Notes on the GSW function gsw_SA_from_Sstar

Notes updated 24th February 2011

Preformed Salinity S_* is designed to be a conservative salinity variable which is unaffected by biogeochemical activity in the ocean; it is defined as Absolute Salinity less the contributions of biogeochemical processes to Absolute Salinity.

The **gsw_SA_from_Sstar**(SA,p,long,lat) function first interpolates the global Absolute Salinity Anomaly Ratio (R^δ) data set using the iinternal GSW library function **gsw_SAAR** to the (p,long,lat) location and then uses this interpolated value to calculate Absolute Salinity S_A according to

$$S_A = S_* \frac{\left(1 + R^\delta\right)}{\left(1 - r_1 R^\delta\right)} , \qquad\qquad \text{non-Baltic} \qquad (1)$$

where r_1 is taken to be the constant 0.35 based on the work of Pawlowicz *et al.* (2011).

If the observation is from the Baltic Sea, Absolute Salinity S_A is simply put equal to Preformed Salinity S_* ($S_A = S_*$) and returned, that is,

$$S_A = S_* . \qquad\qquad\qquad\qquad \text{Baltic} \qquad (2)$$

Note that in the Baltic Sea the deviations of Absolute Salinity from Reference Salinity are not due to non-conservative biogeochemical processes but rather are due to the anomalous composition entering the Baltic from rivers. Since these anomalous constituents are conservative, Preformed Salinity S_* in the Baltic Sea is taken to be the same as Absolute Salinity.

If the latitude and longitude are such as to place the observation well away from the ocean, a flag 'in_ocean' is set to zero as a warning, otherwise it is 1. This flag is only set when the observation is well and truly on dry land; often the warning flag is not set until one is several hundred kilometers inland from the coast. When the function detects that the observation is not from the ocean, R^δ is set equal to zero and **gsw_SA_from_Sstar** returns $S_A = S_*$ in accordance with Eqn. (1).

References

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Feistel, R., S. Weinreben, H. Wolf, S. Seitz, P. Spitzer, B. Adel, G. Nausch, B. Schneider and D. G. Wright, 2010: Density and Absolute Salinity of the Baltic Sea 2006–2009. *Ocean Science*, **6**, 3–24. http://www.ocean-sci.net/6/3/2010/os-6-3-2010.pdf

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Below are appendices A.5 and A.20 of the TEOS-10 Manual (IOC *et al.* (2010)) which discuss the conservative nature of Preformed Salinity S_* and its use in numerical ocean models.

A.5 Spatial variations in seawater composition

When the oceanographic data needed to evaluate Eqn. (A.4.10) for $S_A^{dens} - S_R \equiv S_A - S_R$ is not available, the look-up table method of McDougall *et al.* (2011a) is recommended to evaluate $\delta S_A \equiv \delta S_R^{dens} \equiv S_A - S_R$. The following paragraphs describe how this method was developed.

In a series of papers Millero *et al.* (1976a, 1978, 2000, 2008b) and McDougall *et al.* (2011a) have reported on density measurements made in the laboratory on samples collected from around the world's oceans. Each sample had its Practical Salinity measured in the laboratory as well as its density (measured with a vibrating tube densimeter at 25 °C and atmospheric pressure). The Practical Salinity yields a Reference Salinity S_R according to Eqn. (A.3.3), while the density measurement ρ^{meas} implies an Absolute Salinity $S_A \equiv S_A^{dens}$ by using the equation of state and the equality $\rho^{meas} = \rho\left(S_A^{dens}, 25\,°C, 0\,dbar\right)$. The difference $S_A^{dens} - S_R$ between these two salinity measures is taken to be due to the composition of the sample being different to that of Standard Seawater. In these papers Millero established that the salinity difference $S_A - S_R$ could be estimated approximately from knowledge of just the silicate concentration of the fluid sample. The reason for the explaining power of silicate alone is thought to be that (a) it is itself substantially correlated with other relevant variables (e.g. total alkalinity, nitrate concentration, DIC [often called total carbon dioxide]), (b) it accounts for a substantial fraction (about 0.6) of the typical variations in concentrations $(g\,kg^{-1})$ of the above species and (c) being essentially non-ionic; its presence has little effect on conductivity while having a direct effect on density.

When the existing data on δS_A, based on laboratory measurements of density, was regressed against the silicate concentration of the seawater samples, McDougall *et al.* (2011a) found the simple relation

$$\delta S_A / (g\,kg^{-1}) = (S_A - S_R) / (g\,kg^{-1}) = 98.24\left(Si(OH)_4 / (mol\,kg^{-1})\right). \qquad \textit{Global} \quad (A.5.1)$$

This regression was done over all available density measurements from the world ocean, and the standard error in the fit was $0.0054\,g\,kg^{-1}$.

