Product Information Document (PIDoc)

SeaDataCloud Temperature and Salinity Historical Data Collection for the Black Sea (Version 1)

SDC_BLS_DATA_TS_V1

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Product Name

SDC_BLS_DATA_TS_V1

Extended name

SeaDataCloud Temperature and Salinity Historical Data Collection for the Black Sea (Version 1)

Product DOI

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Short description

The SeaDataCloud Temperature and Salinity Historical Data Collection for the Black Sea includes open access in situ data on temperature and salinity of water column in the Black Sea (and a little in the Sea of Azov) for period 1868 – 2017. The data were retrieved from the SeaDataNet infrastructure at the end of 2017. The dataset format is Ocean Data View (ODV) binary collection. The quality control of the data has been performed with the help of ODV software. Data Quality Flags have been revised and set up using the elaborated by SeaDataNet2 project QC procedures in conjunction with the visual expert check. Data duplicates have been identified and excluded from the dataset. The final number of the Temperature and Salinity profiles (stations) in the collection is 137723.

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Public	

How to Cite

History

Version	Authors	Date	Comments
1.0	V. Myroshnychenko	19/02/2018	
2.0	S. Simoncelli	20/02/2018	General revision
2.1	V. Myroshnychenko	23/02/2018	Formatting and corrections
2.2	V. Myroshnychenko	20/04/2018	Update after adding missing data to the product

2.3	S. Simoncelli	22/06/2018	Final revision

Table of contents

Abstract

The SeaDataCloud Temperature and Salinity Historical Data Collection for the Black Sea includes open access in situ data on temperature and salinity of water column in the Black Sea (and a little in the Sea of Azov) for period 1868 – 2017. The data were retrieved from the SeaDataNet infrastructure at the end of 2017. The dataset format is Ocean Data View (ODV) binary collection. The quality control of the data has been performed with the help of ODV software. Data Quality Flags have been revised and set up using the elaborated by SeaDataNet2 project QC procedures in conjunction with the visual expert check. Data duplicates have been identified and excluded from the dataset. The final number of the Temperature and Salinity profiles (stations) in the collection is 137723.

Whenever SDC_BLS_DATA_TS_V1 product is used, this PIDoc should be cited in any publication. We also ask users to remember that hard-working scientists made these measurements, often under severe conditions. Further, the data providers normally possess insight on the quality and context of the data not always shared with the SeaDataCloud team. Hence, inviting data providers and product leaders to collaborate in scientific investigations that depend on their data and data products is considered good and fair practice. Importantly, this will promote further sharing of data and will be beneficial to science.

1. General description of the data collection

The SeaDataCloud Temperature and Salinity Historical Data Collection for the Black Sea contains data on temperature and salinity of water body (profiles and surface measurements) retrieved from the SeaDataNet infrastructure at the end of 2017. The collection includes non-restricted data obtained from 42 data providers (originators and distributors) listed in Annex 2 – Data providers.

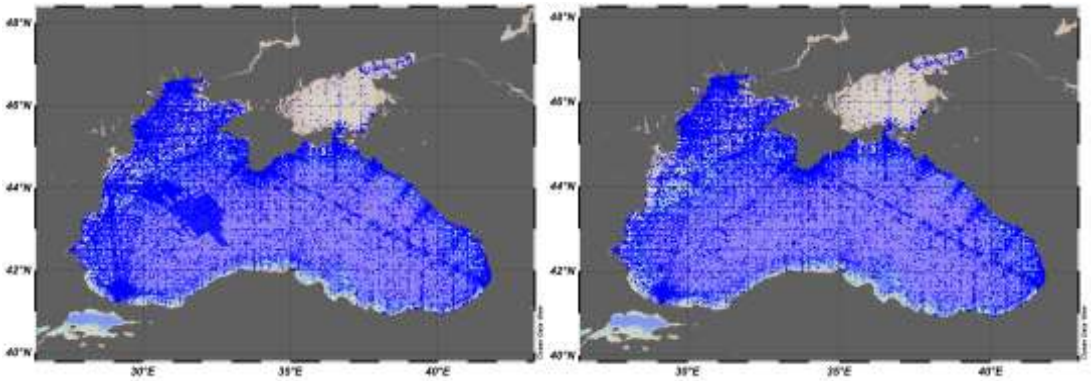
The collection was created, managed and quality controlled with Ocean Data View (ODV) software. The dataset format is ODV binary collection.

The collection covers period 1868 – 2017. All data in the collection have been quality controlled according to procedures described in chapter 2. The duplicates and bad data (e.g. stations on land, empty depth levels and empty profiles i.e. those without Temperature and Salinity) were excluded from the collection. Spatial distribution and data density for final dataset are presented at **Figure 1.1** and **Figure 1.2** below.

The collection includes underway data (surface Temperature and Salinity) from two cruises, which trajectories are easily recognized at **Figure 1.1**. The underway data are obtained with high frequency (e.g. 1 measurements per minute), therefore the number of data points per cruise can be huge. Since every data point has different coordinates and time, in ODV these data points are considered as separate stations. The number of underway stations in the collection is 18563, i.e. stations from 2 datasets represent 13.5% of total! Such large amount of irregularly obtained data introduces bias in data statistics. For better understanding of the dataset the data statistics will be provided further either for the whole collection or excluding underway data where appropriate.

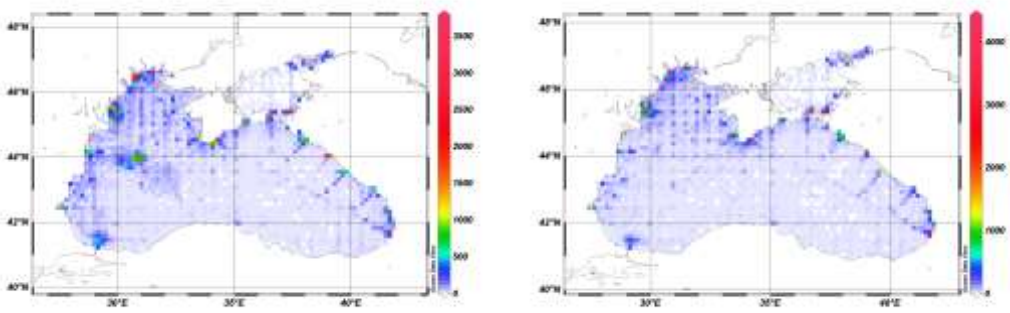
Table 1.1 Data Statistics: total numbers.

