

# **A COMMON PROTOCOL TO ASSEMBLE A COHERENT DATABASE FROM DISTRIBUTED HETEROGENEOUS DATA SETS : THE MEDATLAS DATABASE EXPERIENCE**

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## **SUMMARY**

The MEDATLAS hydrological data base, has been created by a consortium of several data centers, including HNODC (Greece), IEO (Spain), EPSHOM/CMO (French navy), IFREMER/SISMER the coordinating center (France) and ICES (Denmark) as the supervisor of the quality control procedure, in the frame of the MEDATLAS project. This project is a MAST supporting initiative for ocean data and information management. Its objectives were to assemble a comprehensive data base of temperature and salinity profiles collected in the Mediterranean sea by the scientific laboratories and the navies, to check them for quality and to revise the climatological statistics by using this updated date set. An important part of the work has been devoted to define a common protocol to archive the data sets and to ensure a coherent level of quality for the data which originate for various sources within the consortium and from other data centers : ICES, World Data Center A, MODB, BODC, DOD.

The common protocol includes :

- an exchange format (the MEDATLAS/MODB format)
- a quality control procedure.

Both are based on the UNESCO/IOC and MAST recommendations.

This paper describes The MEDATLAS/MODB format, the common quality checks protocol and the hydrological data sets gathered in the frame of the MEDATLAS project.

## **THE MEDATLAS PROGRAM**

Hydrographic (temperature and salinity, TS) data are widely used for varied purposes : scientific studies of climatological changes in water masses, initialization of models, preparation of new field experiments, calibration of sensors like multibeam echo sounders or acoustic tomographers as well as for industrial purpose like cable operators. The most frequent data requests include : comprehensive TS data sets , data of good quality, gridded statistical values, on an electronic support easy to handle. Digitized atlases fulfill these requirements, but it is necessary to update them regularly, and for the Mediterranean region, very few are available.

The access to the existing data sets, which currently date from the beginning of the century, is not easy for the users. Most of the recent data collected in the Mediterranean Sea, and a significant number of historical data have never been archived in a data center and lay dispersed in several European and non European scientific laboratories. Even inventories are not always available. Important temperature data sets, mainly from XBT, have also been

collected by the Navies. A subset of these are classified but can be used for statistics computations.

An easy access to data means also that the data sets are available at a common format, on a digitized support and that no anomalies would impede any further use of them. The Intergovernmental Oceanographic Commission (IOC) and the European Marine Science & Technology Program (MAST) have recommended quality checks procedures to detect outliers (ICES/IOC,1995). Quality checks are particularly crucial for the hydrographic data sets which are delivered at any format, whose validation is not always documented, and whose necessary copying and transcoding can introduce errors.

Creating such an updated and checked data bank is the objective of the MEDATLAS program, which was initiated by a consortium of several Mediterranean Data Centers including the Hellenic Data Center (Greece), the IEO Data Center (Spain), the EPSHOM/CMO (French Navy), IFREMER/SISMER (France, coordinating center), the ICES data center (Denmark, supervisor of the Quality control procedures) and in close relationship with the MAST/MODB project. It is a MAST supporting initiative for ocean data and information management, and is supported jointly by the national agencies in charge of the data centers.

Four tasks have been defined to achieve the program objectives :

- 1 : Compilation of the TS profiles from all sources, European and extra-European.
- 2 : Quality Control of the data according to the IOC and MAST recommendations taking advantage of the regional expertise of the Mediterranean data centers.
- 3 : Updating of the seasonal gridded statistics with a resolution adapted to the Mediterranean space scales, including some classified data sets.
- 4 : Publication of the updated data set by using an electronic publishing technique.

Beyond the short term objective of the program, several long term results are expected : improvement of the data safeguarding and data quality, better preparation of the sea cruises and numerical experiments, getting experience for banking other data types like nutrients, chemicals, time series, floats.., and strengthening of the Mediterranean data centers network to make them ready to participate jointly in further operational international projects.

## **THE MEDATLAS/MODB FORMAT**

Vertical profiles of temperature, salinity, oxygen and nutrients, are basic core parameters which have been widely exchanged since the beginning of oceanography. A common format is necessary to exchange data originating from dispersed sources, to merge them in an integrated data set, and to be able to use any processing software. It is important, to insure the data quality and to avoid the duplicates, not only to archive the data points, but also to keep information (meta-data) about the source and the processing of the data : cruise, laboratory, parameter accuracy, methodology, time and location etc.. According to the ICES/IOC GETADE recommendations (ICES/IOC,1995), a good exchange format must fulfill the following requirements :

- To facilitate the reading of the data, (and not to optimize the data archiving on the magnetic support, neither to speed up the data processing).
- To be independent of the computer.
- To keep track of the history of the data including the data collection and the processing. Then each cruise must be documented.
- To allow the processing of profile independently. Therefore the date, time and geographical coordinate must be reported on each profile header.
- To be flexible and accept (almost) any number of different parameters.
- The real numbers (floating numbers must remain in the same way as they have been transmitted (not transcoded into integer numbers). The number of decimals must implicitly indicate the accuracy of the measurements.

These requirements have been taken into account in the MEDATLAS/MODB exchange format which has been designed by the MEDATLAS and MODB consortia, in the frame of the European MAST II program (MEDATLAS Group,1995).

This format is an ASCII auto descriptive format. A data file consists in :

- a cruise header including a minimum cruise information to track the source of the data
- a profile header including the date and location, the number of observed parameters and the number of record in the profiles, the list of the observed parameters with codes, names, units and default values, some environmental information like bottom depth and any other relevant information on data collection and data processing
- data points in columns with codes of the observed parameters as titles
- at the end of each profiles, a line of default values.

