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Salinity Assimilation using $S(T)$ relationships: Part 1 Theory.

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Abstract

Assimilation of salinity into ocean and climate general circulation models is a very important problem. ARGO data now provide far more salinity observations than ever before. In addition a good analysis of salinity over time in ocean reanalyses can give important results for understanding climate change. Here we show from the historical ocean database that over large regions of the globe (mainly mid and lower latitudes) variance of salinity on an isotherm $S(T)$ is often less than variance measured at a particular depth $S(z)$. We also show that the dominant temporal variability of $S(T)$ is slower than $S(z)$ based on power spectra from the Bermuda timeseries, and from ocean models we show that the horizontal spatial covariance of $S(T)$ often has larger scales than $S(z)$.

These observations suggest an assimilation method based on analysing $S(T)$. We present an algorithm for applying $S(T)$ assimilation and show how it can be made orthogonal to the multivariate assimilation of temperature data which produces its own salinity correction. We argue that the larger space and timescales should allow larger gain matrices to be used for the $S(T)$ assimilation leading to better use of scarce salinity observations.

Finally we show results of applying the salinity assimilation algorithm to a single analysis time within the ECMWF seasonal forecasting ocean model. The separate salinity increments coming from temperature and salinity data are identified and the independence of these increments is demonstrated. Results of an ocean reanalysis with this method will appear in a companion paper.

1 Introduction

As more salinity observations become available from ARGO floats, Roemmich et al (2001), it is becoming more important to develop methods to assimilate salinity profile data into ocean circulation models. Getting the salinity field right is important in a number of contexts. Salinity has an impact on the density field and hence on ocean currents and transports, *e.g.* Cooper (1988), Roemmich et al (1994), Vialard and Delecluse (1998a,b). Salinity is also important in certain places in the mixed layer where it controls the stability of the water column and hence to a degree, mixing and air-sea interaction, eg. in the barrier layer around the western Equatorial Pacific. In addition the relationship between temperature and salinity contains important information about the nature of the thermocline and subduction rates and areas, Iselin (1939). Temperature-salinity scatter-plots are a standard tool in the armoury of physical oceanographers. They are used to track water masses in the deep ocean, and to infer information about mixing rates using end member analyses, Tomczack (1981), and other inverse methods. Temperature and salinity data have also been compared in repeat section work in an attempt to identify climatic changes over decadal timescales, eg. Bindoff and McDougall (1994), Wong et al (1999), Bryden et al (2003). Indeed Dixon et al (2003) and Curry et al (2003) discuss high latitude and global salinity changes as providing the dominant signal of climate change in the oceans over the past few decades. It is important therefore to recognize that the correct treatment of salinity data in the context of ocean data assimilation will allow analysed ocean fields to be used for more detailed studies of all of the above phenomena.

Several methods have been proposed to update salinity in a multivariate fashion during the assimilation of other data, Troccoli and Haines (1999), Vossepoel and Behringer (2000), Maes and Behringer (2000), but there has been very little work so far attempting to assimilate salinity observations themselves. This paper takes as its starting point the conceptual methods advocated in Haines (1994), Cooper and Haines (1996), Troccoli and Haines (1999) and Haines (2004). The aim is to use the salinity data in the most effective way by seeking to identify independent information from that available from other more abundant assimilated data sets. For example, Cooper and Haines (1996) argued that during altimeter data assimilation, water columns should be changed in such a way as not to alter the volume, or the T/S characteristics, of water masses in the model water column. The justification is (1) that these quantities are not directly observed by the altimeter, (2) that much of the sea level variability is due to dynamical advection associated with wave motions, while budgets of water mass volumes and properties are controlled largely by separate thermodynamic processes. Similarly Troccoli and Haines (1999) argued that when temperature profile data are assimilated into models, the volume of water in each temperature range is observed but the T/S relation is not. Therefore it is useful to introduce multivariate salinity changes with the aim of keeping the $S(T)$ relations in model water columns unchanged. This is a better solution than leaving $S(z)$ unchanged when the salinity is not observed. Troccoli et al (2002) and Ricci et al (2004) have shown that this constraint provides many benefits in assimilation of temperature profiles, in particular leading to improvements of both the salinity and temperature fields. Fox and Haines (2003) describe the application of both these methods in a high-resolution global ocean model and discussed the contributions of each data set to the success of the final assimilation. However the above studies, and others, have also shown that even with appropriate constraints, the salinity fields of ocean models tend to drift away from realistic values due to poor knowledge of the surface freshwater fluxes as well as poor representation of other internal processes such as mixing and thermohaline circulation strength. Hence the urgent need for an appropriate salinity assimilation scheme.

This paper aims to demonstrate the value of analysing salinity on surfaces of constant temperature $S(T)$, in comparison to analysing on level surfaces, or $S(z)$. It is argued that this allows the salinity data to provide independent information to the analysis from that inferred from either altimeter or temperature profile data. In section 2 data from the WOD01, from the ARGO array, and from two different ocean models, are used to study the variance and spatial covariance of $S(T)$ compared with $S(z)$. In section 3 we develop a data assimilation scheme for $S(T)$ data. In section 4 we show preliminary results of salinity analyses that result from $S(T)$ assimilation as applied in the ECMWF ocean model. Section 5 provides conclusions and discussion. A companion paper takes the study further and describes the results from running this $S(T)$ assimilation scheme in the ECMWF seasonal forecasting model.

