Empirical reconstruction of salinity from temperature profiles with phenomenological constraints

F. Reseghetti

**Ocean Science
Discussions**

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ENEA-ACS CLIM-MED, Forte S. Teresa – Pozzuolo di Lerici, 19032 Lerici (Sp), Italia

Correspondence to: F. Reseghetti (reseghetti@santateresa.enea.it)

Title Page

Abstract | Introduction

Conclusions | References

Tables | Figures

|◄ | ►|

◄ | ►

Back | Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

EGU

Estimate of salinity from temperature profiles

F. Reseghetti

EGU

Abstract

The problem of estimating the salinity when only temperature profiles are available is having an increasing interest mainly because of multi-parametric data assimilation in ocean forecasting models. In this paper, a new method based on the introduction of a correction factor for salinity deduced from recent measurements is proposed to calculate salinity from temperature profiles and climatological datasets. It is supposed that the seawater potential density in a specific area, as deduced from climatological monthly averaged temperature and salinity values, does not change. A certain but small variability on its values is admitted and estimated combining the uncertainty of temperature and salinity in-situ measurements, and the diurnal variation, as obtained from a set of recent CTD and MedArgo measurements in Tyrrhenian Sea. Then, the deduced range of variability for salinity and potential density is imposed to synthetic values, which are compared with CTD and XCTD data. Finally, this technique is used to calculate salinity profiles from XBT temperature profiles from Ligurian and Tyrrhenian Sea (XBT probes monthly dropped along the transect Genova-Palermo, within the Mediterranean Forecasting System-Toward Experimental Prediction project). Results are analysed and discussed.

1 Introduction

Measurements of seawater temperature (T) are much easier to do and cheaper than the ones of salinity (S). Ships of opportunity have collected a wide amount of temperature profiles, and, consequently, the dataset of temperature values is much bigger than the salinity dataset. The implementation of multi-parametric data assimilation schemes in ocean forecasting models implies the use of realistic S values estimated from T profiles. The usual way-out is based on climatological datasets and some physical assumptions.

The density of seawater at a given depth can be expressed as a function of local

T and S values, but the relationship among salinity, temperature and other variables changes from region to region (Emery and Dewar, 1982), and was used for determining water types since early 40's (Sverdrup et al., 1942). It is useful to introduce the potential temperature (θ) values. It is possible to estimate salinity or potential density (σ) from T
5 profiles, but this is not a very difficult task only where seawater regimes are well known and stable. Under the assumption that a certain θ-S relationship does exist (even if changing in time and space), many authors proposed different techniques in order to calculate S profiles and/or dynamic heights when only T profiles are available, as from XBT measurements (e.g. Hansen and Thacker, 1999).
10 Among several approaches, Sverdrup et al. (1942) proposed to adopt a straight-line T-S representation using end-points for the North Atlantic Central Water, by assuming that intermediate temperature water has salinity value on the straight line. Stommel (1947) supposed that the main part of salinity variability is due to vertical movements of water having that S and T values. Then, he proposed that the expected salinity
15 at a given temperature is more or less the value previously measured at the same temperature.

Emery (1975) utilised mean θ-S diagrams to obtain the salinity corresponding to a measured temperature. Emery and O'Brien (1978) suggested a mean pressure – salinity relationship, in which S was derived from T, and mean local P-S curves; the
20 authors were also able to calculate more accurate geo-potential heights than Stommel's method did. An early version of this approach was developed in Emery and Wert (1976), whereas different upgrades were done in Emery and Dewar (1982), and in Siedler and Stramma (1982). Donguy et al. (1986) introduced in their computations sea surface salinity as deduced from θ-S relationship. The near-surface portion was
25 defined by linear interpolation from T and S monthly average values at surface to the subsurface S maximum, which is usually present in tropical Pacific Ocean, and, one year later, Kessler and Taft (1987) improved this method. Käse et al. (1996) developed a method based on observed horizontal distribution of T and S profiles; they were able to reproduce T and S variations at constant pressure over distance in case of smooth

and monotonic changes between CTD stations. Hansen and Thacker (1999) upgraded the Emery and O'Brien's (1978) proposal, and computed the coefficients relating the estimated S profile with measured "predictor parameters" (T, sea surface salinity, and latitude) by usinga fitting procedure. From the analysis of the influence of assimilation within models, Troccoli and Haines (1999) proposed to derive a T-S relationship from the most recent data in proximity of each T profile, or from the model (Haines et al., 2005).

Each approach presents some problems. Following Käse et al. (1996), the method of Emery and Dewar (1982) can produce large errors in salinity values in regions with mesoscale variability and water mass conversions, and it is not suitable if large anomalies occur. On the other hand, the Sverdrup et al. (1942) method fails in situations where T and salinity do not have a one-to-one correspondence within a T-S relationship.

Empirical Orthogonal Function (EOF) decomposition of historical T and S data offers a completely different way-out: S is reconstructed from a linear combination of the dominant modes. The coefficients are obtained by minimising the difference between modes and data from available observations, namely T and sea level (see Maes, 1999; Maes and Behringer, 2000, and references therein; Maes et al., 2000). Carnes et al. (1994) proposed regression models estimating the coefficients of salinity EOFs from the coefficients of temperature EOFs. Vossepoel et al. (1999) presented a hybrid method, estimating S below the bottom of thermally mixed layer by T-S technique and within the isothermal layer by linear interpolation to a measured sea surface salinity. When a great anomaly occurs, this technique produces fictitious density inversions; therefore a correction, using sea surface heights, mainly from satellite observations, is introduced.

Most of the cited authors (e.g. Vossepoel et al., 1999) showed that σ profiles calculated by means of the synthetic salinity are not guaranteed to be close to the true potential density, but the "mean computed value" is in a good agreement with the "true mean value", due to compensations in the vertical profile. Therefore, the computed

Estimate of salinity from temperature profiles

F. Reseghetti

EGU

surface geo-strophic currents, and dynamical heights are quantitatively good, even if problems arise when a more complete description of the internal dynamics is required.

Recently, the calculation of salinity from T profiles became of paramount importance for the ocean forecasting (e.g. De Mey and Benkiran, 2002) because of multivariate assimilation in numerical models (Demirov et al., 2003; Sparnocchia et al., 2003): in fact, multivariate data assimilation greatly improves the models. In this regard, XBT data are operationally collected, and S profiles are calculated by using historical data, and EOF technique.

MODAS (Modular Ocean Data Assimilation System) approach (Fox et al., 2002) combines the Hansen and Thacker technique (in order to estimate salinity from XBT profiles) with regression models assuming that climatological T and S values agree with observed T-S relationships. More in detail, salinity is computed by a linear function of temperature with coefficients depending on specific area and depth. Recent improvements, i.e. HYCOM (Hybrid-coordinate Ocean Model), see Bleck (2002), and Halliwell (2004), try to include XBT data into the model (Thacker and Esenkov, 2002), and to extend initial steps based on Gulf of Mexico analyses to open oceans such as Atlantic Ocean (Thacker, 2006, Thacker and Sindlinger, 2006).

The different techniques are based on the underlying idea that the relationship between T and S for certain sea areas is seasonally changing, but it shows very small variations over longer time scales, with the "natural" exception of near surface seawater. In many cases, this is a good working hypothesis, but the reliability of the above-mentioned methods is not assured in areas where the seawater physical characteristics are subjected to a high inter-annual variability. This is the case of Mediterranean Sea, having great and rapid changes, a non-simple behaviour probably related to its size, coastal influences, and bathymetry.

Some processes producing temperature instability are not correlated to salinity variability: examples were provided in areas of strong mixing, such as the surface mixed layers, or eddy induced mixing. The θ-S relationship cannot be well defined, and can be strongly time-dependent in isothermal layers presenting salinity stratification. For

EGU

example, Hansen and Thacker (1999) found that CTD profiles from Pacific Ocean show a depth-dependent behaviour: local correlation between θ and S is small in the upper 50 m, small and negative between 50 and 150 m depth, positive below 200 m. It must be noted that θ and S temporal variability decreases with depth; moreover, the θ-S
5 relationships derived from climatological datasets (when and where climatology is representative of an averaged state), are generally valid, and remain almost unchanged over the time. Therefore, they can be used as an approximation estimating salinity from temperature values. Salinity on pressure surfaces at a fixed date can be reproduced in an approximate way by a function of temperature and geographic coordinates (i.e.
10 linear function in MODAS). The use of high degree polynomial of temperature, coordinates, pressure, and so on, does not improve the results as expected. In fact, specific (local) values of data used to compute the coefficients of the polynomial could induce a rough description of independent data.