Hereafter is an example of a file at the MEDATLAS/MODB format :

```
*FI35199100391 CONVHIV1                35LU SUROIT
26/11/1991-07/12/1991 LIGURIAN SEA
35 IFREMER, /INSU, Marine Nationale , Brest (SHOM), Universites de Kiel, d'Athenes
DESAUBIES Yves                          Project=
Regional Archiving= FI                    Availability=P
Data Type=H10 n=28   QC=N
COMMENT
No limitation on the number of the comment lines in the cruise header.
*FI3519910039100010 Data Type=H10
*DATE=27111991 TIME=0730 LAT=N42 45.04 LON=E004 59.92 DEPTH=1250 QC=0000
*NB PARAMETERS=03 RECORD LINES=01083
*PRES SEA PRESSURE sea surface=0        (DECIBAR=10000 PASCALS           ) def.= -999.9
*TEMP SEA TEMPERATURE                   (CELCIUS DEGREE              ) def.= 99.999
*PSAL PRACTICAL SALINITY                 (P.S.U.                      ) def.= 99.999
*GLOBAL PROFILE QUALITY FLAG=0 GLOBAL PARAMETERS QUALITY FLAGS=000
*DC HISTORY=SONDE SEABIRD
*
*DM HISTORY
*
*COMMENT
No limitation on the number of the comment lines in the station header.
*SURFACE SAMPLES=
*
*PRES TEMP    PSAL
  4.0 14.976 38.087 000
  6.0 14.975 38.086 000
  7.0 14.976 38.087 000
  8.0 14.976 38.086 000
.....
-999.9 99.999 99.999 999
```

All the profiles measured with the same instrument (e.g. bottles, CTD, XBT..) are grouped within the same file beginning with the cruise header. The data files begin with a short cruise descriptor based on the ROSCOP information forms. The profiles are attached behind an each of them begins with a profile header giving all the necessary environmental information on the observations. Each observed parameter represent a separate column. There is no limitation to the number of parameters (columns) but the number of parameters within the same cruise must be constant. If a parameter is missing in one station, the corresponding column must be completed with default values.

In order to maintain some flexibility with the format and not to loose existing complementary information on the data processing or any observations not taken into account in the format, three specific fields terminate each header profile :

- \*DC HISTORY for the information linked to the data collection at sea (like instrument, calibration)
- \*DM HISTORY for the information linked to the data management and archiving (like the source latitude if the sign of this one has been changed)
- \*COMMENT for all optional data and meta data like time and location at the end of the profile, meteorological observations... The number of comment lines is not limited.

## **THE QUALITY CHECKS**

The methodology adopted within the consortium involves a regional expertise, and the specification of standard quality checks.

### **1. Regional Expertise**

For the CTD and BOTTLE data set, the implementation of the program is based on a regional sharing of the tasks.

A regional expertise facilitates the usual tasks of data banking by a better local knowledge of where the data are and what the acceptable values are. Each Mediterranean basin has been subdivided into a limited number of rectangular sub-regions (Figure 1). Specifics minimum and maximum values of temperature and salinity are defined for each sub-region.

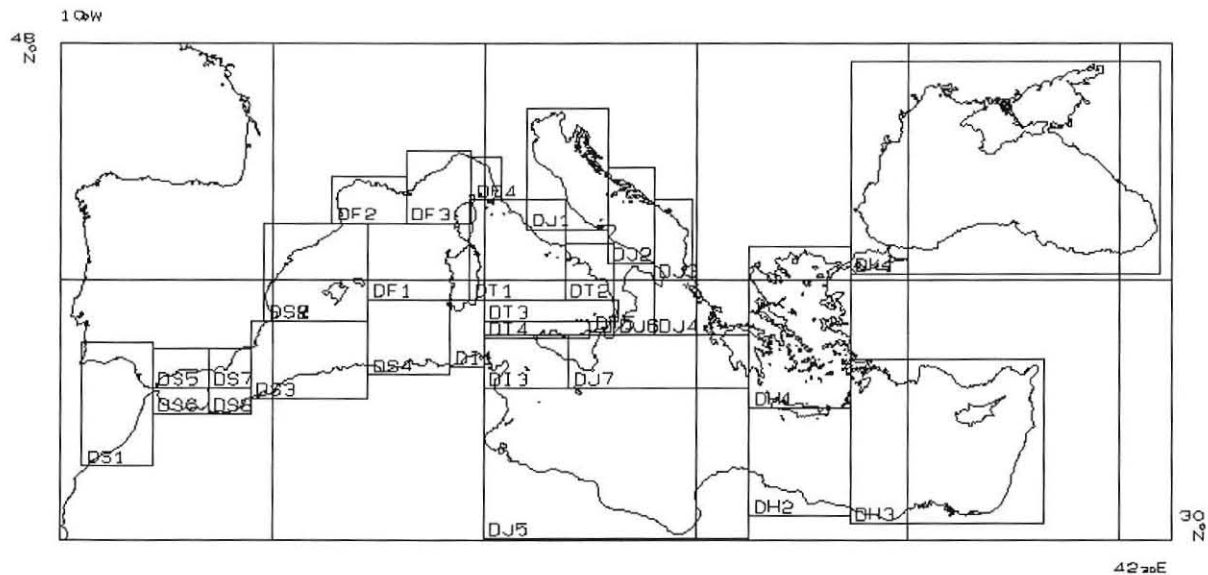


Figure 1. Regional expertise, subdivision into rectangular sub-regions.

The quality checks are under the responsibility of a partner data center, according to their regional expertise : IEO for the Gulf of Cadiz and the west part of the Western basin, SISMER for the central part of the Western basin and the Adriatic sea and HNODC for the Eastern basin and the Black sea.

For the BT data set, SHOM/CMO has performed all the quality checks.

## 2. Standard quality checks

Historical data cannot be used without control. Even validated recent data may have some anomalies get during each processing, copying or transcoding. For practical reasons, QC procedures defined by IOC and MAST (CED/DG XII,1993) have been revisited in the MEDATLAS banking document (MEDATLAS Group, 1995). New software's have been developed on UNIX (IFREMER/SISMER (CURE *et al*, 1995; FICHAUT *et al*, 1996)). and DOS (IEO (GARCIA, NIKOULINE, 1997)). These procedures are briefly described hereafter.

Quality checks consist in comparing the numerical values with the estimated statistical values that are maximum, minimum, mean and standard deviation. Presently available estimates of means are the 1x1 square degree LEVITUS climatology (LEVITUS *et al*, 1994) and the 0.25x0.25 degree MODB (BRASSEUR *et al*, 1996) climatology. Minima and maxima are not known on the same scale. Their first estimate has to be determined prior to the QC, and tuned afterwards, if necessary. This is presently carried out by the regional data centers, according to their geographical expertise. It may be noted that these estimates are useful not only for performing QC, but also for preparing field experiments.