The dependence of δS_A on silicate concentration is observed to be different in each ocean basin, and this aspect was exploited by McDougall *et al.* (2011a) to obtain a more accurate dependence of δS_A on location in space. For data in the Southern Ocean south of 30ºS the best simple fit was found to be

$$\delta S_A / (g\,kg^{-1}) = 74.884\left(Si(OH)_4 / (mol\,kg^{-1})\right), \qquad \textit{Southern Ocean} \quad (A.5.2)$$

and the associated standard error is $0.0026\,g\,kg^{-1}$.

The data north of 30ºS in each of the Pacific, Indian and Atlantic Oceans was treated separately. In each of these three regions the fit was constrained to match (A.5.2) at 30ºS and the slope of the fit was allowed to vary linearly with latitude. The resulting fits were (for latitudes north of 30ºS, that is for $\lambda \geq -30°$)

$$\delta S_A / (g\,kg^{-1}) = 74.884\left(1+0.3622\left[\lambda/30°+1\right]\right)\left(Si(OH)_4 / (mol\,kg^{-1})\right), \qquad \textit{Pacific} \quad (A.5.3)$$

$$\delta S_A / (g\,kg^{-1}) = 74.884\left(1+0.3861\left[\lambda/30°+1\right]\right)\left(Si(OH)_4 / (mol\,kg^{-1})\right), \qquad \textit{Indian} \quad (A.5.4)$$

$$\delta S_A / (g\,kg^{-1}) = 74.884\left(1+1.0028\left[\lambda/30°+1\right]\right)\left(Si(OH)_4 / (mol\,kg^{-1})\right). \qquad \textit{Atlantic} \quad (A.5.5)$$

These relationships between the Absolute Salinity Anomaly $\delta S_A = S_A - S_R$ and silicate concentration have been used by McDougall, Jackett and Millero (2011a) in a computer algorithm that uses an existing global data base of silicate (Gouretski and Koltermann (2004)) and provides an estimate of Absolute Salinity when given a seawater sample's Practical Salinity as well as its spatial location in the world ocean. Version 3.0 of this computer algorithm works as follows. The values of both the Reference Salinity and the

Absolute Salinity Anomaly, calculated from the global Gouretski and Koltermann (2004) hydrographic atlas using Eqns. (A.5.2) – (A.5.5), are used to form the ratio $R^\delta \equiv \delta S_A^{ref} / S_R^{ref}$ of these reference (ref) values of Absolute Salinity Anomaly and Reference Salinity. These values of R^δ are stored as a function of latitude, longitude and pressure on a $4° \times 4°$ grid in latitude and longitude. These values of R^δ are interpolated onto the latitude, longitude and pressure of an oceanographic observation (the details of the interpolation method can be found in McDougall $et~al.$ (2011a)) and the Absolute Salinity Anomaly of the oceanographic observation is calculated from

$$\delta S_A = R^\delta S_R \quad \text{where} \quad R^\delta \equiv \delta S_A^{ref} / S_R^{ref} , \tag{A.5.6}$$

where S_R is the Reference Salinity of the oceanographic observation. For the bulk of the ocean this expression for δS_A is almost the same as simply setting δS_A equal to δS_A^{ref}, but the use of Eqn. (A.5.6) is preferable in situations where the sample's Reference Salinity is small, such as in rivers, in estuaries and after a rain shower at the sea surface in the open ocean. In these situations the influence of the ocean's biogeochemical processes on δS_A should approach zero and this is achieved by Eqn. (A.5.6).

The relationships between the three salinity variables S_A, S_* and S_R are found as follows. First the standard relationships between these salinities are listed (from Eqns. (A.4.2), (A.4.1) and (A.4.6))

$$S_A = S_R + \delta S_A , \tag{A.5.7}$$

$$S_* = S_R - r_1 \delta S_A , \tag{A.5.8}$$

$$S_A = S_* + (1 + r_1) \delta S_A . \tag{A.5.9}$$

Substituting Eqn. (A.5.6) into these equations gives the following simple linear relationships between the three different salinities,

$$S_A = S_R \left(1 + R^\delta \right), \tag{A.5.10}$$

$$S_* = S_R \left(1 - r_1 R^\delta \right), \tag{A.5.11}$$

$$S_A = S_* \frac{\left(1 + R^\delta \right)}{\left(1 - r_1 R^\delta \right)} = S_* \left(1 + F^\delta \right) \quad \text{where} \quad F^\delta = \frac{[1 + r_1] R^\delta}{\left(1 - r_1 R^\delta \right)} . \tag{A.5.12}$$

These three equations are used in the six GSW functions that relate one salinity variable to another, where r_1 is taken to be 0.35 while R^δ is obtained from the look-up table of McDougall $et~al.$ (2011a).