In this paper, an empirical method estimating S from T profiles is presented, by
15 improving the method developed in Vignudelli et al. (2003), where synthetic salinity profiles were computed by modifying climatological profiles through the use of the spline coefficients technique. Unfortunately, climatology seems not to be not able to describe the strong variability recorded in last years in Mediterranean Sea, due either to transient phenomena or to something related to the seawater warming processes. In
20 addition, the robustness of climatological datasets is not homogeneous, both in spatial and temporal sampling.

The underlying idea is that it is possible to calculate more realistic synthetic salinity values in a specific sea area if recent T and S profiles from the same region (better if at a seasonal rate) are available (such as from CTD, ARGO or GLIDER measure-
25 ments). More in detail, it is supposed that the averaged difference between climatology and measurements can describe the main part of the variation with respect to climatological seawater parameters because of temporal evolution. A correction factor is computed and used to improve climatological values of S and σ correspondent to T profiles (such as from XBT probes) from the same area in the period correspondent

to trial measurements. In this work, the inputs are the MEDAR/Medatlas climatological dataset, and recent CTD and MedArgo T and S profiles from Tyrrhenian Sea. Constraints derived from such measurements are imposed on the variability, and the physical meaning of the corresponding σ profile is required. Seasonal evolution is admitted and required; only inter-annual variations, though not large, are reproduced in some ways by the method. After a sensitivity analysis evaluating the impact of uncertainties in the estimate of S and σ, a feedback process involving potential density is used. Then, synthetic S and σ profiles are computed and compared with recent measurements.

The plan of the present paper is as follows: in Sect. 2 the climatological dataset for Mediterranean Sea are considered, whereas in Sect. 3 the available dataset are detailed, including the data preparation and a comparison with the existent climatology. In Sect. 4, the new method is proposed and separately applied to Tyrrhenian and Ligurian datasets, whereas a comparison with a set of XCTD measurements in Tyrrhenian Sea is proposed in Sect. 5. Results of the application of this technique to XBT profiles are reviewed in Sect. 6, whereas discussion and comments are in Sect. 7.

2 Dataset in the Mediterranean Sea

During the last decade, a great effort was made to collect historical data in the Mediterranean Sea: protocols for quality assessment and θ-S climatological datasets were provided (Medatlas Group, 1994; Brasseur et al., 1996). Recently, a project was launched by the European Commission to safeguard all the information on the Mediterranean Sea environment, in the framework of the UNESCO – Intergovernmental Oceanographic Commission program GODAR (Global Oceanographic Data Archaeology and Rescue). The Mediterranean component of such program was called MEDAR (MEditerranean Data Archaeology and Rescue), and involved institutions mainly from countries bordering the Mediterranean and Black Seas, but also included contributions from Belgium, Denmark, and USA (Medar Group, 2001).

Estimate of salinity from temperature profiles

F. Reseghetti

A subset of the MEDAR/Medatlas dataset was recently used to build an improved climatology called MED-6 (Brankart and Pinardi, 2001), providing T and S mean monthly profiles in a regular grid of 0.25 degrees. Unfortunately, the new climatology is not representative of all Mediterranean areas, due to the temporal and spatial coverage.

5 Usually, the global dataset from a selected region is statistically consistent, but monthly and yearly measurements show a great variability both in number and in values, depending on the analysed area.

As an example, many measurements are available for the Ligurian Sea and can provide useful information on temporal behaviour of the T-S characteristics. The amount

10 of historical data is much smaller for other Mediterranean regions: for instance, Ionian Sea and Eastern areas.

The temporal variability of the θ-S relation is generally associated to seasonal changes in the water characteristics. For the Mediterranean Sea, the protracted temporal changes of the θ-S relation can be attributed mainly to temperature trends, since

15 the total salinity is assumed to be almost constant. In addition, it can be assumed that other effects, such as mixing among different water masses, have weak influence, and θ-S properties are almost stable over long time scales.

3 The available dataset

T and salinity profiles collected from 1996 up to 2005 in Ligurian and Tyrrhenian Seas

20 have been used: CTD casts are the most part of them, but since August 2004, profiles from MedArgo floats are available. The main characteristics of the dataset are shown in Tables 1 and 2. All the 1996–1999 profiles are from the MEDATLAS dataset. Many profiles were recorded during URANIA vessel cruises by using a SeaBird SBE 911 *Plus* automatic profiler, calibrated before and after each cruise at NURC, La Spezia (Italy).

25 Its sampling rate is 24 Hz, the adopted falling speed is $1.0\,\mathrm{ms}^{-1}$, and its (static) nominal accuracy is $\delta T = \pm 0.001°\mathrm{C}$ on temperature and $\delta C = \pm 0.0003\,S\,\mathrm{m}^{-1}$ on conductivity. The (static) time responses are $0.065\,\mathrm{s}$ for conductivity and temperature sensors, and

F. Reseghetti

EGU

0.015 s for the pressure sensor.

CTD profiles from Urania dataset data were processed by using standard Seabird's software (Data Conversion, Alignment, Cell Thermal Mass, Filtering, Derivation of physical values, Bin Average and Splitting); then, they were controlled by using Medatlas protocols (Maillard and Fichaut, 2001). MedArgo float consists of two different types of instruments (APEX and PROVOR), both having SBE conductivity sensors. In any case, the vertical stability for all the CTD and MedArgo profiles has been checked and assured.

3.1 Data preparation

As a preliminary step, climatological T, S and σ profiles are prepared for each available profiles in the following way:

- The monthly climatological dataset, which is supposed to be representative of the central day of each month, is re-sampled at every 5 m down to 100 m depth, at each 10 m down to 1000 m depth, at each 150 m down to 2500 m; then, the values at 3000 and 3500 m depth are added. Linearly interpolated in depth and in time T_{CLI} and S_{CLI} profiles are obtained for the area corresponding to the selected measurements;

- Climatological σ profiles are calculated and checked since some σ inversions occur. In such a case, they are corrected in order to have σ values always increasing with depth; then, new S_{CLI} profiles are deduced from the ordered σ profiles;

- CTD and MedArgo T and S profiles are re-sampled at the same depths as the climatological profiles, and the corresponding σ profiles are computed.

3.2 T and S uncertainty and variability

The management of the uncertainty and variability of the physical parameters, which are due to the instrumental errors and environmental changes at daily time scale, is

included. Obviously, the calculation of salinity from climatology cannot be more precise than the differences existing between real data: only if other (external) constraints are available, a fine-tuning can be done.

It has been supposed that the uncertainty is $\delta T = \pm 0.01°C$ for climatological temperatures, and $\delta T = \pm 0.1°C$ for XBT measurements (a value as great as the instrumental sensitivity indicated by manufacturer). In a similar way, an uncertainty of $\delta S = \pm 0.01\,PSU$ is supposed to affect the climatological salinity values. The results are summarised in Table 3.

The uncertainty in σ values induced by the temperature slightly depends on the depth, being associated to the pressure effects on θ, whereas the influence of salinity uncertainty does not change with the depth. The effect of the contemporaneous use of both the uncertainties ranges from $0.0065\,kgm^{-3}$ ($\delta T = \pm 0.01°C$) up to $0.0337\,kgm^{-3}$ ($\delta T = \pm 0.1°C$). Consequently, σ values within that uncertainty have to be thought as equal, or this is the biggest difference between two values in order to quote them as coincident. It has to be stressed that a "noise level" as great as $0.03\,kgm^{-3}$ (up to $0.05\,kgm^{-3}$ in upper layers) was defined as "acceptable" in the protocol for quality control published by Maillard et al. (2001).

The experimental daily variation of S and σ, and its correlation with T, is calculated down to 250 m depth. The available CTD dataset includes hourly repeated measurements in the same geographical position made in January and October 2004 in the Tyrrhenian Sea (two stations, for 24 profiles). The daily T and S oscillations are computed by choosing, at each depth, the half interval of the measured range of variability, the instrumental uncertainty also. Then, they are combined (by adding in quadrature), and their effect on the global σ variability is supposed to represent an upper limit to the daily σ variability. All σ values within the computed range have to be thought as indistinguishable. The oscillation range in upper layers (down to 100 m depth) has been modified, as deduced from daily variability, by introducing a linear interpolation, because of the strong fluctuation occurring at the surface. Moreover, the derived daily variability for all the available measurements, independently on the month, can repre-

sent an even more significant overestimate of the variability in winter or homogeneous water potential density profiles.