As a result, QC do not modify the data values but add to them a quality flag. For simplicity reasons, the GTSP quality flag scale has been adopted with a flag = 0 which means that no QC has been performed. The final flag corresponds to the highest level of anomaly encountered. Automatic checks are followed by visual checks which validate the flags. The operator can only modify the header values (in this case the corresponding flag is 5

"interpolated" and the original value is safeguarded) when obvious errors are met. He cannot modify the data points but can only set the flags. QC are performed into three steps :

### QC 0 : Check of the format

Data sets must be readable at the exchange format, and core information like references, date, time, latitude, longitude, source country and ship must not be missing. The codification (type of data, parameters, ship, country, archiving center, oceanic region) are controlled. As a result, a "list of errors" is displayed and manual corrections are necessary before any further processing. The following QC are implemented when "no error" is returned from QC0.

### QC 1 : Check of the Headers

Automatic checks are made on the date, the ship velocity the location of the station which must not be on land and compare the sounding with the ETOPO5 gridded bathymetry (NOAA/NGDC, 1993). The checks for duplicate data sets are implemented at this step. Visual checks display the ship velocity, station locations for a cruise and, the coastlines and isobathes of the area (JONES, 1994).

| HEADER<br>Control Flags | 1<br>Correct | 2<br>Inconsistent<br>with statistics | 3<br>Doubtful,<br>questionable     | 4<br>Bad, wrong,<br>erroneous | 5<br>Changed or<br>interpolated                 | 9<br>Missing<br>Value          |
|-------------------------|--------------|--------------------------------------|------------------------------------|-------------------------------|---|--------------------------------|
| Date + Time             | No Outliers  |                                      |                                    | out of the<br>cruise duration | - day modulo 24 h<br>- non UT                   | <i>not allowed</i>             |
| Latitude<br>Longitude   | No Outliers  |                                      |                                    |                               | - ship velocity is out<br>of scale<br>- on land | <i>not allowed</i>             |
| Bottom Depth<br>(BD)    | No Outliers  | slope stations<br>(manual checks)    | < (Dmin-20%)<br>or<br>> (Dmax+20%) | out of the<br>regional scale  |   | no bottom<br>depth<br>recorded |

Dmin = minimum, Dmax = maximum of 9 nearest ETOPO5 grid points

## QC 2 : Check of the Data points

The automatic checks on the measured parameters

- search for the impossible regional values, the constant profiles, the spikes, the vertical instabilities
- verify that the reference parameter (pressure) increases, that there is no data points below the bottom depth
- compare the data with the pre-existing statistics

All the controls and the resulting flags are listed in the following table.

| PARAMETER<br>Control Flags               | 1<br>Correct | 2<br>Inconsistent<br>with statistics         | 3<br>Doubtful,<br>questionable                                    | 4<br>Bad, wrong,<br>erroneous  | 9<br>Missing<br>value  |
|--|--------------|--|---|--|------------------------|
| Pressure                                 | No Outliers  |  | - Flag(BD)=3 and<br>P > BD+5%<br>- Flag(BD)=9 and<br>P > Dmax*1.5 | - out of the regional<br>scale<br>- Flag(BD)=1 and<br>P > BD+5%<br>- non increasing        | <i>not<br/>allowed</i> |
| Temperature<br>Salinity<br>Nutrients ... | No Outliers  | out of mean +/-<br>n* standard<br>deviations | - spike   | - out of the regional<br>scale<br>- constant over the<br>vertical<br>- density instability |                        |

The available data to perform the "consistency with pre-existing statistics" (mean and standard deviation) tests are the LEVITUS (LEVITUS *et al*, 1994) and MODB (MODB Group, 1996) climatologies. The number n\* of permitted standard deviations from the mean value depends on the type of the station (over shelf, straits/slope or deep sea) :

|   |         |
|---|---------|
| n = 3 for Bottom Depth (default is the nearest ETOPO5 grid point) | > 400 m |
| n = 4   | < 400 m |
| n = 5   | < 200 m |

Visual checks consists in water fall and superposed vertical profiles displaying. More specifically, they aim at controlling the two following cases :

- 1) when facing a vertical instability between two consecutive levels, to determine which is the wrong level and the wrong parameter;
- 2) when the estimate of the statistics is poor, to compare with other estimates and check the continuity among consecutive profiles.

Doing so, each profile is visualized and compared to the other profiles of the same cruise and to the climatology by the operator.

After the completion of the QC, a global quality flag is assigned to the profile and to each measured parameter according to the following scale :

| Global Flags     | 1<br>Correct                 | 2<br>Inconsistent with<br>statistics | 3<br>doubtful,<br>questionable | 4<br>bad, wrong, erroneous                                |
|------------------|------------------------------|--------------------------------------|--------------------------------|---|
| <b>PROFILE</b>   | Few Outliers                 |                                      | no temperature recorded        | - no pressure recorded (nor depth)<br>- constant profiles |
| <b>PARAMETER</b> | > 80% values with Q flag = 1 | > 20% values with Q flag=2           | > 20% values with Q flag=3     | > 20% values with Q flag=4                                |

For each parameter, if at least 80% of the values are without outliers, the global parameter is flagged to 1 (good); if not, the global flag is assigned to the most frequent error flag.

The final step of the quality checks procedure is the merging of all the data set in one data base with a careful checks of the duplicates.

## THE HYDROLOGICAL DATA SETS

The hydrological data set of the MEDATLAS data bank consists in a collection of temperature and salinity profiles collected with CTD, Bottle, XBT and MBT. The data set originate from various sources which are :

- Direct sources from the partners of the MEDATLAS project :
  - ⇒ French laboratories which released their data to the French data center (IFREMER/SISMER). The data set includes recent data from the MEDIPROD, PRIMO and MAST projects.
  - ⇒ Spanish laboratories which released their data to the Spanish data center (IEO). The data set includes recent data from the GIBRALTAR EXPERIMENT, DONDE VA? and CANALES projects.
  - ⇒ Hellenic laboratories which released their data to the Hellenic data center NCMR/HNODC. The data set includes recent data collected in the frame of the POEM project.
  - ⇒ the French Navy from the Service Hydrographique et Océanographique de la Marine (SHOM) / Centre Militaire d'Océanographie (CMO).
- MODB data bank
 

Only the recent Spanish and Italian cruises have been recovered from the MODB data set, this includes

  - ⇒ Recent Spanish cruises from the Balearic Islands University (BIU).
  - ⇒ Recent Spanish cruises from the Instituto Ciencias del Mar (ICM).
  - ⇒ Recent Italian cruises from the Ente por la Nuove Tecnologie e l'Ambiente (ENEA).
  - ⇒ Recent Italian cruises from the Oservatorio Geofisico Sperimentale (OGS).
- IOC/IODE Network
  - ⇒ Recent German Cruises from the Deutsches Ozeanographisches Datenzentrum (DOD).
  - ⇒ Recent British cruises from the British Oceanographic Data Center (BODC).
  - ⇒ International council for the Exploration of the Sea (ICES) Mediterranean data set.
  - ⇒ World data center A (WDC-A) Mediterranean data set.