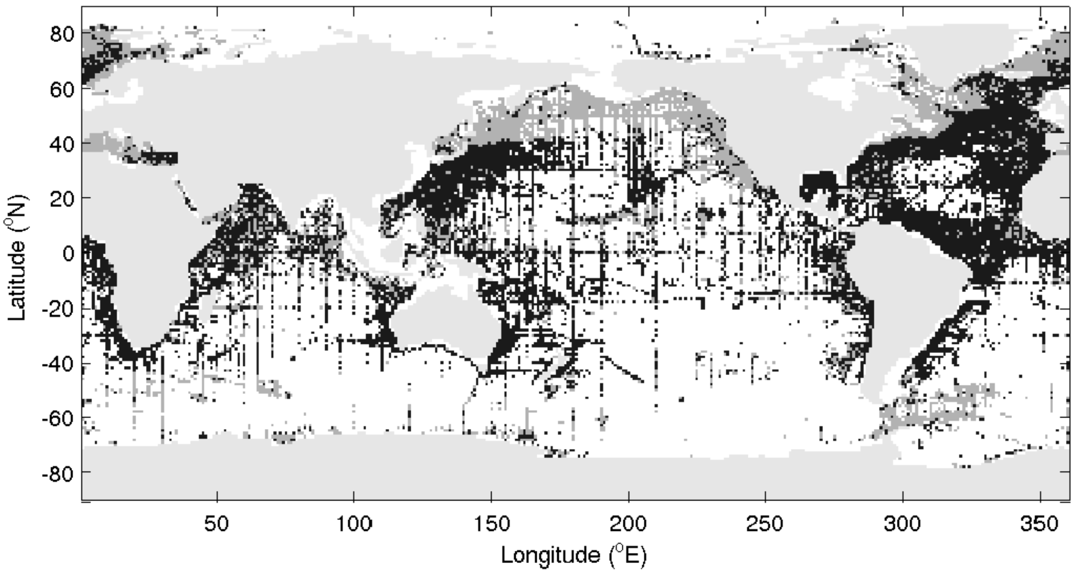
2 Variance and Co-Variance of Salinity from observations and models

2.1 Observed salinity variability

The World Ocean Database 2001 (WOD01) data set has been recently analysed and quality controlled by the Met Office as part of the EU Enact project (Ingleby and Huddleston, 2004). These data cover a period of over 40 years from 1958-2001 and were supplemented by more recent data *e.g.* from the World Ocean Circulation Experiment, WOCE. In order to demonstrate the different results obtained by analysing the salinity variability on depth levels and on temperature surfaces we calculated the salinity variance. The Enact data where first classified into 1x1 bins, where bins with less than 5 samples, or where the variance was in the lowest 5% of values, were omitted. Typically the remaining populated bins contained 10-100 salinity profiles in the upper part of the water column. The $S(z)$ variance was calculated at two different depth levels, 300 and 700m. Then the mean temperature was identified at each of these two depth levels (this mean temperature varies strongly according to location), and the $S(T)$ variance was calculated for these 2 isotherms at each location. This idea was used by Troccoli and Haines (1999) figures 2,3 to demonstrate the reduced variations of $S(T)$ at a couple of isolated locations in the tropical Pacific.

Figures 1a,b show the ratio of the z level salinity variance over the appropriate isotherm variance for the 300 and 700m depth levels respectively, var($S(z)$)/var($S(T)$). For display purposes the black bins have this ratio > 1, i.e. the z level variance is larger, and the shaded bins have a ratio < 1, i.e. the isotherm salinity variance is larger.

The salinity variance on both mean isotherms is reduced compared to that measured on depth levels (ratio > 1) for most of the data bins south of the subpolar gyres in both the N Atlantic and N Pacific oceans. In addition



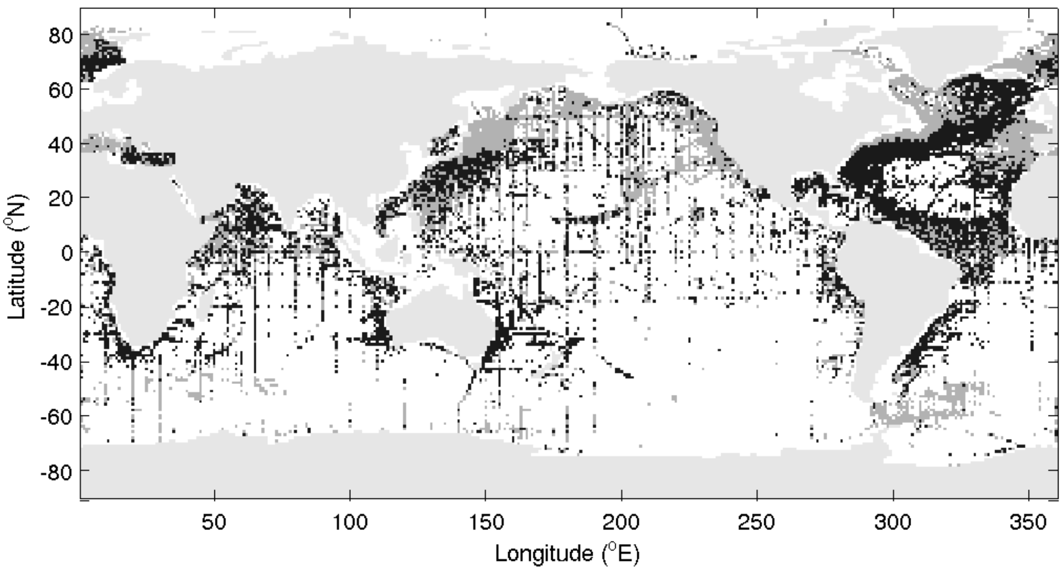


Figure 1: Ratio of $S(z)$ variance over $S(T)$ variance in 1x1 degree bins for the 40 years of Enact data. The top plot (a) is for 300m depth and the mean isotherm at that depth, and (b) is for 700m depth and its mean isotherm. Points where the ration is > 1 are black and points where the ratio is < 1 are dark grey.

at 300m the variance reduction for $S(T)$ is valid right up into the NE Atlantic, in the Indian ocean and down as far south as the Antartic Circumpolar Current fronts. Exceptions are in the western Mediterranean and along the west coast of the US. At 700m the results are less clear cut but still with a predominance of lower $S(T)$ in the subtropical N Pacific and the Indian oceans. However, in the eastern Atlantic near the Mediterranean outflow, the $S(z)$ variance is clearly lower at 700m. By inspecting particular bins, *e.g.* in the Indian ocean, it was determined that there were still some residual bad salinity profiles in this Enact data set, and we would expect that removing these may reduce the $S(T)$ variance still further and extend the black areas in Fig 1.

Overall there is a clear indication of the tendency for S and T to vary together and hence for a reduced $S(T)$ variability in most areas where the water column has a good thermal stratification. This result can be explained by the behaviour of the different kinds of wave motions in the thermocline including internal waves and Rossby waves, as well as mesoscale eddy activity, and seasonal variability due to Ekman pumping. All of these phenomena will contribute to increased salinity variance on a depth surface but have very little impact on salinity variance on a T surface.

It is also relevant to look at the temporal variability of $S(z)$ relative to $S(T)$. There are very few actual timeseries of salinity data available but one place that a reasonably populated series is available is at Bermuda, Joyce and Robbins (1996).