	Cruises	Stations			Values
		All	Profiles	Underway	
All data	2286	137723	119160	18563	4240346
Temperature	2282	137370	118807	18563	4238207
Salinity	2116	129731	111168	18563	4111531



a) b)

Figure 1.1 Spatial distribution of observations: all (a) and excluding underway data (b)

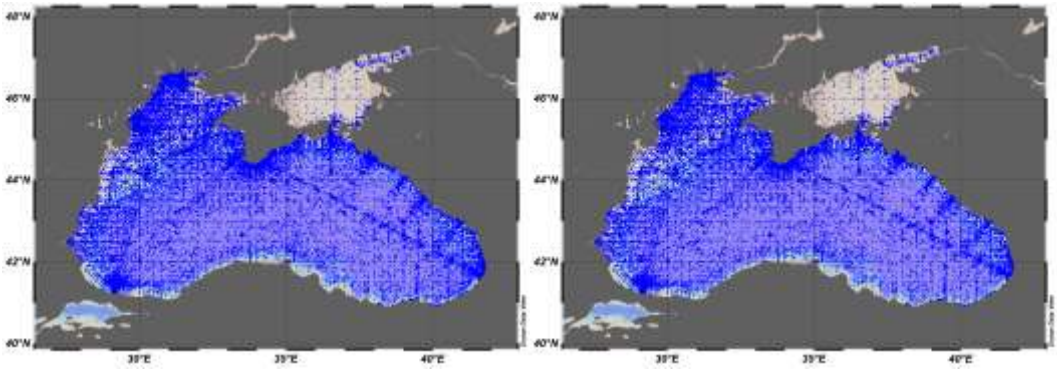


a) b)

Figure 1.2 Data density of observations: all (a) and excluding underway data (b)

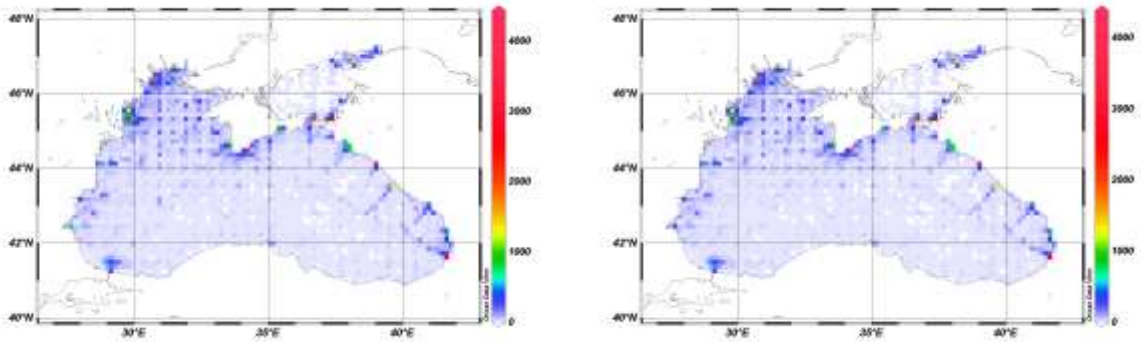
The data distribution in Black Sea is rather uneven: the increased concentration of measurements can be observed in areas of intensive navigation and along the standard oceanographic transects, while the interior of the sea, the areas along southern coast and along the central part of the western coast are covered rather poor. About 9% of stations in the collection belong to the Sea of Azov, however most of them come from several coastal stations while the interior of the sea is covered poorly.

The separate maps for spatial distribution and data density of Temperature and Salinity observations are presented at **Figure 1.3** and **Figure 1.4** respectively. The maps for two parameters are practically identical, the small difference in spatial coverage can be noticed only along the eastern coastline and at the north-western shelf.



a) b)

Figure 1.3 Spatial distribution of Temperature (a) and Salinity (b) observations (excluding underway data)



a) b)

Figure 1.4 Data density of Temperature (a) and Salinity (b) observations (excluding underway data)

Temporal distributions of all observation is presented at Figure 1.5.