- The British Navy from the Hydrographic Office of Taunton (HOT)
- The Spanish Navy from the Instituto Hydrografico de la Marina (IHM)

The distribution of this data set by data type and by data sources is the following :

|              | <b>CTD</b>   | <b>BOTTLE</b> | <b>THERMISTOR</b> |
|--------------|--------------|---------------|-------------------|
| IFREMER      | 1685         | 5901          |                   |
| IEO          | 2763         | 2337          | 29                |
| HNODC        | 2074         |               |                   |
| MODB         | 9429         | 538           |                   |
| WDC-A        | 506          | 21121         |                   |
| BODC         | 132          |               |                   |
| DOD          | 129          |               |                   |
| ICES         |              | 3920          |                   |
| SHOM/CMO     | 31           | 99            |                   |
| <b>TOTAL</b> | <b>16749</b> | <b>33916</b>  | <b>29</b>         |

For the BT data set some of the data have been collected by the navies and are not in the public domain, they have been used for the compilation of the Mediterranean climatology but they are not released in the final data set.

| <b>COUNTRY/SOURCE</b> |        | <b>MBT</b>   |              | <b>XBT</b>    |              |
|-----------------------|--------|--------------|--------------|---------------|--------------|
|                       |        | Usable       | Releasable   | Usable        | Releasable   |
| SPAIN                 | IHM    | 2925         | 0            | 1026          |              |
|                       | BIU    |              |              | 100           | 100          |
| GREECE                | HNODC  | 331          | 331          | 124           | 124          |
| FRANCE                | NAVY   | 6571         | 2152         | 36435         | 0            |
|                       | SHOM   | 886          | 886          | 2360          | 2360         |
|                       | Others | 18249        | 18168        | 804           | 775          |
| UK                    | HOT    | 6841         | 0            | 11371         | 0            |
| Others                | WDC-A  | 54965        | 54965        | 67268         | 67268        |
| <b>TOTAL</b>          |        | <b>90768</b> | <b>76502</b> | <b>119488</b> | <b>70627</b> |

The distribution maps of the CTD, BOTTLE, XBT and MBT profiles (Figures 2, 3 and 4) show a good covering of the Mediterranean sea, and the of Cadiz Gulf. However, along the African coast, the Middle East coast and in the Black sea the data are sparsely distributed.