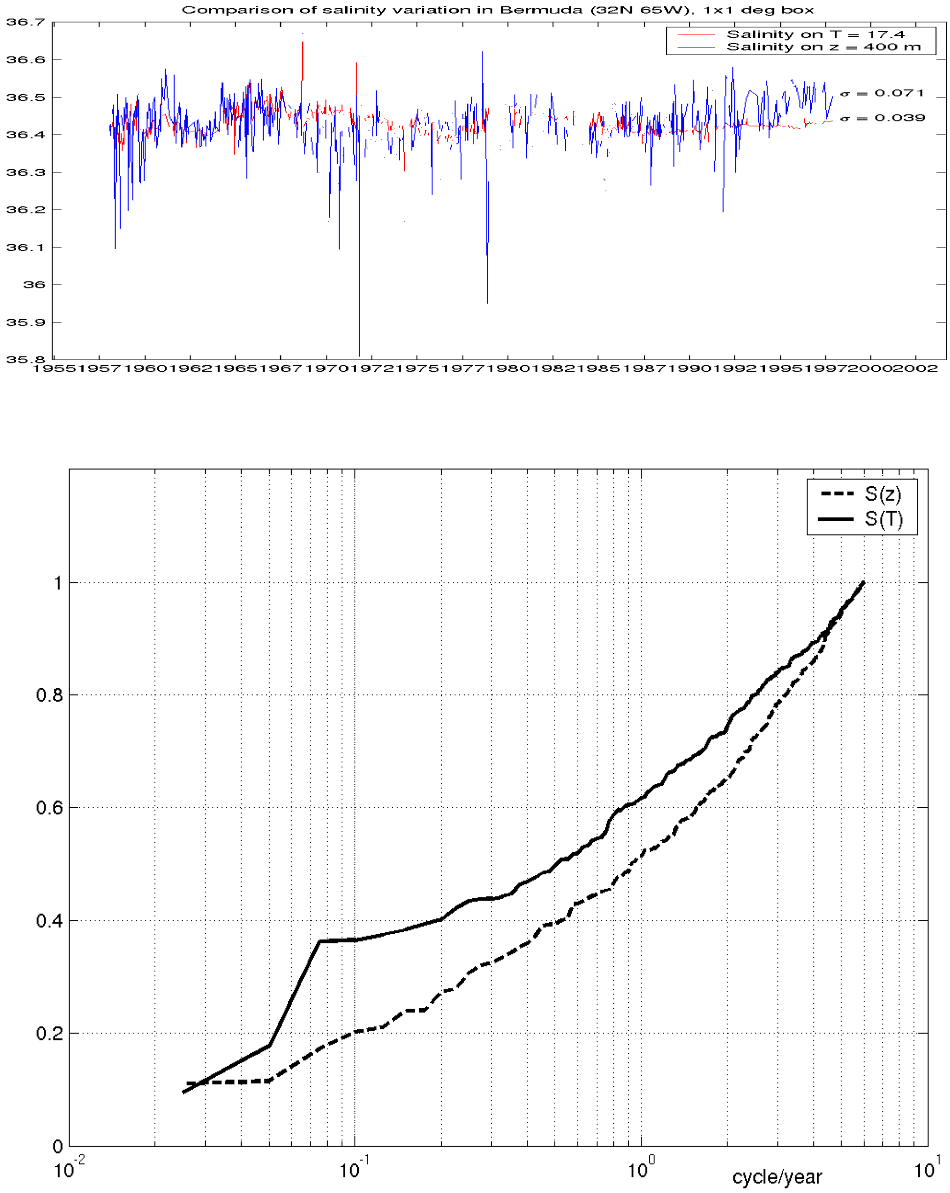


Figure 2: (a) Salinity timeseries at Bermuda. The blue line shows salinity at 400m depth and the red line shows the salinity on the 17.4 C isotherm which is the mean temperature at 400m. (b) Cumulative normalised power spectra for the two time series, showing that a considerably larger fraction of the power in $S(T)$ lies at lower frequencies (the timeseries are linearly interpolated to fill gaps for (b)).

Figure 2a shows the timeseries of salinity at 400m depth at Bermuda, along with the timeseries of the salinity on the 17.4C isotherm, which is the mean temperature at 400m. It is clear from the two timeseries that the variability of $S(z)$ is greater than the variability of $S(T)$, as expected from Fig 1. However we also see that the dominant temporal variability in $S(T)$ occurs on a longer timescale than the dominant variability in $S(z)$. Some of this $S(T)$ variability takes place on very long timescales *e.g.* with salinity on the $S(17.4C)$ during 1968-73 being a little higher for example than in 1995-2000. This dominance of longer timescales in the variability of $S(T)$ is emphasised in Fig 2b which shows the cumulative normalised power spectra of the two timeseries. Clearly a considerably larger portion of the total power occurs at periods longer that 2 years for the $S(T)$ timeseries.

The processes that will change $S(T)$ are processes of horizontal advection along isopycnals bringing in water of a different water type to a region. This ultimately occurs due to changing ventilation patterns at the sea surface where water masses are formed and subducted, or due to large scale changes in mean circulation. Ventilation changes may be larger or smaller in different regions, on different isotherms, and over different time periods. It has been suggested that the $S(T)$ relationships in the North Atlantic have not changed much on inter-decadal timescales, Levitus (1989), but in the Indian and S. Pacific oceans there is evidence of significant inter-decadal change, eg. Bindoff and McDougall (1994), Bryden et al (2003). Ideally one would like to analyse any changes that do occur in $S(T)$ by deriving the spatial covariance structure and, given the different and considerably fewer processes involved in producing $S(T)$ variability, we would expect different scales of spatial variability than found for $S(z)$. However the sparseness of available observational data makes it very difficult to calculate such spatial scales in $S(T)$ variability. Therefore we turn to model data to study spatial covariance.