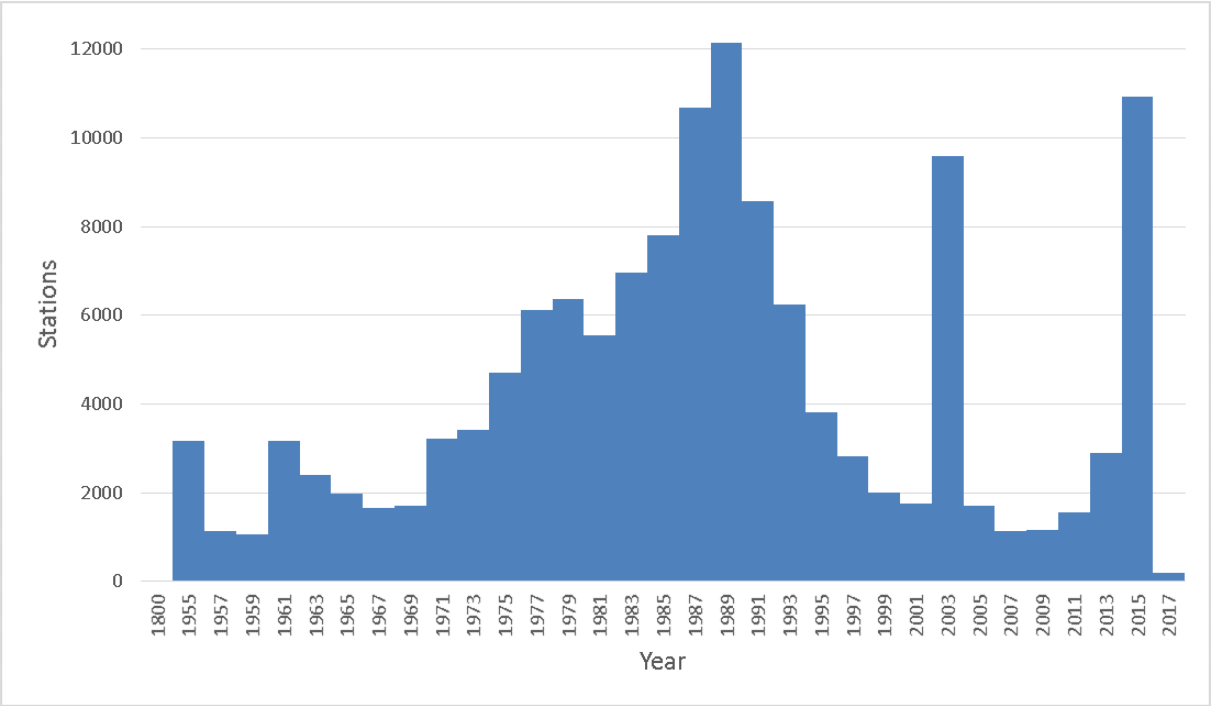


Figure 1.5 Temporal distribution of observations

Though the first oceanographic measurements in Black Sea date from 1868, the total number of observations before 1955 is rather small – just about 3000. The most intensive oceanographic observations were performed in Black Sea in period 1970 – 1995. The peaks in 2002 and in 2015 represent underway data from two cruises: the first one was performed in August – September, 2002, and the second – in August – October, 2015.

Temporal distributions of Temperature and Salinity observation (excluding underway data) are presented at Figure 1.6, Figure 1.7 and at Figure 1.8, Figure 1.9 below. The distributions are practically identical except the small difference in annual distributions in 1960-s, when there were less Salinity observations compared to Temperature.

The amount of observations from recent years (2015 - 2017) is small – just about 300 stations: this could due to overall decrease of observations in Black Sea or due to time lag between sampling and data submission to SeaDataNet or because the recent data have status “restricted” or “moratorium” and therefore could not be included in the current collection.

The monthly and seasonal distributions, as expected, have dome-like shape having maximum in summer (more observations) and minimum in winter (less observations).

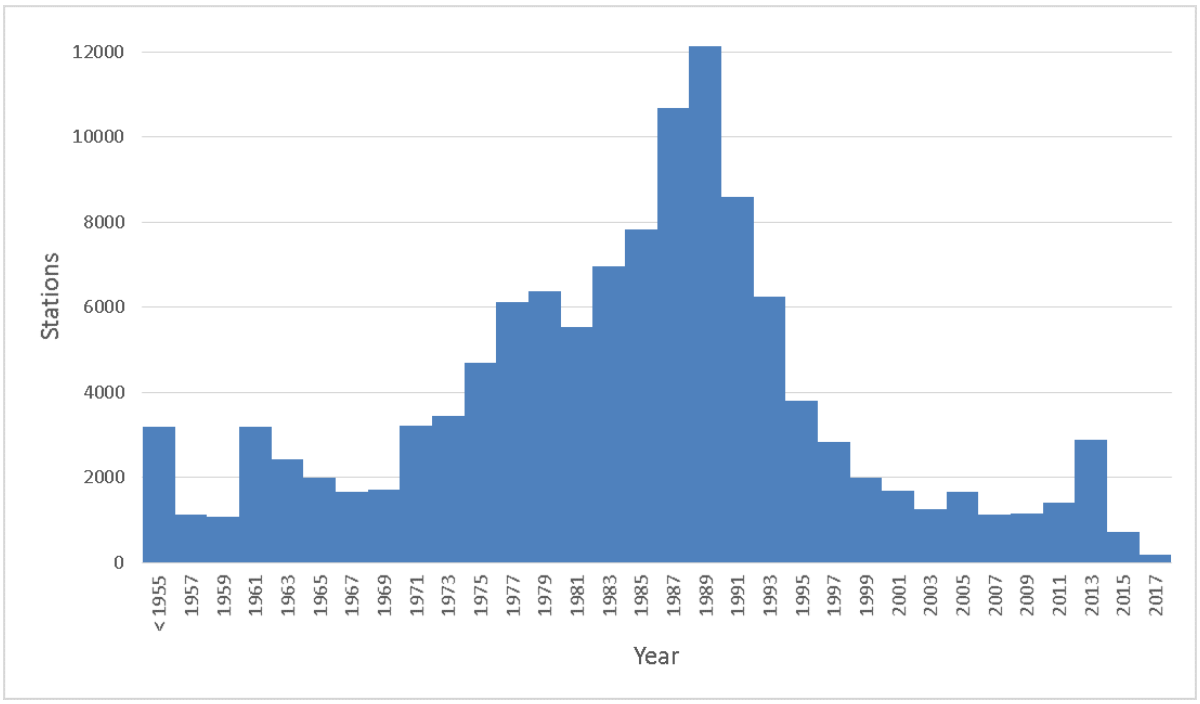
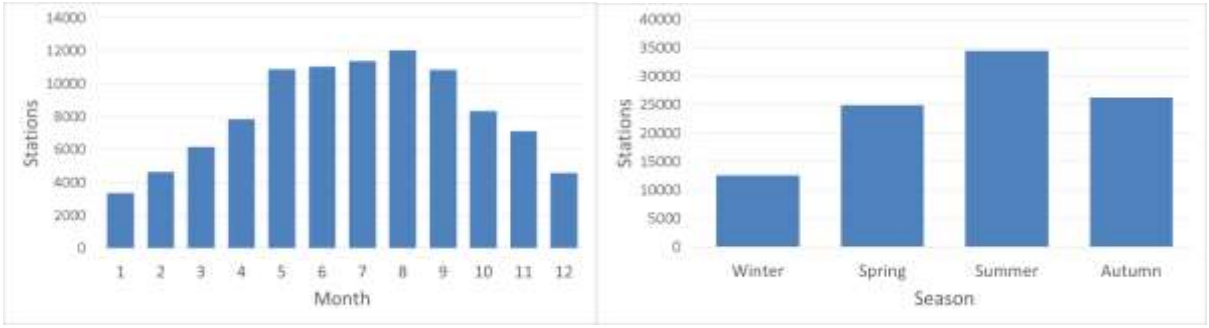