3.3 Differences between climatology and datasets

Climatological and measured T, S and σ profiles have been compared. The correlation between historical and recent data is also computed by plotting historical vs. new measurements, and gives a quantitative parameter of the possible evolution of water characteristics. Results concerning dataset 1996–2001 are plotted in Figs. 1a and b, whereas in Figs. 1c and d, and in Figs. 1e and f dataset 2004–2005 and dataset 1996–2005, respectively, are shown. The fits of T measurements have the same relatively good quality, but the slope of 2004–2005 dataset indicates a deviation from climatological values smaller than in the 1996–2001 one. In fact, when the temperature differences are analysed, the discrepancy between earlier and new measurements is evident. In 1996–2001 dataset, only cooler waters are present at depth ranging between 200 and 500 m, whereas waters at deeper depth are warmer, up to +0.3°C. In recent dataset, both warmer and cooler waters occur in the previous range of depth, and a significant bump is evident below 500 m depth, with temperature differences within the range 0.1–0.4°C.

As a further parameter to check the concordance between climatology and recent measurements, the correspondent σ values are analysed. In Fig. 2, the agreement between climatological and measured σ values, at depths ranging from 5 m down to 2350 m, is specified through the number of values differing less than the uncertainty used in this analysis. If recent values differ less than the allowed variability, such σ values can be thought as constant in time, and the temporal σ stability is verified. Such an assumption is reasonable (at a level of about 80%) down to 100 m depth in both datasets (Fig. 2a and b), mainly thanks to the large admitted variability. At deeper depths, the stability is a robust hypothesis always verified, but the region between 100 and 1000-m depth puts in evidence significant differences, being the agreement at a level of 45% in the whole dataset (Fig. 2e), with a slightly better concordance

Title Page

Abstract | Introduction

Conclusions | References

Tables | Figures

|◄ | ►|

◄ | ►

Back | Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

EGU

of values in more recent dataset. In general, recent measurements show that the water in Tyrrhenian Sea is generally warmer, saltier, and slightly denser than quoted by climatological datasets.

4   Synthetic salinity

The basic assumption of the proposed method is that in each sea region the local θ-S relationship (as deduced from climatological dataset), and the accompanying σ profile evolve at seasonal time scale, but they have not significant variations at inter-annual time scale. This means, for instance, that different profiles as measured in the same day, but in different years, have to be assumed as coincident if their difference at each depth is within the oscillation range (due to instrumental errors and daily variability). Deviations are admitted, and can be recognised and reproduced only when a trend occurs: this requires a transient phenomenon over a significant time interval (at least, more than one year).

The results detailed in Figs. 2a, b, and e indicate that the assumption of σ stability seems to be ruled out mainly at depths ranging from 100 down to 1000 m.

4.1   Proposed technique

Climatological T and S values, as deduced from monthly datasets, represent an average based on a set of data and cannot describe a specific measurement. Therefore, a significant discrepancy between climatological values and real data can occur and, consequently, assimilation of salinity in models can show relevant disagreement and uncertainty. In order to reduce such a discrepancy, modified salinity profiles (S_{CLI}^{*}) have been computed starting from climatological S_{CLI} profiles.

It has been supposed that a synthetic salinity profile (S_{CLI}^{*}) in a specific area can be computed starting from the correspondent climatological profile by introducing a correction factor (CF) deduced from latest measurements in that region, and describing

Title Page

Abstract | Introduction

Conclusions | References

Tables | Figures

◄◄ | ►►

◄ | ►

Back | Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

EGU

12

the difference averaged over time and space. The correction factor is a function f_S depending on measured temperature $T_X(h)$, climatological temperature $T_{CLI}(h)$, and difference $\Delta T(h) = T_X(h) - T_{CLI}(h)$ between climatology and measurements. In short, $S^*_{SYN}(h) = S_{CLI}(h) \cdot f_S(h, T_{CLI}(h), \Delta T(h))$, where the function f_S will be shortly called CF in the paper. The function calculates the ratio between all measured and climatological values of salinity at each selected depth, climatological temperature, and temperature difference with respect to the climatology. The used range of variability is $12.0^\circ C \leq T_{CLI} \leq 27.6^\circ C$ (step $0.2^\circ C$) for temperature, and $-4.0^\circ C \leq \Delta T \leq +4.0^\circ C$ (step $0.1^\circ C$, a value as great as the nominal sensitivity of XBT probes) for temperature difference.

More in detail, each synthetic salinity profile is computed as follows:

1. σ profile is calculated from climatological T and S dataset and from the recent datasets, and its inversion are removed, if necessary;

2. Minimum (and maximum) of salinity and σ diminished (increased) by 0.01 units at each depth within a selected temperature interval is calculated from datasets of recent measurements;

3. The maximum S and σ difference between the values measured at two consecutive depths within the same temperature interval is calculated from recent measurements and increased by 0.01 units.

4. The basis of isothermal waters in upper region (usually in late summer, autumn and winter) is determined by software, then the points 2 and 3 are repeated for this part of the profile.

5. S_{CLI} profile is multiplied by CF, and two conditions are imposed:

   – the difference between the S values at two consecutive depths has to be not greater than the maximum measured at a fixed depth and temperature;

Estimate of salinity from temperature profiles

F. Reseghetti

Title Page

Abstract | Introduction

Conclusions | References

Tables | Figures

|◄ | ►|

◄ | ►

Back | Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

EGU

- the S value at each depth has to be not greater (lower) than the maximum (minimum) measured at a fixed depth and temperature;

6. A σ profile is computed by using such a modified S profile, and the same conditions as at point 5, but for potential density, are applied, also taking into account the occurrence of isothermal profiles. In such a case, σ inversions are eliminated, and the profile is monotonically ordered. This is the "synthetic potential density profiles $\sigma^*_{\mathrm{SYN}}(h)$".

7. From $\sigma^*_{\mathrm{SYN}}(h)$, the salinity profile is computed, and conditions detailed at point 5 are newly applied. This is the "synthetic salinity profile $S^*_{\mathrm{SYN}}(h)$".

4.2 Method validation

In order to check the validity of the proposed technique, the available time ordered dataset of profiles from Tyrrhenian Sea has been divided in sub-samples, and the correction factor has been computed for each subset. Then, synthetic profiles have been obtained by using either the specific CF correspondent to the selected sub-sample or CF deduced from the remaining sub-sample. The comparison has been based on the analysis of the correlation when synthetic values are plotted vs. climatology and measured values, and on the values of averaged differences.

An important step of the proposed method is the capability of reproduction of measured values when CF is not deduced from the analysed dataset. Two are the selected computational ways to verify such a hypothesis, implying the use of CF deduced from a dataset different in time, or from contemporaneous, but independent measurements. For the former, two interpretations are possible, depending on the capability the CF has to allow a right reproduction of measured values. An uncorrected description can be due either to the incapability of the method, or to a peculiar time evolution of physical parameters. In any case, the robustness of the dataset originating CF in order to have right values for the correction factor is fundamental. Afterwards, Ligurian Sea dataset

has been analysed in the same way as the Tyrrhenian one. Results of comparison with such datasets are shortly detailed.

4.2.1 Tyrrhenian Sea

The proposed technique has been checked on time-ordered Tyrrhenian Sea 1996–2005 dataset, and its sub-samples 1996–2001, 2004–2005, and 2004–2005 ODD and 2004–2005 EVEN. The latest datasets were created by extracting from 2004–2005 dataset profiles in position odd or even, respectively.

The analysis of sub-samples 1996–2001 and 2004–2005 highlights some details of the evolution of Tyrrhenian Sea water characteristics. The former confirms the differences with respect to climatological values as evidenced by T profiles (Fig. 1b). Clearly, Tyrrhenian waters are saltier at about 150 m depth (Fig. 3c) and below about 400 m depth (Fig. 3e), and σ values slightly increased (Figs. 3d and f). In this case, synthetic values give a better reproduction of measurements, but the agreement is poor for both S and σ in the region between 100 and 400 m depth. Consequently, only 67% of σ^{*}_{SYN} values in the region 100–1000 m agree with measurements. This could be due to the rough and poor temporal and spatial coverage of the data and makes the CF values at those depths unstable and not sufficiently robust.