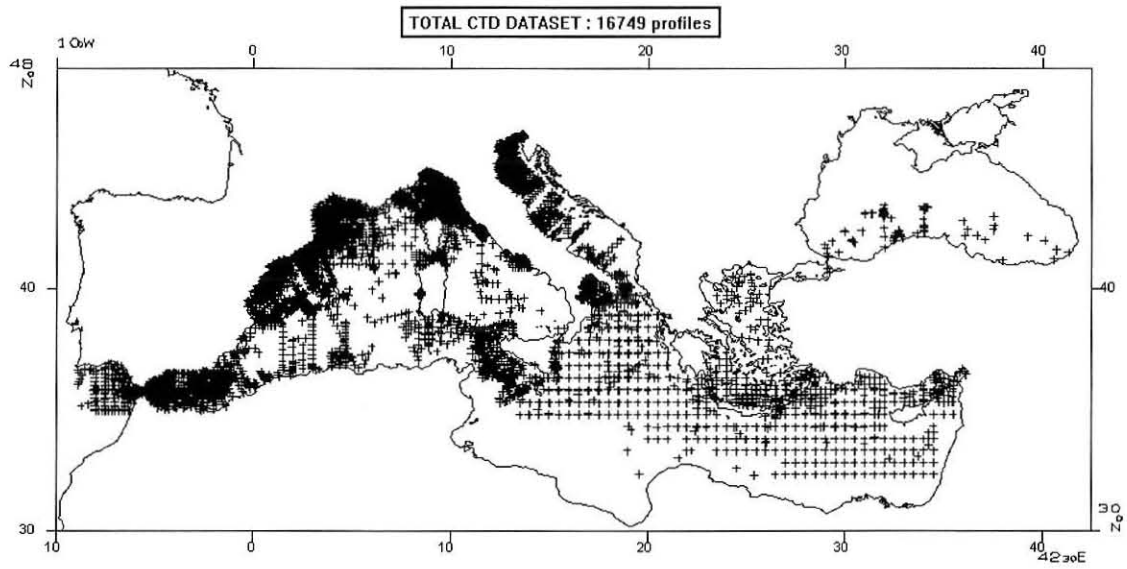


Figure 2. Distribution map of the CTD profiles of the MEDATLAS data set

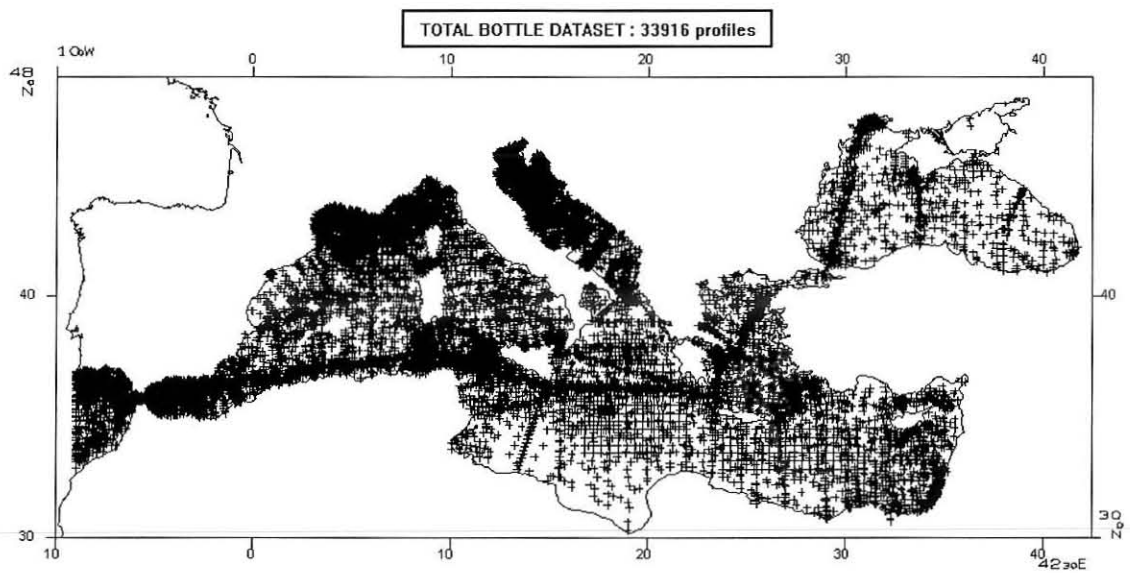


Figure 3. Distribution map of the BOTTLE profiles of the MEDATLAS data set

### XBT and MBT : 147 129 profiles

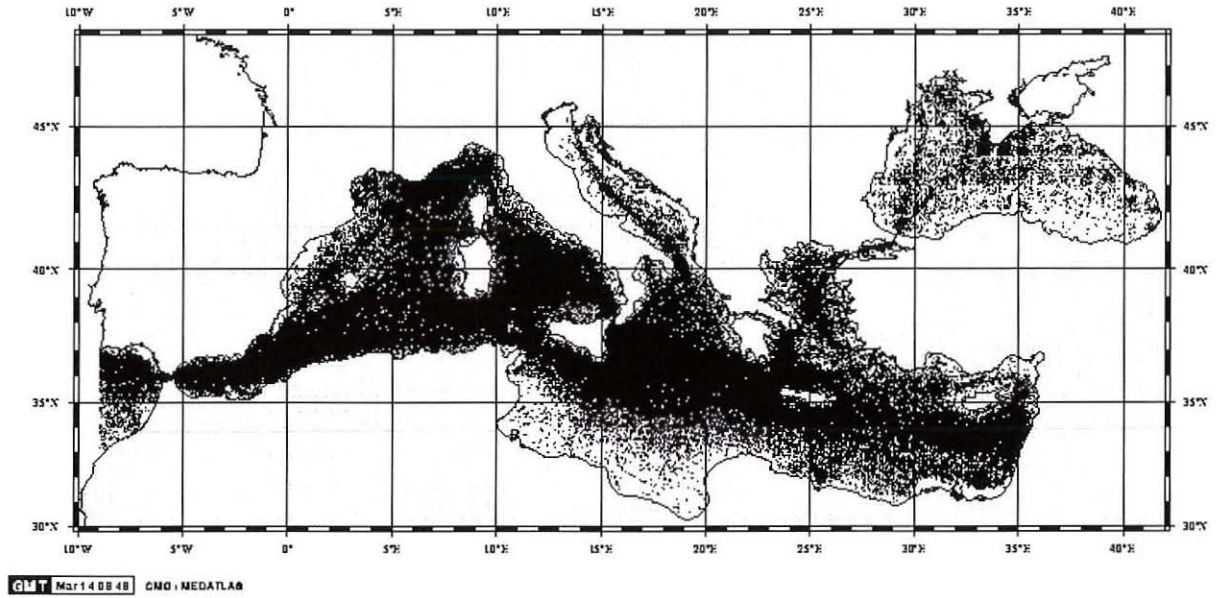


Figure 4. Distribution map of the XBT and MBT releasable profiles of the MEDATLAS data set

The oldest data of the MEDATLAS data set are bottle casts collected at the beginning of the century. The yearly distribution of the data per data type (Figure 5) shows a continuous sampling from the middle forties to nowadays, with a progressive substitution of MBT by XBT since the seventies, and the appearance of the CTD in 1975.

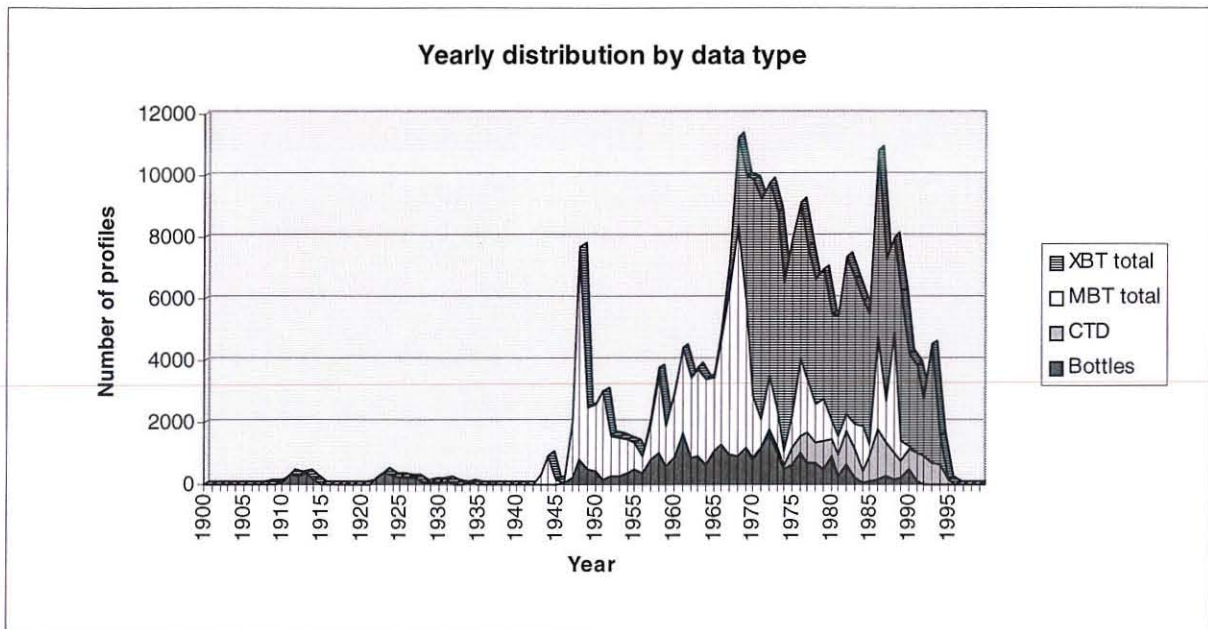


Figure 5. Yearly distribution of the MEDATLAS data set per data type.

The monthly distribution of the data (Figure 6) shows that there is fewer data during winter time (December, January and February) and that the maximum number of profiles is collected during may.