Figure 1.6 Annual distribution of Temperature observations excluding underway data (left bar represents all stations before 1955)



a) b)

Figure 1.7 Monthly (a) and seasonal (b) distribution of Temperature observations (excluding underway data)

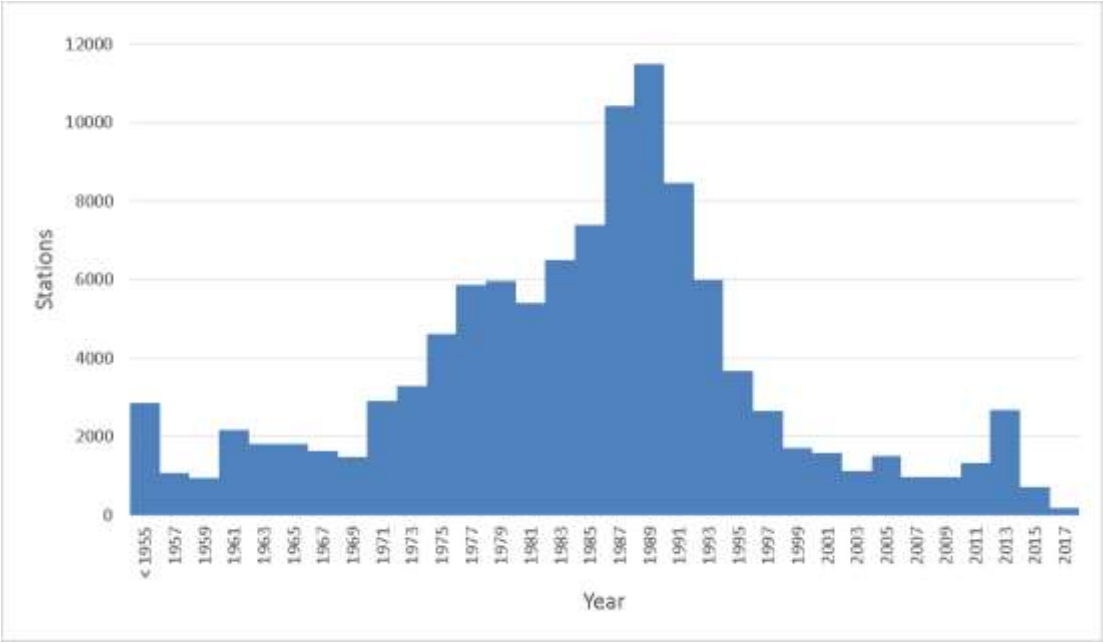
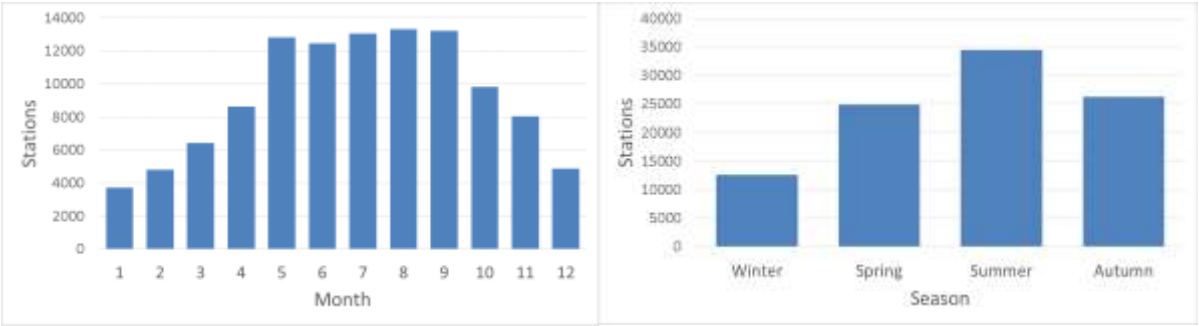


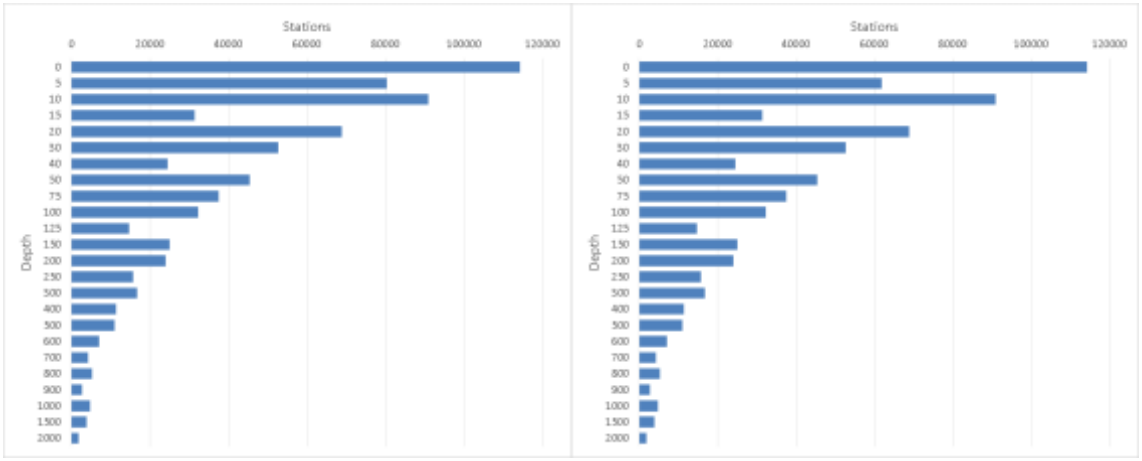
Figure 1.8 Annual distribution of Salinity observations excluding underway data (left bar represents all stations before 1955)



a) b)