The analyses on 2004–2005 dataset reveal a different behaviour. The differences in temperature are lower (Fig. 1c), but a significant bump occurs below about 500 m depth (Fig. 1d), and salinity difference confirms such a variation (Fig. 4e). The capability of synthetic values in reproducing real measurements is evident for both S and σ. The profile of salinity average difference (Figs. 4c and e) underlines a reduced discrepancy in the region between 100 and 300 m depth, mainly due to the influence of 2004 measurements. Similar conclusions are valid for potential density difference (Figs. 4d and f), where the agreement of fit coefficients is very good.

The results of the use in calculation of CFs extracted from a different dataset are explained in Figs. 2a and b, and Figs. 3 and 4 (green lines). The values of fit coefficients are acceptable for both the physical parameters, and improve the results based on

Estimate of salinity from temperature profiles

F. Reseghetti

EGU

climatology. The correlation values indicate a sometimes-significant dispersion in both cases, 1996–2001 dataset with 2004–2005 CF, and 2004–2005 dataset with 1996–2001 CF.

If CFs computed by sorting time-ordered and randomly distributed measurements are applied, interesting results occur. Climatological, synthetic and synthetic with mixed CF plots vs. measurements of salinity for 2004–2005 EVEN dataset are shown in Figs. 5a and b, and in Figs. 6a and b for 2004–2005 ODD dataset. The values of the fit coefficients are in substantial agreement when synthetic salinity mixed results are compared, and well improve the climatology, but the correlation indicates a dispersion of synthetic values bigger than the occurrence when the proper CF is used. The σ values computed with synthetic mixed CF are worse than the ones computed with their specific CF, but much better than the ones deduced from climatology (see Figs. 2c and d, and Figs. 5c and 6c).

The 1996–2005 dataset shows significant discrepancies from climatology in T, salinity and potential density values with interesting depth dependent differences. The fit coefficients and correlation values of Fig. 7a indicate that Tyrrhenian waters are different from climatological waters, with some evident changes in the region between 100 and 1000 m depth (Fig. 2e). In addition, the profile of salinity average difference displays an evident increased salinity value below about 400 m depth with respect to the climatology (Figs. 7c and e); σ values are also greater (Figs. 7d and f). When S^*_{SYN} and σ^*_{SYN} values are considered, the difference with respect to measured values is strongly reduced, and the strength and the depth dependence of the average difference (Figs. 7c and e for salinity, and Figs. 7d and f for potential density).

The analysis on Tyrrhenian datasets indicate that the proposed technique (computing synthetic values for both S and σ starting from T profiles, monthly climatological datasets, and correction factor deduced from recent measurements), greatly improves the climatology, and has usually a good agreement with real data. As a marginal result, in order to obtain a robust CF it is fundamental to have a dataset homogeneous in space and time or, at least, with a good seasonal sampling.

Title Page

Abstract | Introduction

Conclusions | References

Tables | Figures

|◄ | ►|

◄ | ►

Back | Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

EGU

4.2.2 Ligurian Sea

The strong discrepancy between climatology and measurements in Ligurian Sea datasets is evident in plots concerning 1996–2005 dataset (see Fig. 8a for temperature, c for salinity, and e for potential density), as well as the bad quality of the related fits. Recent measurements and climatology disagree, both for S (Figs. 8c and d), and σ (Figs. 8e and f). Bad values of fit coefficients for both S and σ and of the correlation clearly confirm the visual results (Figs. 8c and e).

In addition, 2004–2005 measurements indicate discrepancies of different kind with respect to the previous ones, and significantly saltier and denser waters appear in region down to 300 m depth (see Fig. 9a for temperature, c and d for salinity, and e and f for potential density). The values of fit coefficients and of the agreement between measurements and σ_{CLI} values (Figs. 9c and e) indicate the occurrence of relevant physical phenomena in such a region.

5 Comparison with XCTD measurements

Synthetic values of salinity (and potential density) have been compared with profiles obtained in Tyrrhenian Sea by using 21 Sippican XCTD-1 Digital probes (manufactured by TSK, Yokohama – Japan) dropped in May, September and October 2004. Such expandable instruments have improved uncertainty in temperature values when compared to XBT probes ($\delta T \sim 0.01°$C instead of $\delta T \sim 0.10°$C), whereas the uncertainty on S is about 0.03 PSU. Climatological and measured values are compared with synthetic values as computed by using Tyrrhenian 2004–2005 dataset and the related CF, and the results are shown in Fig. 10. Despite the small available sample, T values are in general greater than climatology states (Fig. 10b), even if the fit does not display strong disagreement (Fig. 10a). Similar behaviour occurs when salinity is analysed: the fit coefficients show that saltier values occur mainly below 200 m depth, but the quality of fits is bad (Fig. 10c). In general, synthetic values seem to be able to repro-

duce measured values better than climatology, but a disagreement remains (Fig. 10d). Synthetic values overestimate real measurements, even if the disagreement is more or less constant below 200 m depth, at a level of about 0.05 PSU. The results of analyses on potential density are similar (Fig. 10e), even if σ^*_{SYN} well fits the measurements (Fig. 10f): in fact, σ^*_{SYN} values overestimate measurements, but the difference is practically constant below 200 m depth, at a level of about 0.03 kgm^{-3}.

6 Application to XBT profiles

The proposed technique has been applied to T profiles obtained from XBT probes dropped along the transect Genova-Palermo, from May 2004 to December 2005, during 15 monthly cruises, with the exception of June, July and August 2004, and of July and August 2005. The sample consists of 414 profiles from Tyrrhenian Sea and of 119 profiles from Ligurian Sea, the maximum depth being 890 m and 770 m, respectively. The advantage in having such repeated measurements done by VOS activity is just the possibility to study the time evolution of water characteristics, but only T values are recorded by XBT probes, a similar monitoring activity being much more expensive when XCTD probes are dropped.

The measured T values have a not negligible difference with respect to the climatological values (Fig. 11a), and all the measurements at depth deeper than 500 m indicate values warmer than before, within the range of 0.1–0.4°C (Fig. 11b). The corresponding CTD sample has a lower difference, but the sampled area is slightly different. When S^*_{SYN} and σ^*_{SYN} are compared with results obtained by using Tyrrhenian 2004–2005 dataset, a general concordance appears. More in detail, salinity shows larger discrepancy (Fig. 11c and d vs. Figs. 4c and d) than potential density has (Figs. 11e and f vs. Figs. 4e and f), both in fit coefficients and average differences. This could be partially attributed to the characteristics of available sample of CTD casts, which is highly inhomogeneous in time and in space, with respect to the XBT dataset, which includes T profiles monthly recorded on the same transect.

OSD

4, 1–39, 2007

Estimate of salinity from temperature profiles

F. Reseghetti

Title Page

Abstract | Introduction

Conclusions | References

Tables | Figures

◄◄ | ►►

◄ | ►

Back | Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

EGU

The comparison of XBT profiles in Ligurian Sea with climatological T profiles shows a not negligible difference (Fig. 12a), even if the quality of the fit is good. Unfortunately, few profiles have depth deeper than 550 m (Fig. 12b), but the available data put in evidence a clear seawater warming process, less evident in near surface layers. When S^*_{SYN} profiles are analysed, a significant difference appears in the fit, which has a rough quality (Fig. 12c), but results shown in Fig. 9c are confirmed. The difference profiles (Fig. 12d) also confirms the previous results on Ligurian Sea (Fig. 9d). Analyses on σ^*_{SYN} profiles indicate that the fit seems to be acceptable, but not excellent (Fig. 12e). More in detail, slightly lower σ values occur in the region between about 200 and 400 m depth, whereas there is a small increment at deeper depth (Fig. 12f).

7 Discussion and conclusion

Very recently, the need of contemporaneous and co-located T and S profiles has increased significantly in ocean forecasting, due to the multivariate data assimilation schemes, which are still in progress. In general, models assimilate satellite data (sea surface temperature and height), and T profiles (e.g. Pinardi et al., 2002), whereas S values are measured only by Argo, GLIDER and CTD (or XCTD). Because of the large difference between the cost of T and S profiles, T measurements are much more than S profiles. In addition, the confidence in salinity climatological dataset is lower than in the temperature dataset. In any case, S profiles are usually "extracted" from climatological datasets, even if the applied technique is quite different (i.e. De Mey and Benkiran, 2002; Fox et al., 2002; Thacker, 2006).