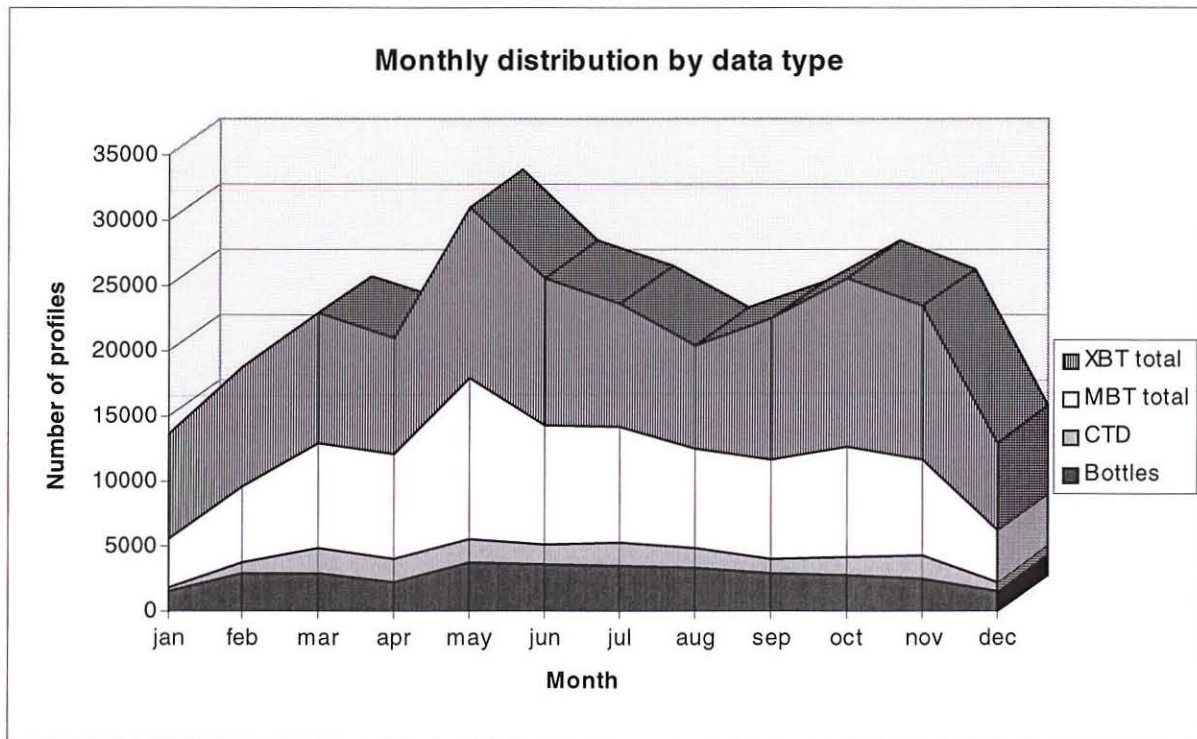


Figure 6. Monthly distribution of the MEDATLAS data set per data type.

The vertical distribution of the data (Figure 7) allows to compute a mensual climatology down to 300 m, a seasonal one from 400 to 800 m, and an annual one down to the bottom for the temperature. Concerning the salinity collected with the CTD and the BOTTLE, only an annual climatology has been computed.

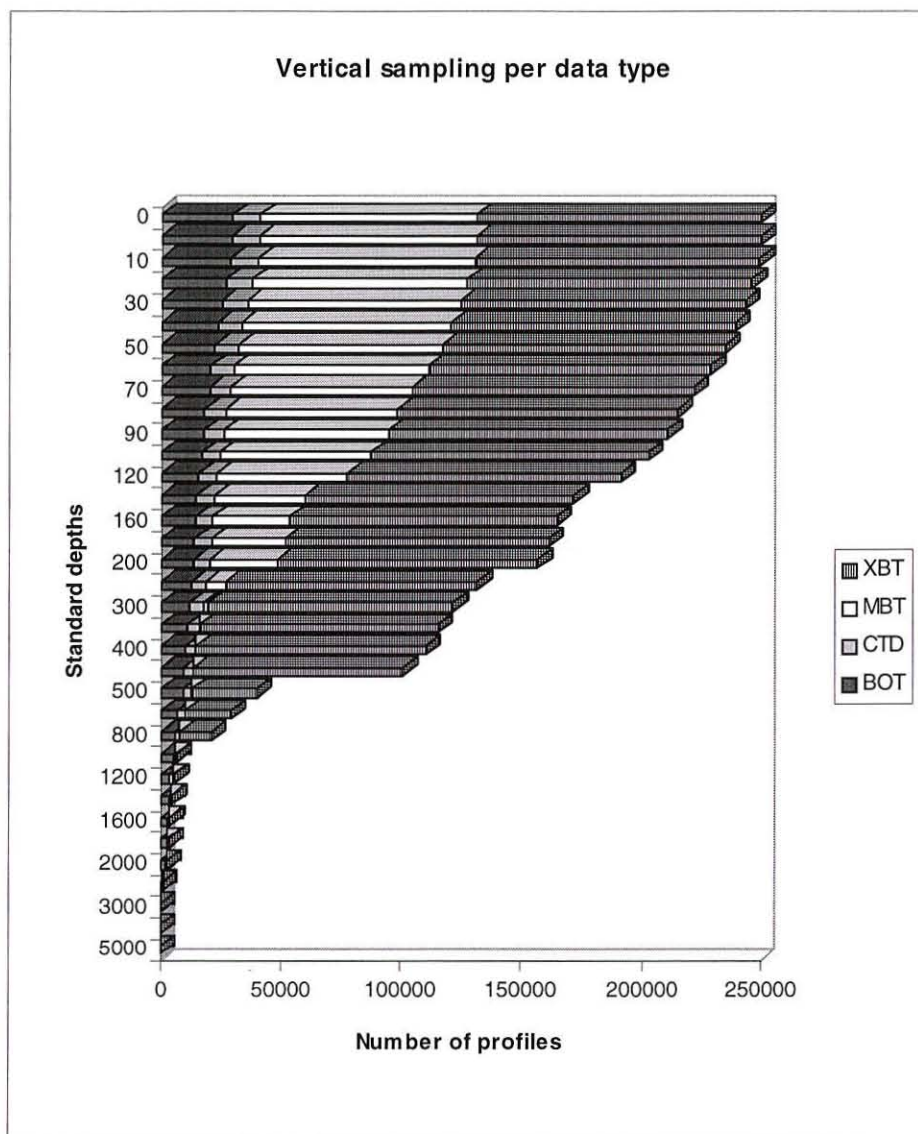


Figure 7. Vertical distribution of the MEDATLAS data set per data type.