Figure 1.9 Monthly (a) and seasonal (b) distribution of Salinity observations (excluding underway data)

Figure 1.10) shows that data availability drastically decreases with depth. The difference between all data and data without underway data appears at 5 m depth level. As the significant part of the collection is bottles data there are also gaps at non-standard depth levels, e.g. at 5, 15, 40, 125 m.



a) b)

Figure 1.10 Vertical distribution of observations: all (a) and excluding underway data (b)

2. Quality Control Procedure

Prior performing quality control of data the collection was checked for presence of duplicates. The initial collection contained data at 151,530 stations from 2550 cruises (datasets). Analysis revealed presence of more than 12,000 duplicate stations. The duplicates were excluded (deleted) from the collection along with stations having wrong location (on land) or being out of region (e.g. Bosporus stations). **The final collection contains 137723 stations from 2286 cruises**.

The quality control of the Temperature and Salinity data was performed following the guidelines in Annex 1 to this document and taking into account peculiarities of the Black Sea water masses such as permanent halocline and a two-layered structure of the waters, presence of **Cold intermediate Layer (CIL)**, conservativeness of properties of deep water layer (below 200 m), etc. The physical properties of the Black Sea water masses remain the same practically through the whole basin except the North-Western shelf, which is under influence of inflow from large rivers, and area of "Bosporus plume", where saline Mediterranean waters flow to the Black Sea.

Despite the efforts undertaken in SeaDataNet2 project to improve the overall quality of data within the SeaDataNet infrastructure the initial Black Sea data collection still contained significant amount of not QC-ed data (i.e. having QF=0) as well as wrongly flagged data (i.e. bad data flagged as good and vice versa). Prior performing quality control the QF=1 (good) was assigned to all data having QF=0 (not checked), then the results of data flagging in SeaDataNet2 project were applied to the data in the current collection where possible, and then the quality of data flagged as good was revised with the help of ODV [3] software.

The following simple range check procedures were applied to the whole data array, allowing to identify and flag obvious erroneous data:

- Depth < 0,
- Temperature < 0 and QF<>4,
- Temperature > 30 and QF<>4,
- Salinity < 0 and QF<>4,
- Salinity S > 39 and QF<>4,
- Salinity > 23 out of "Bosporus plume" area (28.8<Longitude<29.3, Latitude <41.6),
- Temperature < 6 at depth > 200,
- Temperature > 10 at depth > 200.

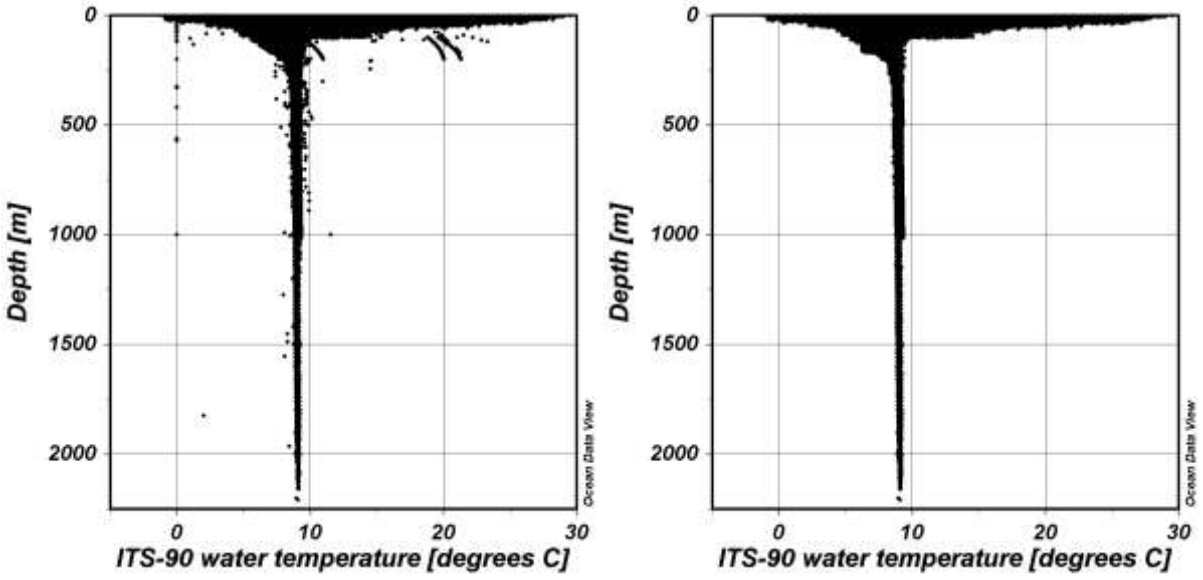
Further the profiles were analysed for spikes (using both gradient plots and visual checks), and for stability with the help of plots of density derivative. In addition to duplicates and location checks described above the following metadata checks were performed for informing data providers about found mistakes and requesting for corrections:

- Identification of stations with Bottom Depth < 0,
- Identification of stations with profile depth > Bottom Depth,
- Identification of stations with wrong date,
- Identification of stations with missing time.

The collection contains some amount of data from stations located in river estuaries. Data values at such stations can vary in wide range depending on season and weather conditions.