MEDATLAS/MED6 climatological monthly dataset is a reference dataset for Mediterranean Sea, but it does not reproduce local and peculiar situations, and the derived σ profiles (even if an oscillation band, due to the addition of daily variation and instrumental uncertainty, is added), indicate a significant difference from recent measurements. When a day-by-day linear evolution during a month is applied to the seawater σ values, the improvements are negligible.

In general, synthetic values computed by applying the technique proposed in this paper have a good agreement with measured S and σ values: the fit coefficients and the correlation confirm it. The proposed correction factor seems to be able to describe the main part of the difference that recent measurements in Tyrrhenian and Ligurian Seas show with respect to the climatological values. The addition of other recent T and S profiles, assuring a more homogeneous temporal and geographic coverage, improves the stability and the robustness of the correction factor. In this case, σ^*_{SYN} and S^*_{SYN} profiles should have a further reduced discrepancy with respect to the experimental data. Analyses on Tyrrhenian and Ligurian Seas seem to indicate that measurements seasonally repeated can check the variability of water characteristics, and allow the computation of a sufficiently robust correction factor.

A significant check of the validity and robustness of S values obtained by applying this method could be done by comparing dynamical height values with sea level anomalies and heights as deduced from satellite measurements. In this case, the transect Genova-Palermo is nearly coincident with the pass number 44 of the JASON-1 satellite. Aiming to this further but significant control, all the cruises along that transect were made within 24 h from the passage of satellite, in order to minimize the possible difference of sea conditions.

The major problem discussed in this paper is the implementation of a methodology capable to estimate S from climatological data. The proposed method is based on the θ-S relationship and the stability of water properties: it allows the estimate of S and σ from T profiles with the addition of few phenomenological constraints. The obtained results are in general good agreement with measurements.

The most significant deviations can occur in regions of particular vertical movements: in such cases, the θ-S characteristics do not respect the basic hypothesis of relatively small mixing. It must be underlined that even other methods based on EOF technique require a basic long-term stability, but the reconstruction of salinity remains a not completely solved problem, that must be addressed to provide "good" data for multiparametric data assimilation.

It has to be pointed out that one of the properties of this technique is the rapidity in calculation. If datasets for climatology and for the computation of the correction factor are available, some minutes are required to calculate S^*_{SYN} and σ^*_{SYN} profiles from a set of XBT profiles. Therefore, in this case it should be possible to release at the same time quality checked XBT T profiles with estimated S and σ associated profiles.

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Title Page

Abstract | Introduction

Conclusions | References

Tables | Figures

|◀ | ▶|

◀ | ▶

Back | Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

EGU

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Estimate of salinity from temperature profiles

F. Reseghetti

Title Page

Abstract | Introduction

Conclusions | References

Tables | Figures

|◄ | ►|

◄ | ►

Back | Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

EGU

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Estimate of salinity from temperature profiles

F. Reseghetti

Title Page

Abstract | Introduction

Conclusions | References

Tables | Figures

◄ | ►►

◄ | ►

Back | Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

EGU

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Estimate of salinity from temperature profiles

F. Reseghetti

Title Page

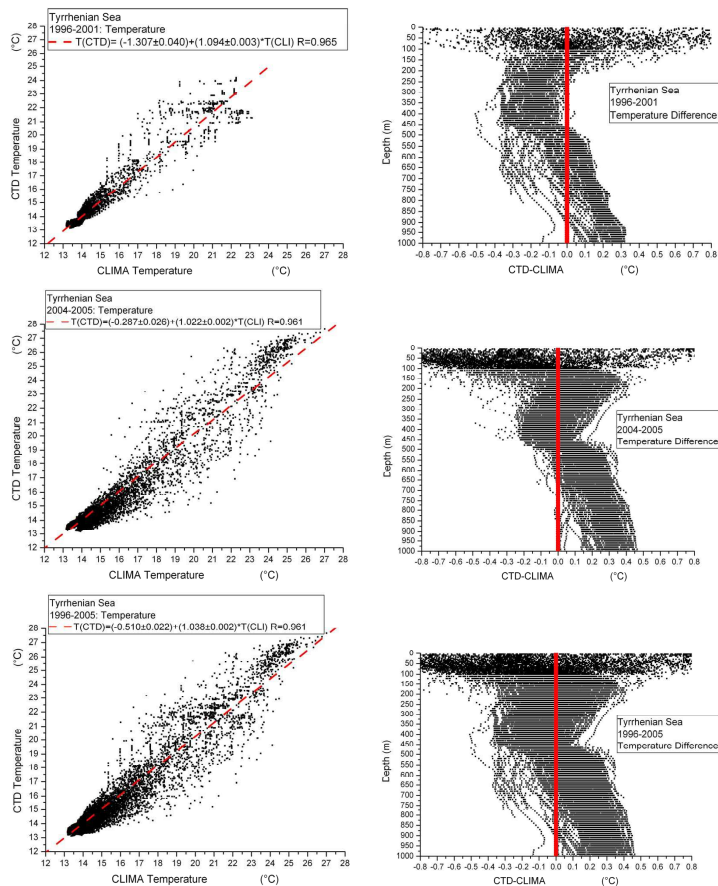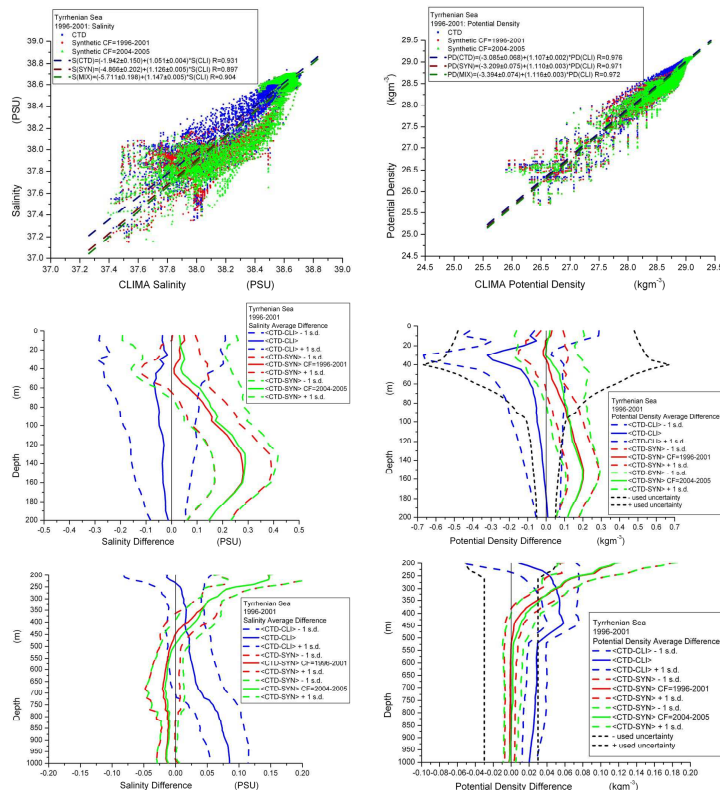| Abstract | Introduction |
| Conclusions | References |
| Tables | Figures |

|◀ | ▶|

◀ | ▶

Back | Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

EGU

Estimate of salinity from temperature profiles

F. Reseghetti

Title Page

Abstract | Introduction

Conclusions | References

Tables | Figures

◄◄ | ►►

◄ | ►

Back | Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

EGU

Table 1. Temporal distribution of profiles from Tyrrhenian Sea.

Year	Jan	Feb	March	April	May	June	July	Aug	Sep	Oct	Nov	Dec	Total
1996	–	–	–	4	4	24	–	–	17	–	–	–	49
1997	16	–	–	–	–	–	–	–	–	19	5	–	40
1998	–	–	–	–	15	–	–	–	–	–	–	–	15
1999	–	–	–	–	–	–	–	–	–	–	–	8	8
2001	2	–	–	–	–	–	–	–	–	5	–	–	7
2004	24	–	–	–	34	–	–	90	14	16	12	7	197
2005	6	3	9	13	45	9	6	8	9	7	5	5	125
Total	48	3	9	17	98	33	6	98	40	47	22	20	441

Table 2. Temporal distribution of profiles from Ligurian Sea.

Year	Jan	Feb	March	April	May	June	July	Aug	Sep	Oct	Nov	Dec	Total
1996	–	8	–	7	–	1	–	–	3	–	–	–	19
2000	–	–	–	–	–	–	–	–	32	–	–	–	32
2001	3	–	–	–	–	–	–	–	–	4	–	–	7
2002	–	–	–	–	–	26	20	–	–	8	–	–	54
2003	–	–	–	9	6	–	–	–	43	–	–	–	58
2004	–	–	–	–	3	–	–	–	7	–	–	–	10
2005	–	–	3	69	5	2	–	1	–	–	–	–	80
Total	3	8	3	85	14	29	20	1	85	12	–	–	260

EGU

Table 3. Influence of uncertainties of temperature and salinity on potential density (σ) (the values are in kgm^{-3}).

