth to detect a spike together with the density profile. After testing, this method can effectively detect continuous and obvious spike abnormalities (Figure 2).

(11) Digit rollover. There is a problem caused by insufficient float data (or code) storage, which leads to large data differences in adjacent levels. If the temperature difference between two adjacent observation levels was greater than 10 $^{\circ}$ C or the salinity difference was greater than 5 psu, its quality flag was marked as "4".

(12) Frozen profile. If all temperatures or salinities in the observation profile were equal to the same value, its quality control flag was marked as "4".

(13) Density inversion. A universal seawater toolkit was used to calculate the water density from shallow to deep. If the density of the current layer minus the density of the next layer was greater than 0.03 kg/m^3 , both temperature and salinity of the two layers were marked as "4". Conversely, from deep to shallow, if the density of the current layer minus the density of the next layer was less than -0.03 kg/m^3 , the temperature and salinity of these two layers were also marked as "4".



Figure 2 MEDD test example using the 163th salinity profile from float 3901496. The open circles represent the original data, 'x' indicates detected abnormal data, and the solid line is the median value obtained from the MEDD method with dotted lines representing the left and right boundaries

(14) Deepest pressure: If the pressure was greater than 1.1 times the maximum pre-set observation depth of the float, then the corresponding

pressure, temperature and salinity values were all marked as "4".

(15) Climatology. The test searches for nearby historical CTD data (or historical Argo data, Fig. 3) provided by the Coriolis Data Center for Argo delayed-mode quality control based on the position of each profile; they calculated the standard deviation of temperature and salinity at different depths. When the temperature or salinity value of the float was outside of the range of ± 6.5 times the standard deviation, its quality was marked as "3" (i.e. suspicious data). When a profile had more than 33% of its data (temperature or salinity) marked as "3", all of the data from the whole profile were marked as "3".

Figure 4 displays the climatology test results of a salinity profile (No. 93) of a float (No. 2902581). The salinity below 463×10^4 Pa falls outside ± 6.5 times the historical CTD standard deviation, demonstrating that the salinity profile may have drifted. In this case, delayed-mode quality control (salinity correction) or additional input from personnel with professional knowledge would be required.



Figure 3 Geographical distribution of historical CTD data for Argo delayed-mode quality control. The colors represent the year when the CTD data were acquired



Figure 4 Example of the climatology test (the 93^{th} salinity profile from float 2902581). The gray dotted lines indicate historical CTD data, the black dotted lines represent ± 6.5 times the standard deviation calculated by historical CTD data and the solid black line is the average calculated by historical CTD data. The open circles represent Argo salinity data falling within ± 6.5 times the standard deviation and the filled

circles represent Argo salinity data falling outside the range of ±6.5 times the standard deviation

5 Dataset Results and Verification

5.1 Data Results

Overall, 2,373,923 temperature and salinity profile files were obtained from GDAC from July 1997 to December 2020, and, of these, about 2,244,712 files were retained after the post-quality control procedure^[17], accounting for about 94.5% of the total profiles (Fig. 5). With the addition of new Argo floats and the increase in float lifetimes, more than 100,000 temperature and salinity profiling files have been received each year from the observation network since 2008. By the end of 2020, the global Argo network constituted about 4000 active floats that can obtain at least 150,000 temperature and salinity profile files annually. In other words, the current global Argo network can obtain one million temperature and salinity profile files in less than 7 yrs.



Figure 5 Number of temperature and salinity profiles provided by the global Argo real-time ocean observation network from 1997 to 2020. The gray bars indicate the number of profiles after post-quality control measures while the black bars show the number of profiles before post-quality control

5.2 Evaluation of Data Accuracy

At present, Argo floats are normally equipped with SBE41 or SBE41CP CTD sensors (Sea Bird Inc.), with a laboratory calibration accuracy of pressure of $\pm 2.0 \times 10^4$ Pa, temperature of ± 0.002 °C and conductivity of ± 0.0003 S/m (equivalent to salinity of ± 0.0035 psu). It should be noted that this level of accuracy cannot be reached in actual observations. In particular, the Argo float is an expendable instrument, which cannot re-calibrate the CTD sensor after recovery, unlike shipboard CTD instruments or underwater gliders. Wong et al. (2020)^[12] analyzed the results of 10,048 floats and found that less than 10% required salinity corrections through delayed-mode quality control after 2 yrs of deployment. However, about 40% of floats required salinity correction after the float observed 280 profiles. Undoubtedly, there have been batches of pressure and conductivity sensor technology problems in the implementation of the International Argo Program, leading to large errors in the data. Some of these errors cannot be corrected via the delayed mode. In this case, the ADMT placed these floats into a gray list and gave uniform quality control flags to the observational elements where problems arose (see Table 2).

The International Argo Program proposed an observation accuracy targeted at a pressure of $\pm 2.4 \times 10^4$ Pa, temperature of ± 0.005 °C and salinity of ± 0.01 psu at the initial implementation stage. In general, the temperature sensor is more stable and accurate and could more easily meet the accuracy requirement, whereas pressure and salinity had more difficulty in meeting the observation accuracy requirements. To assess the observation accuracy of the global Argo dataset over the past two decades, Wong et al. (2020)^[12] paired the global ocean transect data of GO-SHIP and adjacent Argo salinity profiles and found that pressure and salinity values in the global ocean Argo dataset reached the target observation accuracy of pressure and salinity upon application of delayed-mode quality control measures. Thus, Argo data of reliable quality are backed by the global ocean Argo temperature and salinity profile scattered dataset made by CARDC using the post-quality control method.

6 Discussion and Conclusions

The International Argo Program has been deployed more than 16,000 Argo profiling floats in the global ocean, it obtained at least 2.3 million temperature and salinity data profiles. It is one of the most successful global ocean observation systems. The data have been widely used in operational forecasting for the ocean, atmosphere and climate. Although strict Argo data quality controls are in place, various data quality problems have resulted from the profiling floats themselves as well as their hosted CTD sensors, which can be affected by sea surface oil pollution, biological fouling and electronic device aging, limiting the promotion and application of Argo data in basic research.

In 2019, CARDC developed and implemented a global Argo data fast access and post-quality control system that used the quality controls of ADMT and combined them with the practices and improved techniques and methods proposed by DACs and their data quality control technicians. With this new system, global ocean Argo temperature and salinity profiling scattered datasets at various time periods can be regularly or irregularly reorganized and provided based on user needs and made freely available through the network¹.

The global ocean Argo temperature and salinity profile scattered dataset compiled from 1997 to 2020 were originally from GDAC, and processed by CARDC under strict post-quality control operations. The post-quality control method is performed automatically by a computer, and can quickly identify profiles that have drifted or are offset in the conductivity sensor without delayed-mode quality control. It appears that the dataset quality is superior to the Argo profile data that are open and shared on the GDAC website, which aids user demands for high-quality Argo data.

Author Contributions

Liu, Z. H. was responsible for developing the systems and algorithms; Xu, J. P. was in charge of the post-quality control and manual review methods of the dataset; Li, Z. Q. collected and reorganized the dataset as well as oversaw the manual review; Wu, X. F. was responsible for conducting delayed-mode quality control for all Argo float observation data in the Argo observation network in China; Lu, S. L. verified the data; Sun, C. H. conducted the information statistics of the dataset.

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¹ ftp://ftp.argo.org.cn/pub/ARGO/global/

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Conflicts of Interest
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The authors declare no conflicts of interest.

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