2.2 Modelled salinity variance and covariance

As suggested above, much of the variability of salinity on temperature surfaces within the thermocline occurs on long timescales and comes about because of variability in surface flux conditions where the isotherms (and isopycnals) outcrop. Through slow processes of ventilation the changes in $S(T)$ then penetrate into the subsurface ocean through advection. We therefore expect that models exhibiting such variability would have to be run for long periods. The Hadley Centre coupled climate model HadCM3 has been run for more than 1000 years without flux correction, Gordon et al (2000). The model climate is reasonably realistic and the drifts are very small after the preliminary adjustment, especially within the thermocline, making this model suitable for studying natural variability of water properties on long timescales. The ocean component is 1.25x1.25 with 20 vertical levels and it is therefore not eddy permitting. Monthly mean temperature and salinity data from this model were available for a 100 year period from the NERC COAPEC program. A second Hadley Centre coupled model, HadCEM Roberts et al (2004), is an ocean eddy-permitting version of HadCM3 with an ocean resolution of 1/3x1/3 and 40 vertical levels, but with the same atmospheric model as HadCM3. HadCEM has been run for 150 years as a free coupled model and the last ten years of these data were also available to us as monthly mean fields.

Figure 3 shows a set of four one-point correlation maps for salinity variability $S(z)$ at a depth of 400m from two locations in the Pacific and Indian oceans, based on these HadCM3 and HadCEM data. Figure 4 shows the equivalent one-point correlations for salinity variability on an isotherm. In each case the isotherm chosen (shown in the legend) corresponds to the mean temperature at 400m for the same locations as Fig 3.

First of all it can be seen in Fig 3 that the spatial covariance scales of the HadCM3 model and the HadCEM model for $S(z)$ are quite different, with the HadCEM model showing much smaller spatial covariances. This is the result of the HadCEM model being eddy-permitting and therefore the spatial scale is dominated by the mesoscale variability at the Rossby deformation radius. There is therefore every reason to believe that the $S(z)$ covariances in the real world wherever mesoscale variability is strong, would be dominated by these same short

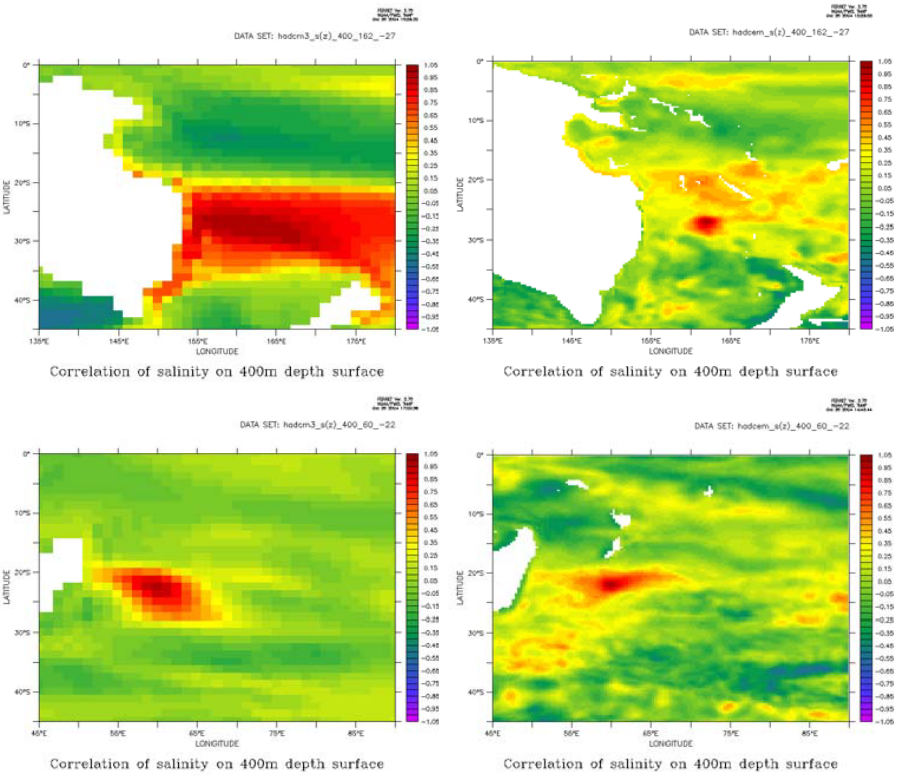


Figure 3: One-point correlation maps for $S(z)$ at 400m. The left panels show results from 100 years of the low resolution climate model HadCM3, and the right panels show results from 10 years of the higher resolution HadCEM model at the same locations. The upper panels are located at 162E, 27S in the south Pacific off Australia, and the lower panels are located at 60E, 22S in the Indian Ocean east of Madagascar.

spatial scales.

However, when we look at the correlations for $S(T)$ variability in Fig 4, the spatial scales from HadCEM and HadCM3 are much more similar to each other, and these scales are much larger than for the $S(z)$ correlations, especially those in the HadCEM model. Even when the $S(z)$ and $S(T)$ correlation scales are compared within the HadCM3 model, the spatial scales for the $S(T)$ covariances are a little larger than for $S(z)$. There are some spuriously large remote covariances detected in these plots, particularly for the HadCEM data set. This is due to only using 10 years of monthly data which is really a fairly short period of time to quantify $S(T)$ variability accurately, for some of the reasons discussed previously. However the data are sufficient to demonstrate that there are scale differences between the $S(z)$ and $S(T)$ variations. The 400m depth level of this comparison is within the main thermocline at both the locations, and temperature will dominate the stratification.

It is the covariance scales detected in Figs. 3 and 4 that would normally be used for the assimilation of observations. Typically if the spatial covariance scales for $S(T)$ are 3 times larger than for $S(z)$, then each observation of $S(T)$ can be used to influence an area of ocean which is 9 times the area that an observation of S(z) at the same location would influence. Effectively this is achieved because the error covariance for $S(T)$ will be naturally flow dependent, since the T field is flow dependent, whereas the $S(z)$ covariances are not naturally flow dependent. Therefore as far as assimilation is concerned the results of this section demonstrate two important facts:

(1) At mid and lower latitudes a significant fraction of the salinity variability on a depth level can be modelled by re-referencing the salinity properties to an isotherm. This is achieved by the Troccoli and Haines (1999)