## ANALYSED CLIMATOLOGICAL DATA

Once all the data set has been quality checked, only the « good » data (flag 1) are kept to compute the climatology.

The data are interpolated to standard levels (MEDATLAS Group, 1996) in two different ways. For CTD and Bottle data the interpolation is performed following the Reininger and Ross method (REINIGER & ROSS, 1968), and for the BT data a linear regression has been preferred since it is coherent with the way original profiles are subsampled before the storage in the data base.

After the QC, the number of profiles usable to compute the climatology amounts 260 136 (including the classified profiles).

A further automatic control has been performed for the computation, which rejected 0.45% of the total number of profiles. As a comparison, the same processing applied to a data set without any preliminary QC gives a rejection rate around 10%.

The gridded data have been calculated through a neural gridding and kriging method and then reinterpolated on a regular grid of a constant 0.25 degree step in longitude and in latitude a slowly varying step from 0.28 degree at 30.00 N to 0.22 degree at 47.78 N. The methodology is described in (JOURDAN, 1997).

Each processing level requires a new check for quality. The analyzed data have been controlled subjectively by mapping the parameters at different levels. It has been successfully checked that : (Figure 8)

- no methodological artifact was met : neither small scale noise, neither erroneous closure of the isolines in the vicinity of the shoreline or the empty regions;
- the main dynamic features like the modified Atlantic water of the Algerian current, the gyres of the Gulf of Lion and of the Levantine Basin, were properly reproduced;
- the slow variations of these features according to the seasonal cycle and the depth seemed coherent and robust.

Furthermore, a preliminary intercomparison with the MODB results has shown an overall good agreement between both methods, however it appeared small discrepancies over some regions of high variability where this method gave smoother distributions. A possible explanation is the difference in the data preprocessing which, in the present method, aims to avoid to give more weight to some years with larger data sets, but further study will be necessary to complete the intercomparison.

The MEDATLAS data set, climatology and maps will be available on CD-ROM by the end of 1997 (MEDATLAS Group, 1997). A user interface to select the data following several criteria (geographical area, ship, country, data quality, time/period, ...) is released on the CD-ROM (FICHAUT *et al*, 1997).

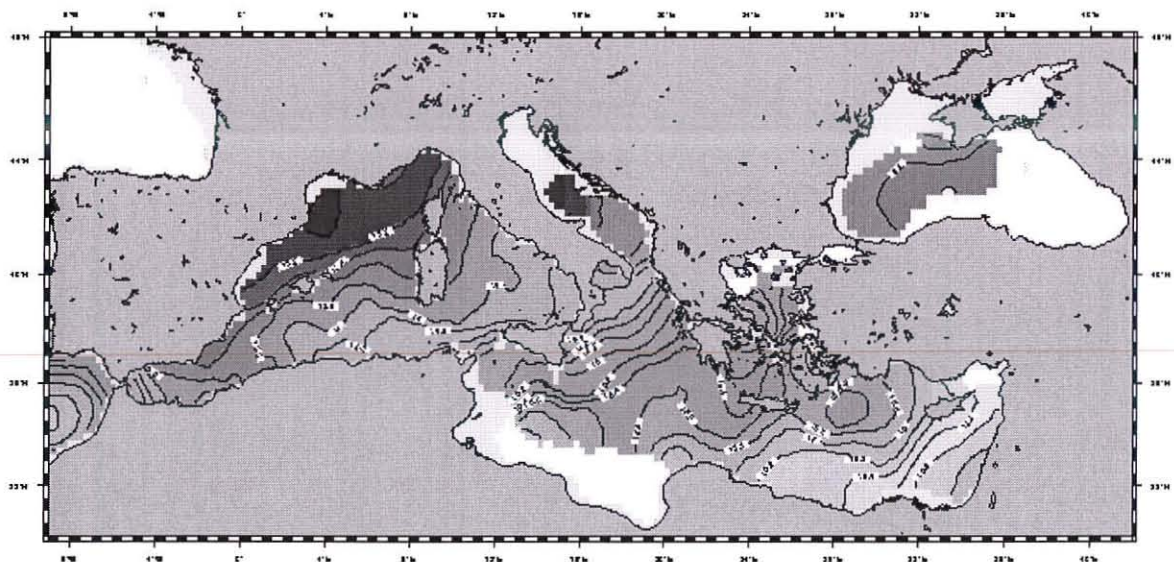


Figure 8A. Temperature distribution in FEBRUARY at Depth = 100 m.

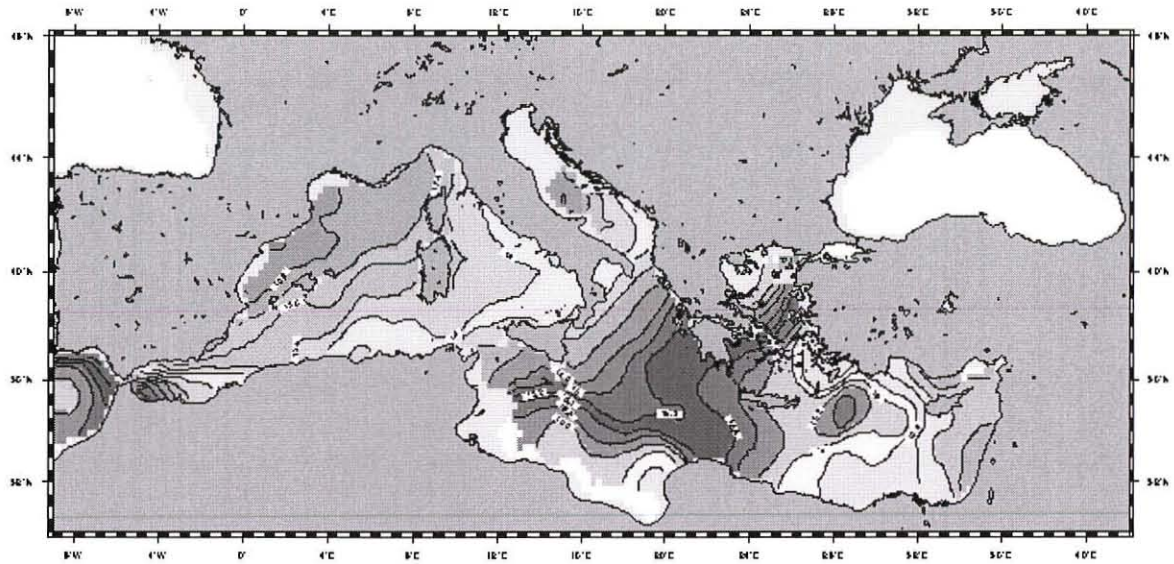


Figure 8B. Temperature distribution in MAY at Depth = 100 m.