	$\delta T = \pm0.01°$C	$\delta T = \pm0.10°$C	$\delta S = \pm0.01$ PSU	$\delta S = \pm0.01$ PSU $\delta T = \pm0.01°$C	$\delta S = \pm0.01$ PSU $\delta T = \pm0.10°$C
0–100 m	$\delta\sigma = \pm0.0026$	$\delta\sigma = \pm0.0265$	$\delta\sigma = \pm0.0078$	$\delta\sigma = \pm0.0065$	$\delta\sigma = \pm0.0337$
>100 m	$\delta\sigma = \pm0.0021$	$\delta\sigma = \pm0.0208$	$\delta\sigma = \pm0.0078$	$\delta\sigma = \pm0.0065$	$\delta\sigma = \pm0.0290$

EGU

Fig. 1. Climatological vs. measured temperatures from Tyrrhenian Sea for different datasets, on left column, and the differences of temperature between CTD measurements and climatology, right column. In order to enhance the differences, only values down to 1000 m depth have been plotted, the same as in the following figures.

28
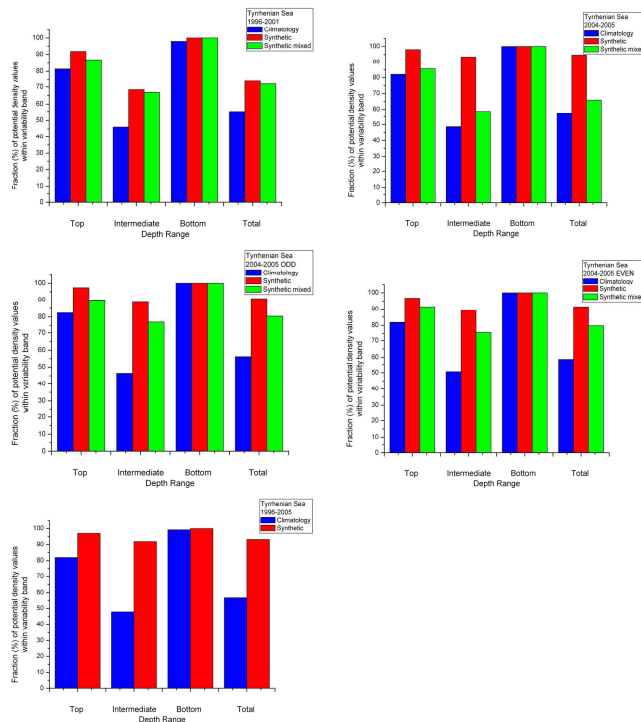
Fig. 2. The robustness of potential density stability hypothesis for the Tyrrhenian Sea, at depths ranging from 5 m down to 2350 m, is verified through the evaluation of the number of climatological and synthetic values having a difference, with respect to the measured ones, smaller than the uncertainty used in the analysis. The percent ratio between the number of climatological (or synthetic) values satisfying the request and the measured values is plotted. If such a case occurs, the values are undistinguishable: consequently, the physical properties of water should be not significantly changed (constancy in time). Synthetic Mixed values are computed by using CF from a different dataset. The depth interval has been shared as follows: Top (0–100 m), Intermediate (100–1000 m), and Bottom (1000–2350 m).

Fig. 3. Comparison among climatology, measured and synthetic values of salinity (left column) and potential density (right column) for Tyrrhenian 1996–2001 dataset. The average differences are also plotted. Synthetic values have been computed both by using the specific CF (red), and from other dataset (green). Synthetic values offer a better description of measurements, mainly at depth deeper than 400 m: fit coefficients give a confirmation of such an improvement. For potential density, the uncertainty values used in calculations are shown.

Estimate of salinity from temperature profiles

F. Reseghetti
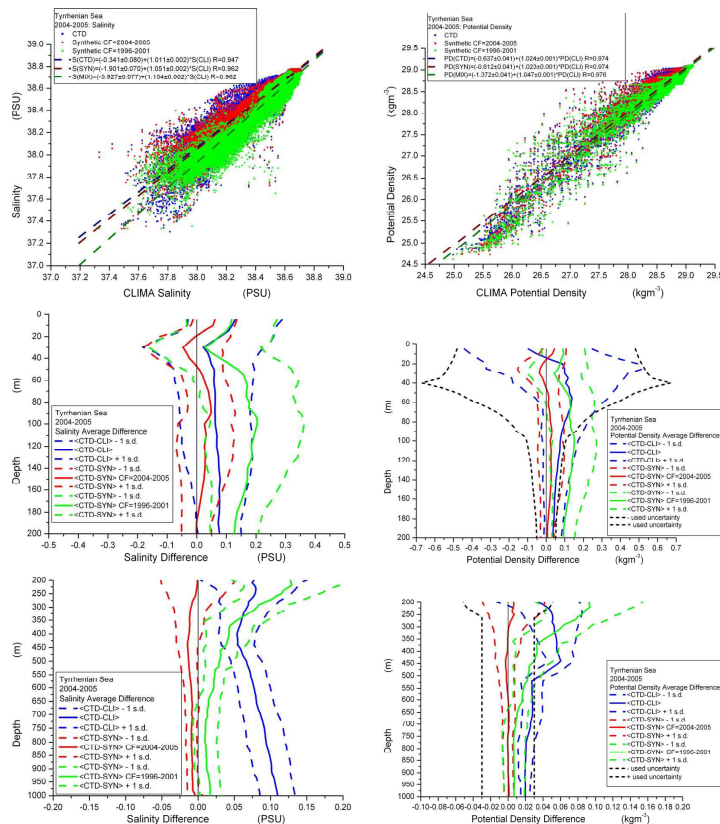
Fig. 4. The same as in Fig. 3, but for Tyrrhenian 2004–2005 dataset, which will be the basis of correction factor for the analyses on XBT data. The good agreement between CTD measurements and synthetic S and σ values is evident.