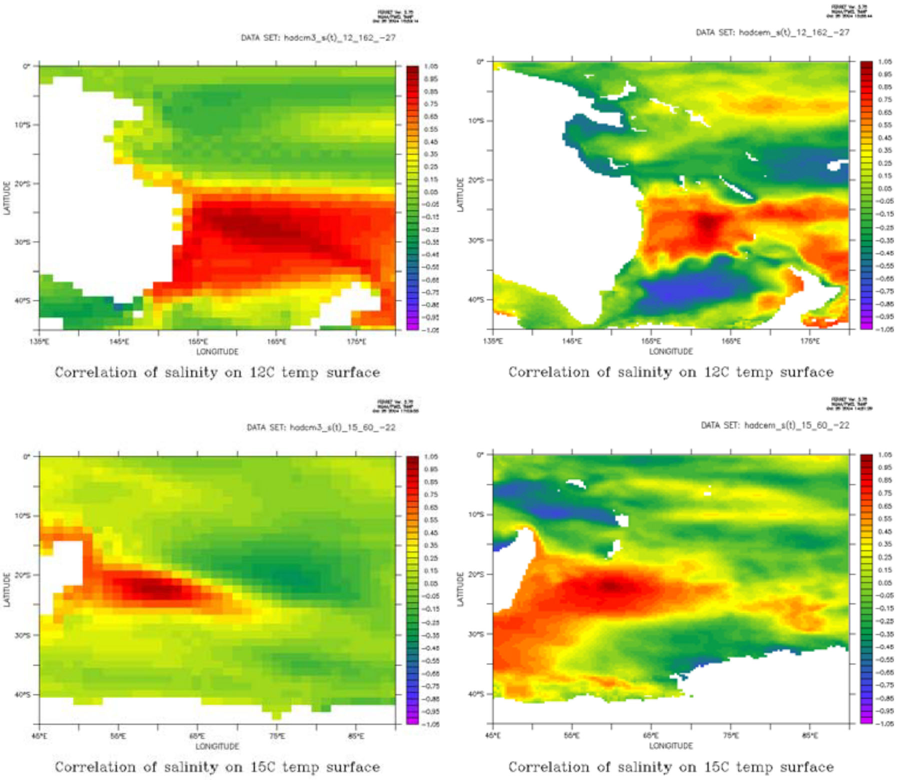


Figure 4: One-point correlation maps at the same locations as in Fig 3 but now for $S(T)$ variations. The left panels are for the HadCM3 low resolution model and the right panels are for the HadCEM high resolution model. The 12C temperature surface is used in the upper panels being the mean temperature at 400m in the Pacific. The 15C isotherm is used in the lower panels being the mean temperature at 400m in the Indian Ocean.

assimilation method in which salinity is modified to remain unchanged on an isotherm during temperature profile assimilation.

(2) When attempting to assimilate salinity observations, the key additional information is the $S(T)$. This $S(T)$ information exhibits larger spatial covariance scales than $S(z)$ (or $T(z)$) which are both dominated by the mesoscale. Thus $S(T)$ data can be given a wider influence radius during the salinity data assimilation step. In the following section we show how an assimilation method for $S(T)$ can be constructed.

3 Salinity Assimilation Methods

All the assimilation methods described here are presented in the context of simple OI methods. Nonetheless this does not detract from the physical content and indeed makes the consequences rather easier to explore. There is no reason why these ideas should not be extended to 3d and 4d Var methods of assimilation with the correct developments of the covariance matrices.

3.1 Salinity OI on z levels; $S(z)$

We begin by assuming a univariate assimilation scheme for observed $S_o(z)$ profiles, which will mirror the OI assimilation normally performed on T profiles. We can write the salinity assimilation analysis, S_a, as;

$$S_a = S_b + \mathbf{K}_1[S_o + HS_b]$$

where H is the projection operator to convert the predicted model background salinity S_b to the location of S_o. The gain matrix, $\mathbf{K}_1$, reflects several important effects: (1) It accounts for relative errors in the background and observations, (2) it reflects a representivity error or filter to remove elements of the data which cannot be modelled, (3) it reflects the projection from the observation location onto the model grid, which includes spreading the influence of each observation profile quasi-horizontally over a considerable area. The spatial weighting of each column in the gain will typically reflect the horizontal distance, r, between the analysis and the observation locations, for example;

$$\mathbf{K}_1 \sim \exp(-r^2/R^2)$$

where R represents a correlation scale on which the influence of the observations decay. Other structure functions, which may be anisotropic, are also possible. In another simplification (currently used in the ECMWF seasonal forecast system) this analysis is only performed level by level so that $\mathbf{K}_1$ would not reflect vertical correlations, and only salinity observations at the same level would be used in the analysis,

$$S_a(z) = S_b(z) + \mathbf{K}_1[S_o(z) - HS_b(z)] \tag{1}$$

This salinity analysis can be carried out entirely independently of the simultaneous measurement and analysis of temperature; however in doing so it misses the opportunity of taking full advantage of the relationships between them.

Troccoli et al. (2002) have already shown that temperature assimilation can considerably improve the salinity field of an ocean model by taking advantage of the large fraction of salinity variance that is strongly correlated with temperature variance, as demonstrated in Figure 1. Let us now consider that a T analysis has been carried out prior to assimilating salinity data. Assume that salinity has been updated as part of this, using the Troccoli and Haines (1999) method which keeps the $S(T)$ relationship of the background unchanged. If the temperature analysis is denoted T_a then we already have a preliminary analysis of salinity;

$$S'_a(z) = S_b(z) + \Delta S_T(z) \tag{2}$$

where ΔS_T ensures that

$$S'_a(T_a) = S_b(T_a)$$

within any model profile. This preliminary salinity analysis now becomes the background for the assimilation of the observed salinity data;

$$\begin{aligned} S_a(z) &= S'_a(z) + \mathbf{K}_2[S_o(z) - S'_a(z)] \qquad (3)\\ &= S_b(z) + \Delta S_T(z) + \mathbf{K}_2[S_o(z) - H\{S_b(z) + \Delta S_T(z)\}] \qquad (4) \end{aligned}$$

Notice the 2 separate increments to the background salinity with the second term on the right of Eq (4) coming from the T assimilation and the third term coming from the S assimilation. However the contribution of $\Delta S_T(z)$ to the final analysis will disappear if we choose to make $\mathbf{K}_2 = \mathbf{K}_1$ and the results will then become the same as in Eq (1). However there are reasons why this does not seem to be a good choice. Given the known improvement of salinity arising from the temperature assimilation step we might have expected to give a smaller error to the background in the salinity assimilation step, i.e. make $\mathbf{K}_2 < \mathbf{K}_1$. Is the solution in Eq (4) with $\mathbf{K}_2 < \mathbf{K}_1$ better than in Eq (1)? We would hope to get a better solution from allowing temperature information to influence the final salinity given that T and S do co-vary.