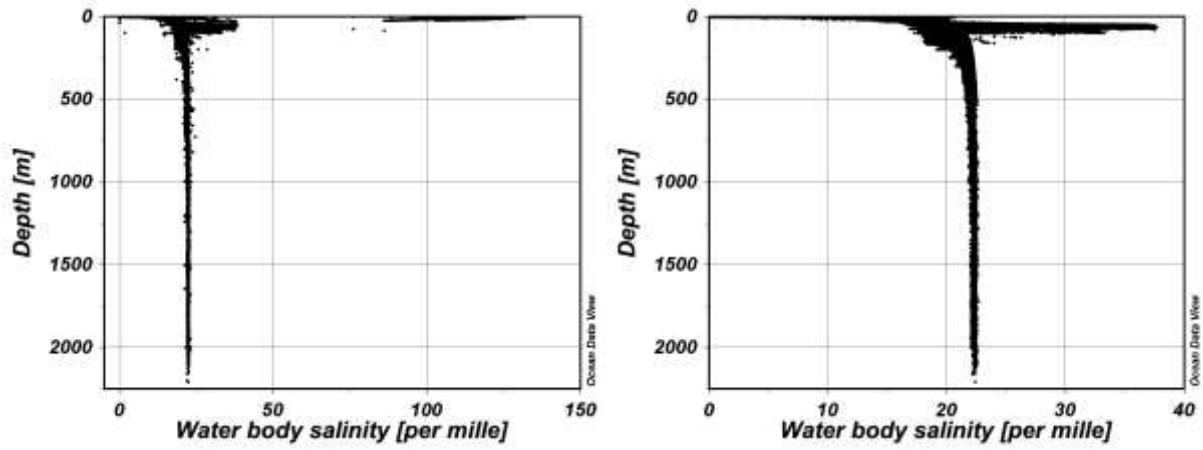
3. Quality assessment results

The initial data collection contained about 12% of non-controlled data as well as a number of bad data flagged as good that can be seen at scatter plots of Temperature, Salinity and TS diagram at Figure 3.1 - Figure 3.3 a). The scatter plots for QC-ed data are presented at Figure 3.1 - Figure 3.3 b) respectively for comparison.



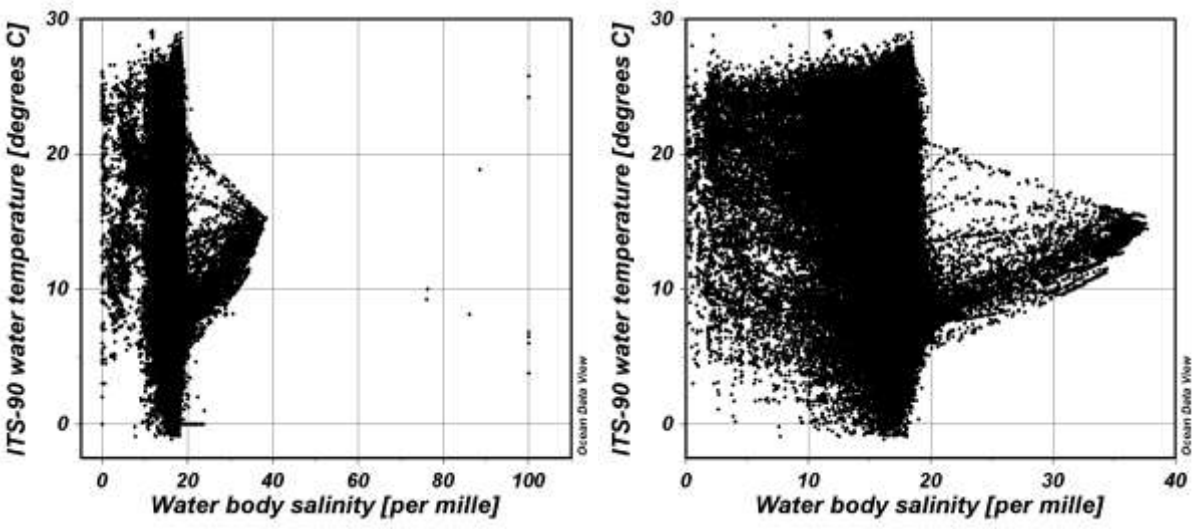
a) b)

Figure 3.1 Scatter plots of Temperature before (a) and after (b) quality control



a) b)

Figure 3.2 Scatter plots of Salinity before (a) and after (b) quality control



a) b)

Figure 3.3 TS diagram plots before (a) and after (b) quality control

The statistics of the quality flagging in the initial and final collections are presented in Table 3.1 and Table 3.2 respectively. About 96% of data in the final collection have QF=1 ("good"). Another 2-3% of data are flagged as "probably good" (QF=2). Thus in total about 98-99% of the collection data can be considered as valid for usage in different studies and applications.

Table 3.1 Data quality flagging statistics in initial collection

QF	0	1	2	3	4	Total
	not checked	good	probably good	probably bad	bad	
Depth	500240	3575857	72266	91973	10	4240346
	11.80%	84.33%	1.70%	2.17%	0.00%	
Temperature	491550	3470913	195737	75114	4893	4238207
	11.60%	81.90%	4.62%	1.77%	0.12%	
Salinity	491915	3448470	118380	48207	4559	4111531
	11.96%	83.87%	2.88%	1.17%	0.11%	

Table 3.2 Data quality flagging statistics in final QC-ed collection

QF	0	1	2	3	4	Total
	not checked	good	probably good	probably bad	bad	
Depth	0	4073158	131197	35702	289	4240346
	0.00%	96.06%	3.09%	0.84%	0.01%	
Temperature	0	4045723	131358	56030	5096	4238207
	0.00%	95.46%	3.10%	1.32%	0.12%	
Salinity	0	3956660	74707	71960	8204	4111531
	0.00%	96.23%	1.82%	1.75%	0.20%	

Special cases of QC:

1. The big dataset “AQUALOG Moored Profiler” of P.P.Shirshov Institute of Oceanology, RAS contains raw data, i.e. data that did not undergo typical CTD post processing such as filtering, alignment, loop-edit, bin-averaging etc. According to the description of Aqualog, “the profiler makes repeated round trips up and down a taut mooring wire between the subsurface flotation and the anchor”. Judging from the data the profiler stays for a while at the end points of its trips generating significant amount of data. When imported to ODV these data are automatically sorted by depth. As a result the data points are getting mixed up, and, consequently, the test of profile for stability fails. Nevertheless, these data were not flagged as bad except the obvious outliers.
2. A number of profiles originating from the Institute of Fishery Resources, Bulgaria also contain raw data for which stability test fails. As in previous case the data were not flagged as bad except the obvious outliers.