Estimate of salinity from temperature profiles

F. Reseghetti

EGU
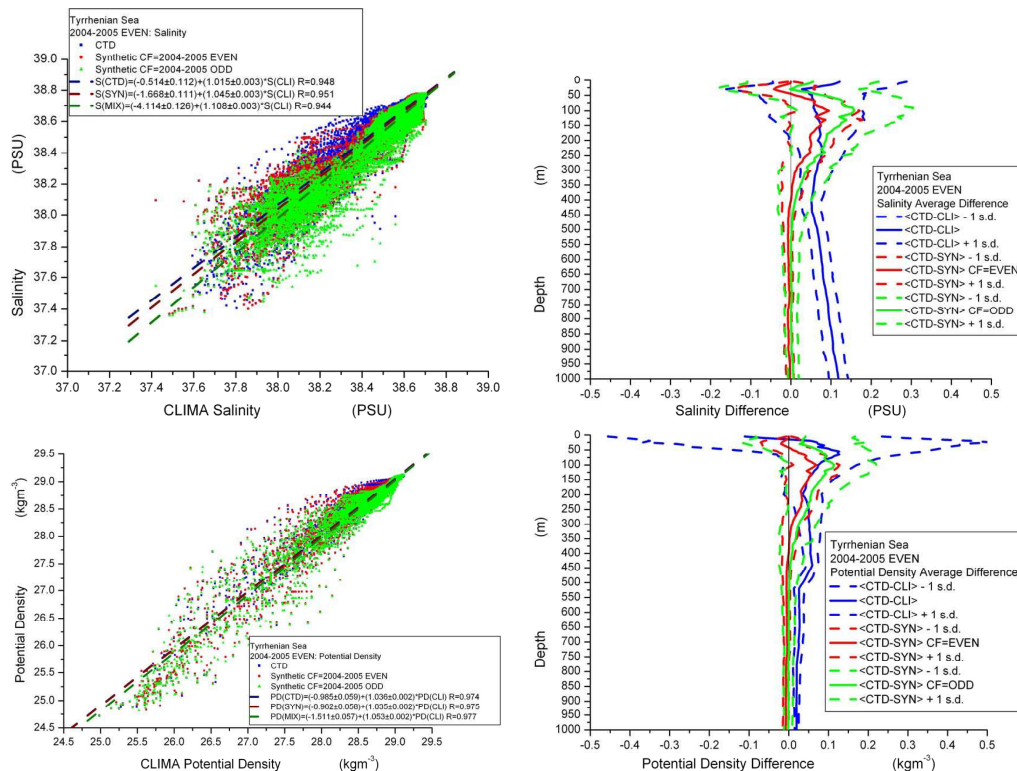
Fig. 5. Salinity and potential density results for Tyrrhenian 2004–2005 EVEN dataset. Here and in Fig. 6, results of analyses with correction factors from independent, but contemporaneous and co-located measurements are detailed. The obtained results well improve the climatological dataset, even if an unexpected significant difference occurs at depth lower than 300 m for salinity and potential density.
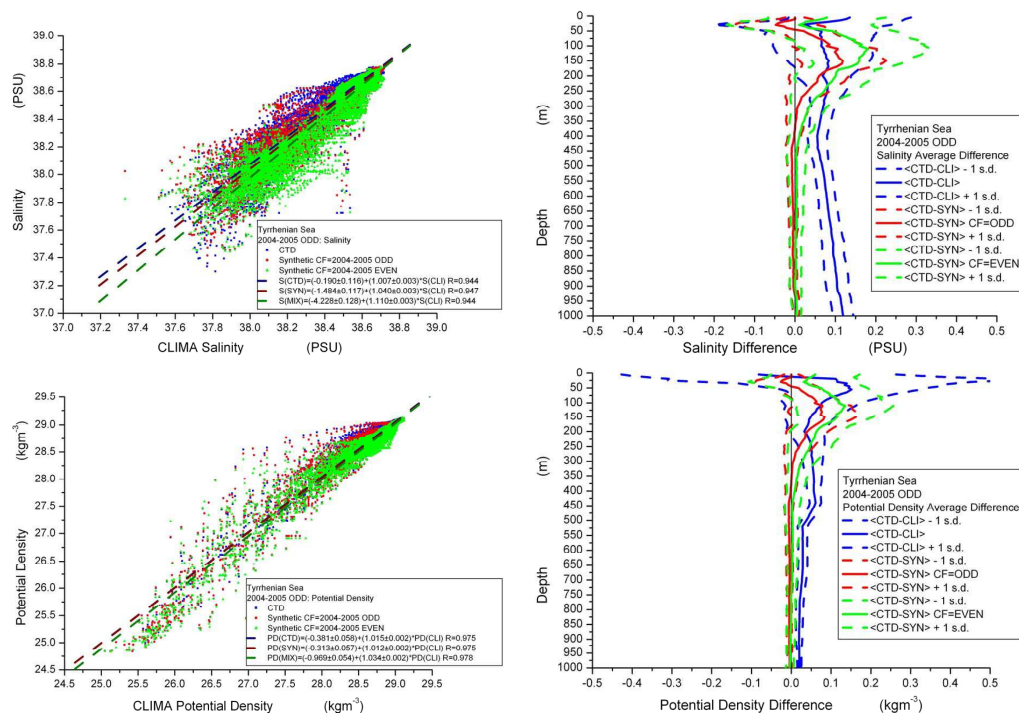
Fig. 6. The same as in Fig. 5, but for Tyrrhenian 2004–2005 ODD dataset. The results are nearly coincident.

EGU

Estimate of salinity from temperature profiles

F. Reseghetti
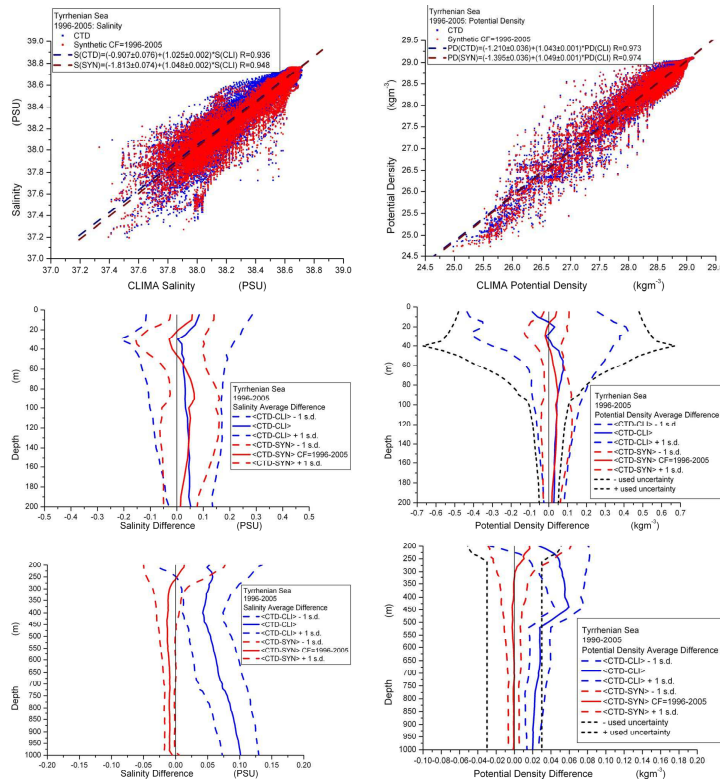
Fig. 7. The same as in Fig. 3, but for Tyrrhenian 1996–2005 dataset, the full available sample. Because of a larger (both geographically and temporarily speaking) dataset, the correction factor includes a more complete set of physical states, allowing the synthetic values to give a more precise reproduction of real seawater characteristics.

EGU
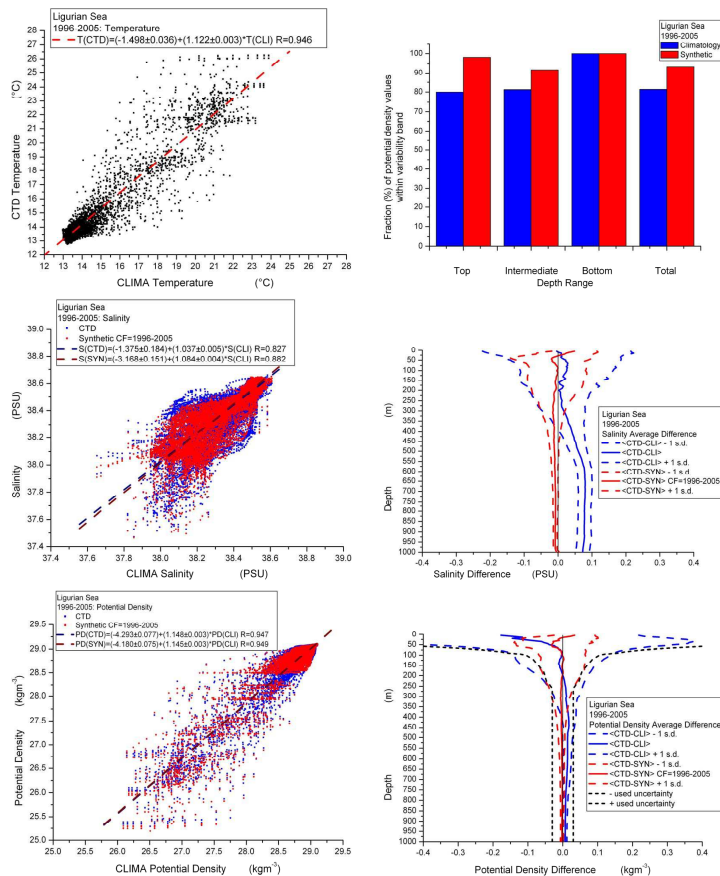
Fig. 8. The plots describing the main results on Ligurian 1996–2005 dataset are shown. CTD temperature values have a well identifiable difference from climatological dataset. Both salinity and potential density synthetic values well reproduce CTD measurements, and put in evidence a different behaviour with respect to the climatology.