The problem is that by doing the analysis in z coordinates we are not taking advantage of the fact that the salinity increments in the Troccoli and Haines (1999) scheme leave the salinity unchanged on T surfaces. If we did so we could use the new salinity measurements to provide entirely orthogonal information to that provided by the temperature data. This method is outlined below and we refer to it as $S(T)$ assimilation.

3.2 Salinity OI on temperature surfaces; $S(T)$

The temperature and salinity provide two separate pieces of information about the hydrographic structure of the ocean but since temperature is always available whenever salinity is measured it is possible to consider that the two separate pieces of information are $T(z)$ and $S(T)$. Provided we do not have temperature inversions, then this information will always allow $S(z)$ to be reconstructed. Other considerations suggest that $S(T)$ and $T(z)$ are much more independent than are $S(z)$ and $T(z)$ since $T(z)$ and $S(z)$ profiles are both strongly influenced by fast dynamical processes, while $S(T)$ is only affected by slow thermodynamic processes.

The more common approach to considering the relationship between S and T is to use covariance relationships, but these are nearly always defined in conventional z coordinates and would not therefore be well conditioned to describing the separate aspects of the $S(z)$ and $S(T)$ variability described above. The separation here is a physically based choice and provides an alternative way of representing the relationship between S and T, see the discussion section for more on this. Assume that at a particular location at level z the temperature analysis has already been performed and has yielded the temperature T_a. What we would really like to be able to do when assimilating the salinity data is;

$$S_a(T_a) = S_b(T_a) + \mathbf{K}_3[S_o(T_a) - HS_b(T_a)] \tag{5}$$

Written in this way in temperature coordinates the orthogonality with the Troccoli and Haines (1999) scheme is clear because $S_b(T_a)$ and $S'_a(T_a)$ are the same so that Eq (5) is correcting an entirely different aspect of the salinity field error. This elegant property means that the appropriate gain $\mathbf{K}_3$ can be set without reference to the $\mathbf{K}_1$ used in the temperature assimilation. As was argued in section 2 this is entirely appropriate given the different decorrelation scales associated with variability in $S(T)$, and the different representivity errors associated with $S(T)$ data. This seems to be a highly desirable approach to the assimilation of salinity data. In practice we need to express the result of Eq (5) in z level coordinates. In z level coordinates Eq (5) implies a second salinity increment which is additive to the first salinity increment of Eq (2). This can be defined as;

$$\Delta S_S(z(T_a)) = \mathbf{K}_3[S_o(T_a) - HS_b(T_a)] = \mathbf{K}_3 \delta S(T_a) \tag{6}$$

that will be applied in addition to the first salinity increment $\Delta S_T(z)$ associated with temperature assimilation.

The key novel step to apply $S(T)$ assimilation is to calculate innovations;

$$\delta S(T_o) = (S_o(T_o) - HS_b(T_o)) \tag{7}$$

which compares the observed salinity, not with the model background at the same z level, but with the model background salinity associated with each observation isotherm at the location of the profile. In practice it makes sense to store a finite number of these salinity innovations $\delta S(T_o)$ for a finite number of isotherms T_o, from each observation profile, probably reflecting the finite number of model levels from which independent background data can be assumed. This set can then be used to infer salinity increments on all intermediate isotherms, see below. This is the most critical step which makes the salinity increments associated with $S(T)$ assimilation orthogonal to the Troccoli and Haines (1999) salinity increments associated with the $T(z)$ assimilation, since both will be required to give the best analysis of the final salinity.

In application it is likely that the $\delta S(T_o)$ innovations from any observation profile will need to influence the salinity corresponding to other analysed temperatures, T_a, surrounding the observation profile. This could be done by interpolation;

$$\delta S(T_a) = \delta S(T_o^-) - (T_a - T_o^-)[\delta S(T_o^+) - \delta S(T_o^-)]/T_o^+ - T_o^-). \tag{8}$$

Alternatively if only a single $\delta S(T_o)$ value is available to infer $\delta S(T_a)$ (as is true in the current seasonal forecasting system at ECMWF where assimilation is done level by level) then it is possible to modify the gain matrix by writing, for example;

$$\mathbf{K}_3 \sim exp(-r^2/R^2)exp(-(T_a - T_o)^2/T_R^2) \tag{9}$$

where the r_2/R_2 factor is the normal decay of influence with horizontal distance, but now T_R is an additional 'temperature scale that determines how salinity measurements on one temperature surface should influence salinity on another temperature surface. These interpolation methods are presented as alternatives, but the key advance is the use of Eqs (5,6) defining salinity increments on isotherms. We now discuss the factors affecting the gains in the above assimilation methods and consider how the different properties of $S(z)$ and $S(T)$ variability discussed in section 2 impact on these gains.

3.3 Determining the Gain for $S(z)$ and $S(T)$ assimilation

There are two principal reasons why we should choose to make the gain larger for $S(T)$ assimilation than for $S(z)$ assimilation, and this is advantageous because it will mean that the observations have a larger impact on the analysis. The first is that $S(T)$ measurements should be usable with a smaller representivity error than measurements of $S(z)$. This is because $S(T)$ is not altered by passing gravity, inertial wave and Rossby wave oscillations that cause variability on short timescales. This is reflected in time variability and the power distribution in the two timeseries in Fig 2. The second reason lies in the larger decorrelation scales for $S(T)$ measurements relative to $S(z)$ measurements, as discussed in section 2.2. Therefore the $S(T)$ gain, $\mathbf{K}_3$ can remain larger as we move away from an observation profile. These two effects are related because it is clear that the expected a priori spatial scale for $S(z)$ and $T(z)$ data in mid-latitudes will be the Rossby deformation radius reflecting the rapidly varying ocean mesoscale. However for $S(T)$ data the mesoscale eddies have only a small signature, just as the gravity and inertial oscillations have a very small signature on $S(T)$. The formulation of $S(T)$ assimilation should therefore be very valuable in assimilating scarce historical salinity data (pre-ARGO) and may also point the way to better methods for assimilating other Lagrangian tracers whose variability could reasonably be determined to first order from the temperature field. We leave to the discussion at the end of the paper the relative merits of using isotherms rather than isopycnals as the basis for the assimilation.

In the next section we go on to look at the results of salinity analyses using the scheme proposed in (3.2).

4 Implementation of $S(T)$ assimilation at ECMWF

In order to demonstrate the application of the $S(T)$ assimilation method it has been implemented within the ECMWF seasonal forecasting system. In this section we focus on the results of the two separate salinity assimilation increments associated with temperature and salinity data and show the differences and also demonstrate that both are required in order to achieve a good analysis. The results of applying this scheme repeatedly in a model integration are left to a companion paper.