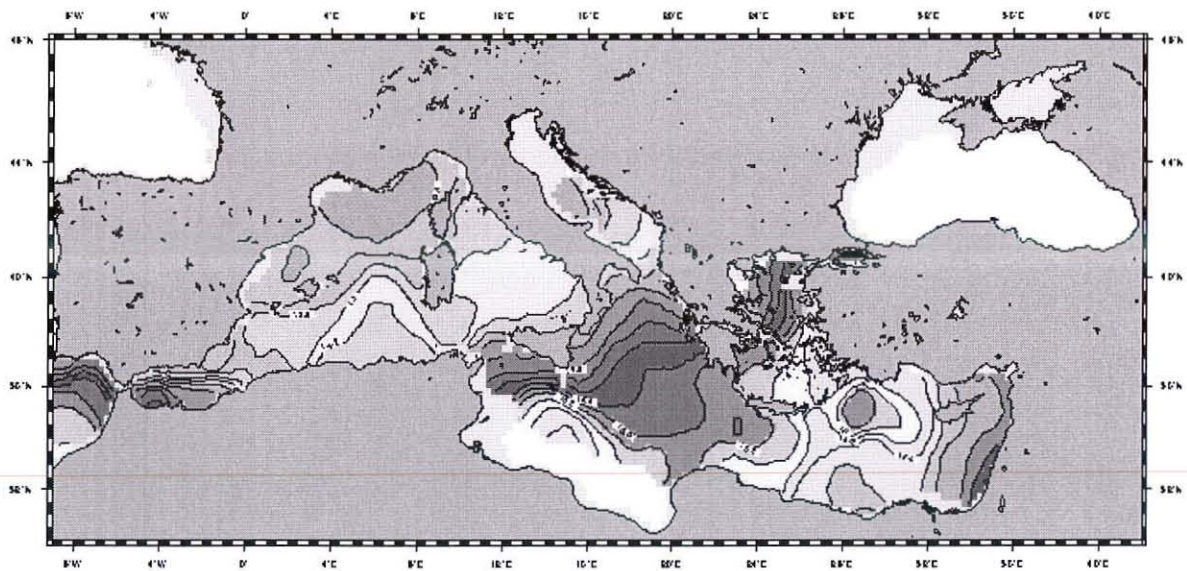


Figure 8C. Temperature distribution in AUGUST at Depth = 100 m.

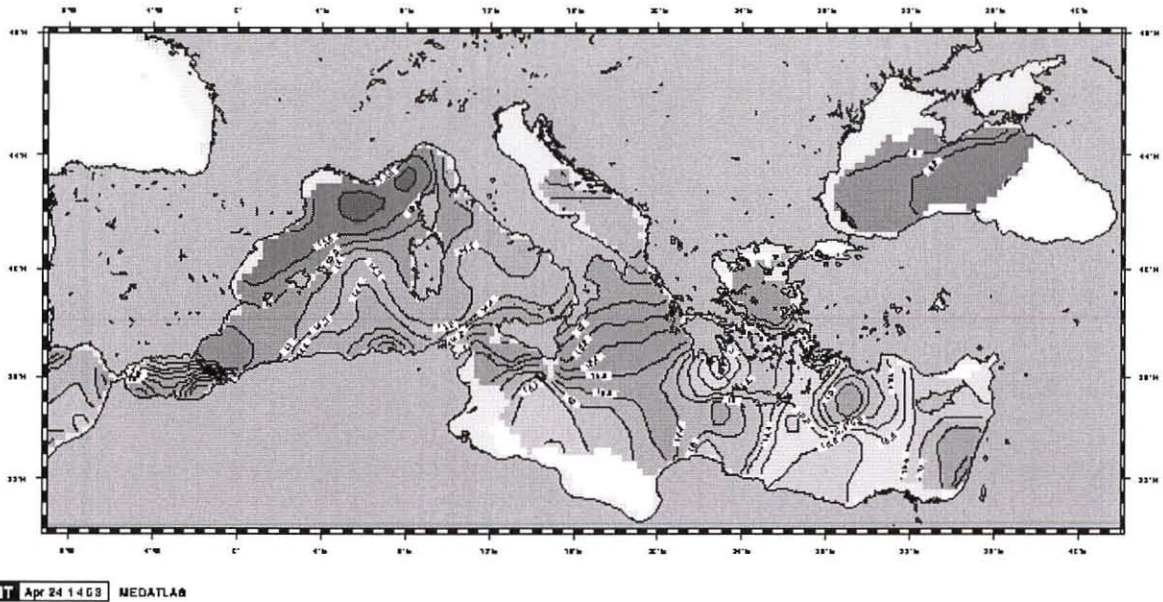


Figure 8D. Temperature distribution in NOVEMBER at Depth = 100 m.

Figure 8. Temperature distribution along the annual cycle. The step between the isotherms is

## CONCLUSIVE REMARKS

The MEDATLAS initiative not only has highly increased the available data set, but also has allowed four different data centers to perform quality checks of high level in a fully coherent and compatible way. These quality checks are more adapted to the local conditions, which represent an improvement from the previous methods, and have been performed by regional experts.

The two systems developed by IFREMER (SCOOP) and IEO (QCMED) respectively on UNIX and DOS have been intercompared to confirm that they provide identical control of data. Both systems provide a flexible interaction between visual and automatic checks and it was recognized that this is an important feature that will be required if additional chemical parameters as to be assessed.

However, the sparseness of data in the Eastern and Southern Mediterranean sea and in the Black sea show that the data set still has to be improved. Furthermore there is a need of climatological statistics on others parameters like dissolved oxygen and nutrients. In this perspective, a new program, MEDAR/MEDATLAS is in preparation.

## ACKNOWLEDGMENTS

This work has been undertaken in the frame of a MAST supporting initiative for ocean data and information management under contract MAS2-CT93-0074. The participants acknowledge with gratitude the financial and technical support of the EC, IFREMER, IEO, HNCMR, and SHOM.



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