35

EGU
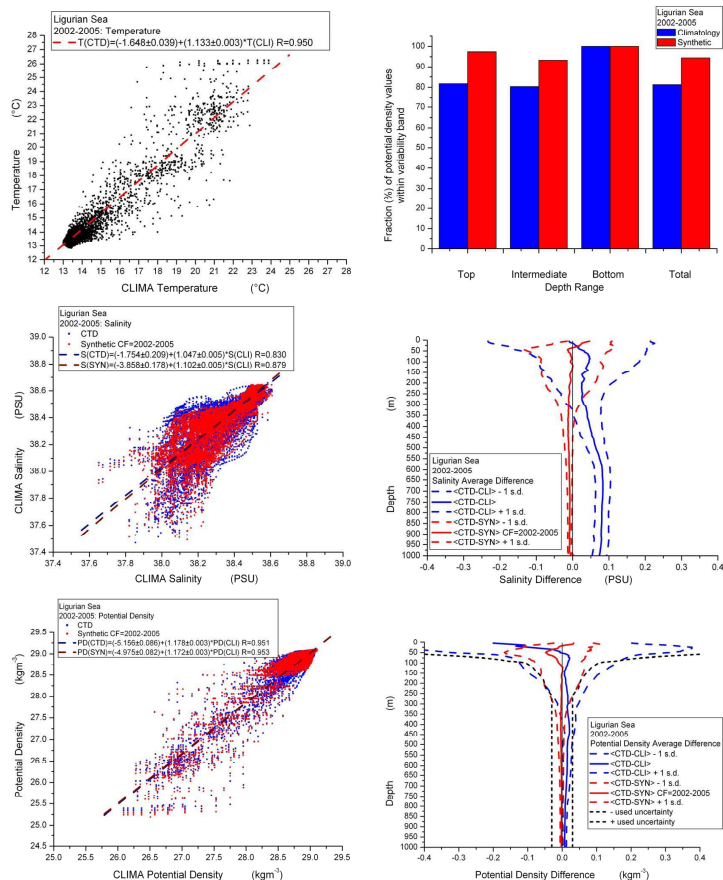
Fig. 9. The same as in Fig. 8, but for Ligurian 2002–2005 dataset, which will be used in analyses on XBT from Ligurian Sea. Similar conclusions with respect to the whole 1996–2005 are possible, mainly for the bad quality of the fit of *S* values.
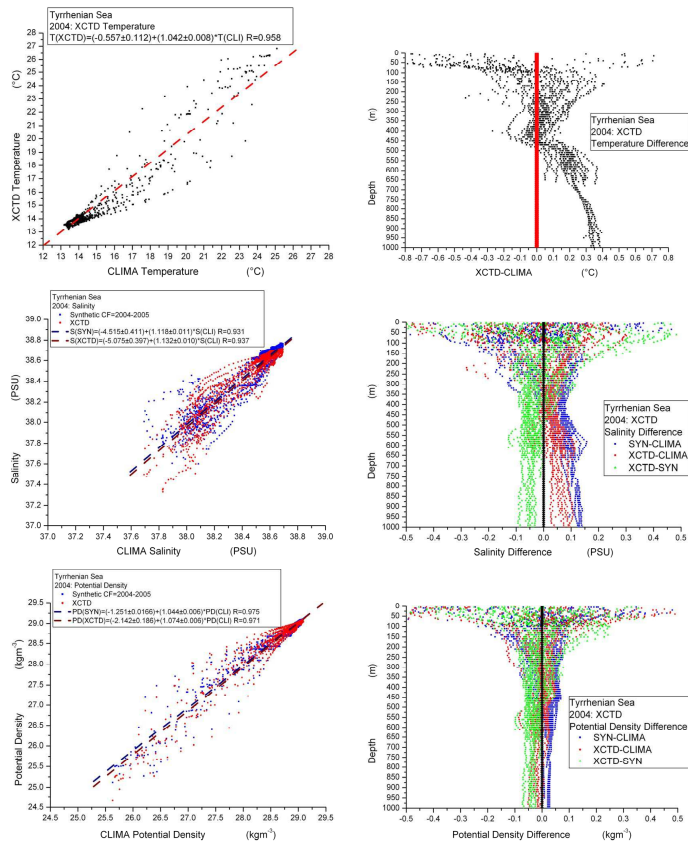
Fig. 10. Main results of analyses on 2004 XCTD dataset (21 profiles) from Tyrrhenian Sea. Almost all the probes were dropped in May and September 2004, the used correction factor is from 2004–2005 dataset. This could explain some small differences, mainly in S values, between synthetic and XCTD measurements. The systematic overestimate that S^*_{SYN} and σ^*_{SYN} values have with respect to the XCTD measurements has to be pointed out.

OSD

4, 1–39, 2007

Estimate of salinity from temperature profiles

F. Reseghetti

Title Page

Abstract   Introduction

Conclusions   References

Tables   Figures

|◄   ►|

◄   ►

Back   Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

EGU

EGU
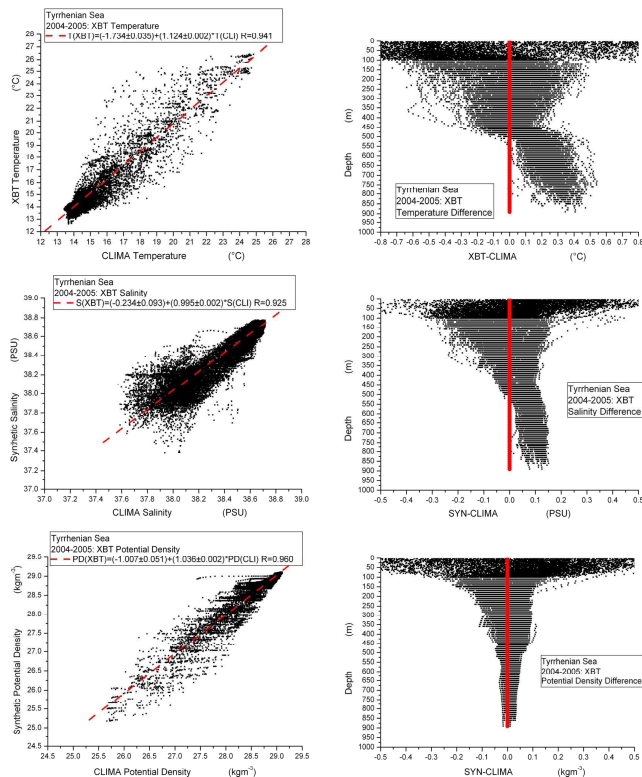
Fig. 11. Main results of analyses on Tyrrhenian 2004–2005 XBT dataset. A comparison can be done with Figs. 1c and d for temperature and Fig. 4 for salinity and potential density plots. The temperature difference has similar behaviour, but the fit puts in evidence a stronger increment in XBT temperature values than in CTD measured, even with different sampling strategy (the same repeated transect for XBT dataset and "random strategy" for CTD dataset). Salinity values indicate a complicate variability down to about 400 m depth, and a well evident increment at deeper depth is strongly confirmed. On the other hand, σ values show a better global agreement.
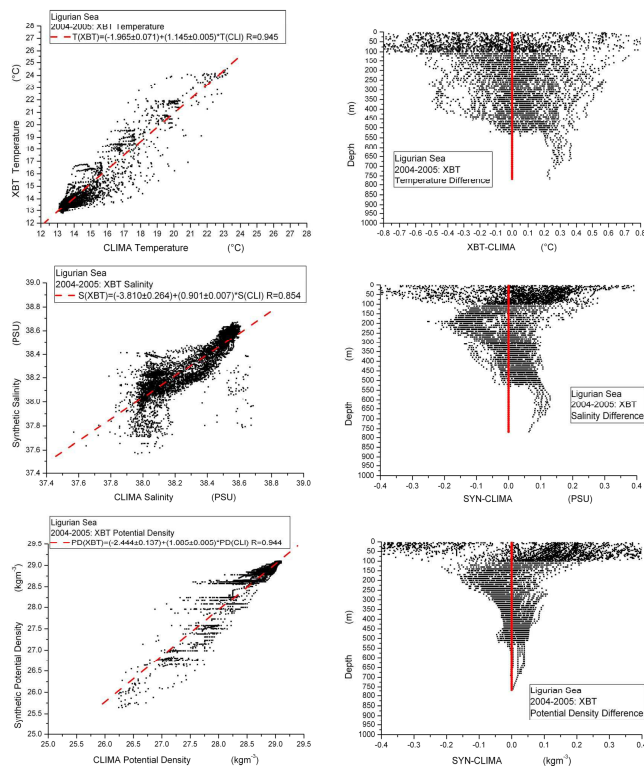
Fig. 12. The same as in Fig. 11, but for Ligurian 2004–2005 XBT dataset. In this case, results have to be compared with Fig. 9. It has to be remarked the difference in available depth between the dataset and the different sampling strategy (the same repeated transect for XBT dataset and "random strategy" for CTD dataset). A substantial agreement in temperature fit appears, whereas S values show a different behaviour both in the fit and in the difference plot down to 350 m depth. On the other hand, σ values have a smaller discrepancy.