The ocean model used at ECMWF is the Hamburg Ocean Primitive Equation model, HOPE. The model uses an Arakawa E grid with a horizontal resolution of $1^o \times 1^o$ (latitude.longitude) plus a refinement to 0.3^o meridionally within 10^o of the equator. In the vertical there are 29 levels, 21 of which are in the upper 425 m. Vertical mixing uses a Richardson number dependent diffusivity based on Pacanowski and Philander (1981). The model is forced by daily average momentum, heat, and fresh water fluxes taken from the ECMWF atmospheric analysis system. More details of the model set up can be found in Anderson et al (2003).

The model was initialised from climatological T and S from the World Ocean Atlas (WOA98, Levitus et al 1998) data and run for a period of five years forced by climatological forcing and then run for 20 more years, until 4th August 2002, forced by ERA40 and ECMWF operational fluxes with a weak relaxation (3 years) to WOA98's subsurface T and S. At this point a first assimilation of both temperature and salinity data was carried out. This period was chosen because by this time the data from the ARGO float network had become quite extensive giving considerably more salinity data than was available in previous periods. The implementation of salinity adjustments, $\Delta S_T(z)$, as part of the temperature assimilation process was already available as part of the operational seasonal forecasting suite, Troccoli et al (2002). The new salinity assimilation scheme was implemented as described in section 3.2 above.

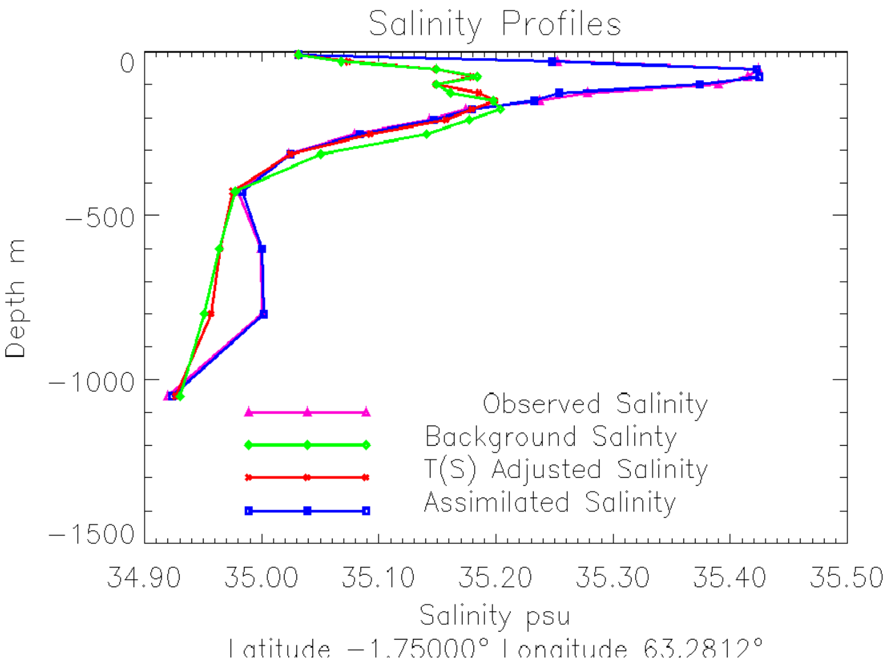


Figure 5: Salinity profiles at a salinity assimilation point near the Equator in the Indian ocean. The $T(S)$ adjusted salinity is the profile that can be deduced from temperature assimilation alone, while the blue line, marked assimilated salinity, shows the result of both the $T(S)$ adjustment and the salinity assimilation itself.

Figure 5 shows for a single water column just south of the equator in the Indian ocean how the salinity is altered by data assimilation. For convenience this observation profile is fairly isolated and we analyse the model changes at the location of the profile so that the assimilation impact is not reduced by distance. In addition the error associated with the observations is made small so that the assimilation is made to reproduce the observation profile. The green line shows the model background while the purple line shows the observed salinity profile. These two profiles have some level agreement at the surface, between 150-450m depth and at 1000m, but largely disagree elsewhere. The red line shows the profile resulting from temperature data assimilation using the $S(T)$ preserving salinity increment $\Delta S_T(z)$. It can be seen that this gives a clear improvement in the salinity profile over the 150-450m depth range but does not have a significant impact outside this depth range. The blue line shows the profile after also applying the $\Delta S_S(z)$ salinity increment, and this now agrees very well with the observed profile at all depths. Note that both assimilation increments are needed especially within the 150-450m depth range, since the $\Delta S_S(z)$ increment is doing very little in this depth range. This means that $S(T)$ is already correct for the waters in this depth range and it is only the depth of the isotherms that needs to be assimilated.

Figure 6 shows the impact of the two salinity increments as spatial fields over the top 300m of the water column over the whole globe. In this case the errors associated with the observations are chosen to give the more typical 50% weighting to the new data. Notice that the increments associated with salinity assimilation are considerably larger than those associated with temperature assimilation outside the tropical band, and they also tend to influence a larger spatial area. We suggest that this is indicative of the poor salinity of the background model state and the poor $S(T)$ relationships within that state. The surface forcing of salinity is probably rather poorly represented in the model and also the WOA98 initial conditions are a poor representation of actual salinity conditions in August 2002. Notice also that there is no obvious correspondence between the two salinity increments shown in Fig 6. If the correlation coefficient between the two salinity increments is calculated the value is very low, < 0.1. This emphasises the fact that the two salinity increments are correcting for quite different processes causing variation in the error field of the model background salinity state. This is further justification of the suggestion of this paper that the salinity assimilation be treated in this way. Further results from salinity assimilation within the ECMWF model will be found in a companion paper.

5 Conclusions and Discussion

In this paper we have first explored some of the variability present in the observational record of ocean salinity and also in salinity within ocean circulation models. We have demonstrated that the different processes involved in controlling salinity measured on a depth surface, z, and salinity measured on a temperature surface, T, are reflected in the different amplitude, space and timescales which dominate the salinity variability on z and T surfaces. In particular salinity variability on T surfaces shows smaller amplitudes and larger spatial and temporal correlations than does salinity variability on a z surface, at least for middle and lower latitudes and at depths with a well stratified water column.