4. Technical Specifications

Product Format

Ocean Data View (ODV) collection.

Data Policy

No limitations on usage, however for data access the registration is required at http://www.marine-id.org.

Product Usability

The collection contains unique large array of QC-ed data on Temperature and Salinity of Black Sea waters for period 1868 – 2017 that can be used as to support the general oceanographic studies, such as investigation of variability of physical properties, as well as applications, such as circulation models. The collection contains a number of data from observations done in river estuaries, firths and ports. Such data should be used with precaution in a certain cases, for example in climatic studies.

Please consider that the SDC_BLS_DATA_TS_V1 data set contains:

- underway data at reduced resolution, since only one sample over seven have been included in this data collection. New releases will keep the original data resolution.
- XBT data without any depth correction.

Whenever SDC_BLS_DATA_TS_V1 product is used, this PIDoc should be cited in any publication. We also ask users to remember that hard-working scientists made these measurements, often under severe conditions. Further, the data providers normally possess insight on the quality and context of the data not always shared with the SeaDataCloud team. Hence, inviting data providers and product leaders to collaborate in scientific investigations that depend on their data and data products is considered good and fair practice. Importantly, this will promote further sharing of data and will be beneficial to science.

Changes since previous version

The previous version of the product was released in framework of the SeaDataNet2 project and available at SEXTANT Catalogue (http://sextant.ifremer.fr/en/web/seadatanet) under the name "Black Sea - Temperature and salinity observation collection V2" (SDN_V2, *Simoncelli et al. 2015*). Compared to SDN_V2 collection there is significant increase at all levels: cruises, stations and data (Table 4.1). The new type of data (for Black Sea collection) – the underway data give about half of increase in number of stations, however practically not affecting statistics on cruises and values. The significant increase of the of data values (57%) is due to adding CTD profiles with high vertical resolution: 1 m, 0.1 m or even raw data.

Table 4.1 Data statistics of previous (SDN2_V2) and current (SDC_V1) versions of collections.

Cruises			Stations			Values (data)		
SDN2_V2	SDC_V1	±%	SDN2_V2	SDC_V1	±%	SDN2_V2	SDC_V1	±%
1723	2284	+32.6%	96487	137723	42.7%	2696215	4240346	+57.2%
Excluding underway data								
1723	2282	+32.5%	96487	119160	23.5%	2696215	4221783	+56.6%

The statistics on data quality of two collections are very similar, therefore the comparison is not provided hereby - please see the Table 3.2 instead.

Annex 1 - QC Best Practices

The basic QC analysis steps applied during SeaDataNet2 Project using ODV were:

- **Data coverage**;
- **Data distribution maps** per Temperature, Salinity and TS couples;
- **Data density maps** (domain binning);
- **Time coverage and time distribution** → histograms with annual, seasonal and monthly data distribution;
- TS scatter plots of the entire dataset;
- Scatter plot of observations with QF=1 (good) and QF=2 (probably good);
- Scatter plot observations with QF=0 (no quality check);
- **Gross range check** to detect observations with temperature and salinity out of reasonable values;
- Visual control of scatter-plots to identify wrong profiles (outliers);
- Identification of stations falling on land;
- Identification of stations having unreal depth;
- Identification of wrong or missing data;
- Stability check on density

Additional checks are advisable per specific:

- **areas** with similar hydrodynamic characteristics;
- **layers** (surface, intermediate, bottom);
- **time periods** (decades, or specific periods i.e. Eastern Mediterranean Transient, Western Mediterranean Transition, Norther Ionian Reversal);
- **Instrument type** → consistency issue of historical data;

Duplicate Check is another important step when performing SDC data integration with external data sources for climatologies and new data products generation.

Table 2 lists the Quality Flags (QF) adopted by SeaDataNet and their definition. QF assigned by the data centers are modified by the regional products' leaders when/if a data anomaly is detected. The data anomaly is reported to the data center asking for correction in the central CDI.

Key	Entry Term	Abbreviated term	Term definition
0	no quality control	none	No quality control procedures have been applied to the data value. This is the initial status for all data values entering the working archive.
1	good value	good	Good quality data value that is not part of any identified malfunction and has been verified as consistent with real phenomena during the quality control process.
2	probably good value	probably_good	Data value that is probably consistent with real phenomena but this is unconfirmed or data value forming part of a malfunction that is considered too small to affect the overall quality of the data object of which it is a part.
3	probably bad value	probably_bad	Data value recognised as unusual during quality control that forms part of a feature that is probably inconsistent with real phenomena.
4	bad value	bad	An obviously erroneous data value.
5	changed value	changed	Data value adjusted during quality control. Best practice strongly recommends that the value before the change be preserved in the data or its accompanying metadata.
6	value below detection	BD	The level of the measured phenomenon was too small to be quantified by the technique employed to measure it. The accompanying value is the detection limit for the technique or zero if that value is unknown.
7	value in excess	excess	The level of the measured phenomenon was too large to be quantified by the technique employed to measure it. The accompanying value is the measurement limit for the technique.
8	interpolated value	interpolated	This value has been derived by interpolation from other values in the data object.
9	missing value	missing	The data value is missing. Any accompanying value will be a magic number representing absent data.
A	value phenomenon uncertain	ID_uncertain	There is uncertainty in the description of the measured phenomenon associated with the value such as chemical species or biological entity.