The paper then uses these results to develop a new data assimilation algorithm for application to salinity data. A two stage salinity assimilation algorithm is advocated in which the first salinity increment ΔS_T allows the $S(T)$ functional relationship to remain fixed when temperature data are assimilated. This first increment was already advocated in Troccoli and Haines (1999). A second assimilation increment ΔS_S is derived here using the observational salinity itself, and this allows the $S(T)$ of the model to be updated. The earlier results on variability suggest that a larger gain can be used for deriving the ΔS_S increments, thus extracting more information from the measurements and increasing the influence of the scarce salinity observations on the final analysed model fields. Some preliminary test results from implementation in the ECMWF seasonal forecasting model are also shown.

It might be argued that a better physical separation to impose upon the two hydrographic variables T, S would be to assimilate potential density $\rho(z)$ and then assimilate $S(\rho)$ or equivalently $T(\rho)$, ignoring cabbeling effects. This probably would be a better separation but it ignores the fact that at least historically we have far more T data than S data and therefore we simply do not have observations in many cases. In future with ARGO coming to dominate the hydrographic record we may seek to implement a scheme focussed on the potential density variable.

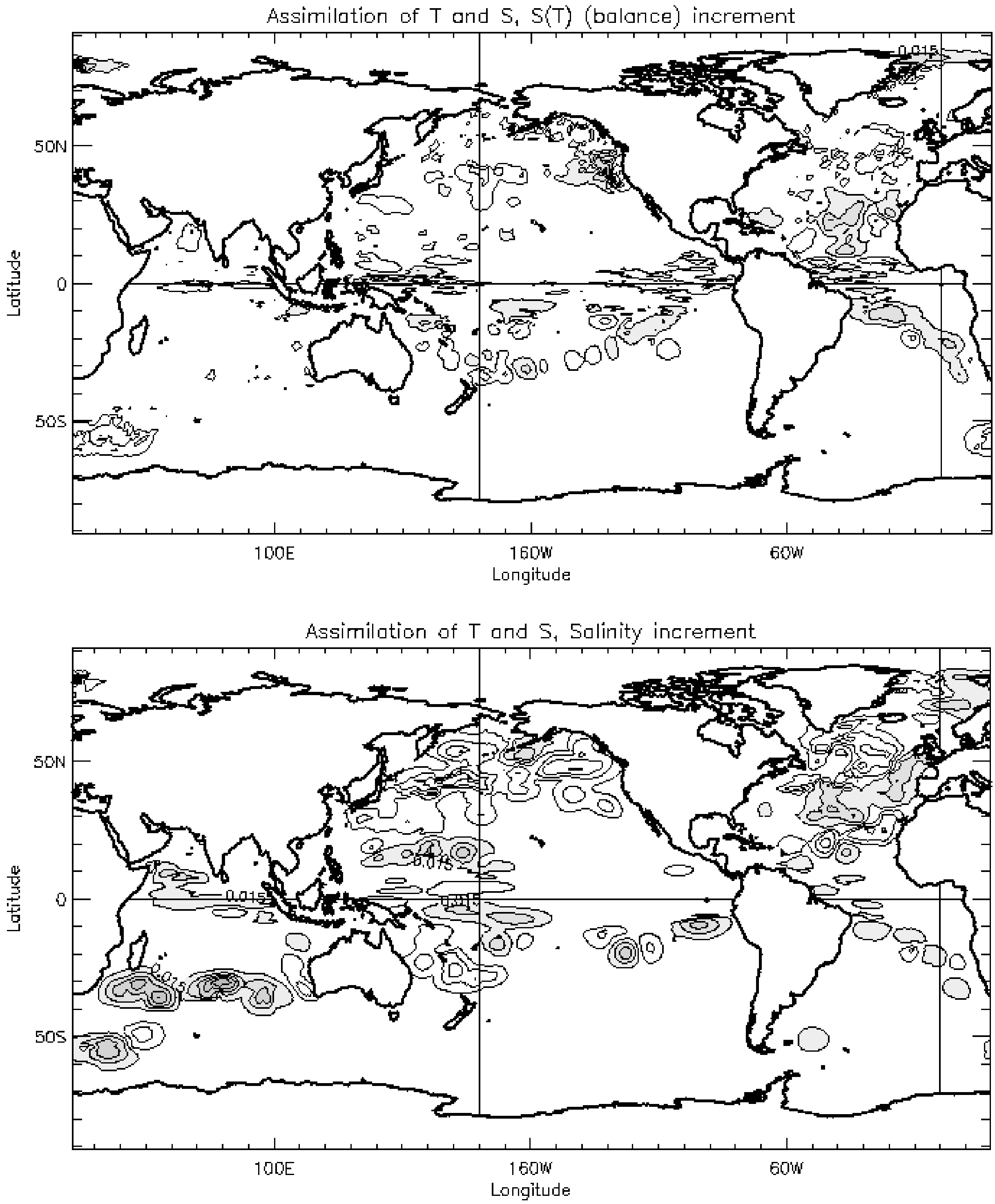


Figure 6: Upper panel shows the salinity increments ΔS_T over the top 300m of the water column on the first assimilation step, that can be deduced from the temperature assimilation using the preservation of the $S(T)$ relationship within the model background. Lower panel shows the salinity increments ΔS_S over the top 300m of the water column deduced from the salinity observations calculated to update the background $S(T)$ relationship. Contour interval is 0.1 psu starting at 0.05 psu.

A more conventional assimilation approach to account for the covariability of S and T would simply be to define a background error covariance matrix reflecting the appropriate level of correlation. However this approach has its own weaknesses. Covariances nearly always need to be derived from models and thus may not reflect true covariance. Also the covariances may need to be space and time varying, because they are really flow dependent and not fixed to the Eulerian reference frame. Again it becomes difficult to define such covariances accurately and a big job to store them. It will also be harder (although perhaps not impossible) to recover the elegant result of a larger gain for the assimilation of $S(T)$ data compared with $S(z)$ using the more conventional multivariate error covariance approach. This increase in the gain when assimilating salinity data should have a big impact when preparing ocean reanalyses for climate purposes where the salinity observations are very scarce.

For all the above reasons we believe it is worth pursuing the approach to data assimilation presented in this paper, for the new physical insights which it brings. It is for this reason that ECMWF have shown interest in implementing it within their ocean analysis system and in a companion paper the results of running this assimilation scheme over a period of time will be shown.

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