Table 2 List of SeaDataNet Quality Flags (QF) used to describe the data value; no changes are made to the original data values.

https://www.seadatanet.org/content/download/596/3118/file/SeaDataNet_QC_procedures_V2_%28May_2010%29.pdf?version=1

Annex 2 – Data providers

EDMO code	Data Originator	Stations	CDIs
841	Ukrainian Hydrometeorological Institute - Marine Branch	34346	34346
727	Marine Hydrophysical Institute	22403	22403
688	Southern Scientific Research Institute of Marine Fisheries and Oceanography	21889	21889
486	IFREMER / IDM / SISMER - Scientific Information Systems for the SEA	18563	2
910	North-Caucasus Regional Administration of Hydrometeorology of Roshydromet	7807	7807
1167	Ukrainian scientific center of Ecology of Sea (UkrSCES)	6303	6303
931	Odessa Branch of SOI (State Oceanographic Institute)	5665	5665
696	Institute of Marine Sciences, Middle East Technical University	3295	3295
697	National Institute for Marine Research and Development "Grigore Antipa"	2995	2994
914	Odessa branch of IBSS (Institute of Biology of Southern Seas)	2412	2412
692	Bulgarian National Oceanographic Data Centre(BGODC), Institute of Oceanology	1903	1903
891	Kuban offing station, North-Caucasus HMS	1694	1694
685	P.P.Shirshov Institute of Oceanology, RAS	1296	1296
871	Donskaya offing station North-Caucasus HMS	1207	1207
731	Department of Navigation and Hydrography and Oceanography, Turkish Navy	671	671
192	Laboratory of Marine Ecology-Central Laboratory of General Ecology	663	600
540	Shom	354	354
120	OGS (Istituto Nazionale di Oceanografia e di Geofisica Sperimentale), Division of Oceanography	334	334
733	Sinop University, Fisheries Faculty	330	330
840	Institute of Biology of the Southern Seas, NAS of Ukraine	324	324
907	Navy Main Administration of Navigation and Oceanography, Ministry of Defence	304	304
191	Institute of Fishery Resources (IFR)	275	275
1054	IFREMER	259	259
942	Tuapse Hydrometeorological Bureau, North-Caucasus Centre	209	209
1265	Scientific - Research Firm "GAMMA"	198	198
913	Nothern Regional Administration of Hydrometeorology of Roshydromet	189	189
2121	Georgian Institute of Hydrometeorology of Georgian Technical University	179	72
4614	ERIC Euro-Argo	126	126
2122	Georgian Institute of Water Management of Georgian Technical University	92	92
693	Iv.Javakhishvili Tbilisi State University, Centre of Relations with UNESCO Oceanological Research Centre and GeoDNA (UNESCO)	52	52
1680	"State Oceanographic Institute, Sebastopol Branch (SB SOI)	48	48
802	Istanbul University, Institute of Marine Science and Management	40	40
2187	Zoological Institute of the Russian Academy of Sciences	36	36

EDMO code	Data Originator	Stations	CDIs
2267	National Environmental Agency of the Ministry of Environment Protection and Natural Resources	32	32
164	Hellenic Centre for Marine Research, Institute of Oceanography (HCMR/IO)	28	28
901	Mariupol Marine Hydrometeorological Station, Ukrainian HMS	25	25
2176	Ankara University	23	23
732	Karadeniz Technical University, Faculty of Marine Sciences	21	21
485	IFREMER / GM-MARINE GEOSCIENCES	7	7
756	Far Eastern Regional Hydrometeorological Research Institute	3	3
	Unknown	1123	1123
	Total	137723	118991

EDMO code	Data Distributor	Stations	CDIs
727	Marine Hydrophysical Institute	75784	75784
486	IFREMER / IDM / SISMER - Scientific Information Systems for the SEA	18975	414
681	All-Russia Research Institute of Hydrometeorological Information - World Data Centre	17697	17697
841	Ukrainian Hydrometeorological Institute - Marine Branch	7820	7820
1167	Ukrainian scientific center of Ecology of Sea (UkrSCES)	3590	3590
696	Institute of Marine Sciences, Middle East Technical University	3295	3295
697	National Institute for Marine Research and Development "Grigore Antipa"	2996	2995
692	Bulgarian National Oceanographic Data Centre(BGODC), Institute of Oceanology	1903	1903
840	Institute of Biology of the Southern Seas, NAS of Ukraine	1322	1322
685	P.P.Shirshov Institute of Oceanology, RAS	1046	1046
731	Department of Navigation and Hydrography and Oceanography, Turkish Navy	671	671
961	National Institute of Meteorology and Hydrology, Bulgarian Academy of Sciences	663	600
540	Shom	354	354
120	OGS (Istituto Nazionale di Oceanografia e di Geofisica Sperimentale), Division of Oceanograph	334	334
733	Sinop University, Fisheries Faculty	330	330
693	Iv.Javakhishvili Tbilisi State University, Centre of Relations with UNESCO Oceanological Research Centre and GeoDNA	327	220
191	Institute of Fishery Resources	277	277
1265	Scientific - Research Firm "GAMMA"	194	194
802	Istanbul University, Institute of Marine Science and Management	40	40
2267	National Environmental Agency of the Ministry of Environment Protection and Natural Resources	32	32
164	Hellenic Centre for Marine Research, Institute of Oceanography (HCMR/IO)	28	28
2176	Ankara University	23	23
732	Karadeniz Technical University, Faculty of Marine Sciences	22	22
	Total	137723	118991

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List of acronyms

Acronym	Definition
ARC	Arctic ocean
BAL	Baltic Sea
BLS	Black Sea
CDI	Common Data Index
CLIM	Climatology
CMEMS	Copernicus Marine Environment Monitoring Service
DATA	Aggregated Dataset
DIVA	Data-Interpolating Variational Analysis (software)
DOI	Digital Object Identifier
EC	European Commission
EDMO	European Directory of Marine Organisations (SeaDataNet catalogue)
GLO	GLobal Ocean
IOC	Intergovernmental Oceanographic Commission
IODE	International Oceanographic Data and Information Exchange (IOC)
MED	Mediterranean Sea
NAT	North Atlantic Ocean
NWS	North West Shelf
ODV	Ocean Data View Software
QC	Quality Checks
QF	Quality Flags
SDC	SeaDataCloud
SDN	SeaDataNet
TS	Temperature and Salinity
WOA	World Ocean Atlas
WP	Work Package