This approach has so far assumed that the Absolute Salinity Anomaly in fresh water is zero. This is usually a good assumption for rainwater, but is often not true of water in rivers. For example, the river water flowing into the Baltic has an absolute Salinity Anomaly of approximately $0.087~\text{g kg}^{-1}$. When one has knowledge of the Absolute Salinity Anomaly due to river water inflow, this can be incorporated as follows

$$\delta S_A = R^\delta S_R + \delta S_A^{river} , \tag{A.5.13}$$

leading to (using Eqn. (A.5.7))

$$S_A = S_R \left(1 + R^\delta \right) + \delta S_A^{river} . \tag{A.5.14}$$

In turn, an estimate for δS_A^{river} might be constructed in the vicinity of a particular river from prior knowledge of the Absolute Salinity Anomaly at the river mouth $\delta S_A^{river\_mouth}$ (this is actually the Absolute Salinity Anomaly appropriate for river water extrapolated to $S_R = 0$) by a formula such as (drawing inspiration from the formula for the Baltic, see below)

$$\delta S_A^{river} = \delta S_A^{river\_mouth} \left(1 - S_R / S_R^{ref} \right). \tag{A.5.15}$$

The computer algorithm of McDougall *et al.* (2011a) accounts for the latest understanding of Absolute Salinity in the Baltic Sea, but it is silent on the influence of compositional variations in other marginal seas. The Absolute Salinity Anomaly in the Baltic Sea has been quite variable over the past few decades of observation (Feistel *et al.* (2010c)). The computer algorithm of McDougall *et al.* (2011a) uses the relationship found by Feistel *et al.* (2010c) that applies in the years 2006-2009, namely

$$S_A - S_R = \delta S_A = 0.087 \, \text{g kg}^{-1} \times \left(1 - S_R / S_{SO}\right), \qquad \textit{Baltic} \text{ (A.5.16)}$$

where S_{SO} = 35.165 04 g kg^{-1} is the standard-ocean Reference Salinity that corresponds to the Practical Salinity of 35. The Absolute Salinity Anomaly in the Baltic Sea is not due to biogeochemical activity, but rather is due to the rivers bringing material of anomalous composition into the Baltic. Hence Absolute Salinity in the Baltic is a conservative variable and Preformed Salinity is defined to be equal to Absolute Salinity in the Baltic. That is, in the Baltic $S_* = S_A$, implying that $r_1 = -1$ (see Eqns. (A.5.7) – (A.5.9)).

In order to gauge the importance of the spatial variation of seawater composition, the northward gradient of density at constant pressure is shown in Fig. A.5.1 for the data in a world ocean hydrographic atlas deeper than 1000m. The vertical axis in this figure is the magnitude of the difference between the northward density gradient at constant pressure when the TEOS-10 algorithm for density is called with $S_A \equiv S_A^{\text{dens}}$ (as it should be) compared with calling the same TEOS-10 density algorithm with S_R as the salinity argument. Figure A.5.1 shows that the "thermal wind" is misestimated by more than 2% for 58% of the data in the world ocean below a depth of 1000m if the effects of the variable seawater composition are ignored.
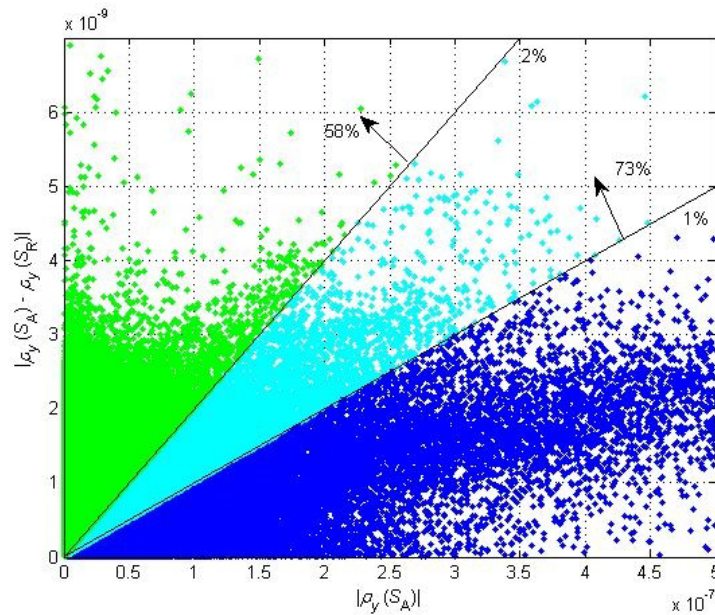

Figure A.5.1. The northward density gradient at constant pressure (the horizontal axis) for data in the global ocean atlas of Gouretski and Koltermann (2004) for $p > 1000$ dbar. The vertical axis is the magnitude of the difference between evaluating the density gradient using S_A versus S_R as the salinity argument in the TEOS-10 expression for density.

The importance of the spatial variations in seawater composition illustrated in Fig. A.5.1 can be compared with the corresponding improvement achieved by the TEOS-10 Gibbs function for Standard Seawater compared with using EOS-80. This is done by

ignoring spatial variations in seawater composition in both the evaluation of TEOS-10 and in EOS80 by calling TEOS-10 with S_R and EOS-80 with S_P. Figure A.5.2 shows the magnitude of the improvement in the "thermal wind" in the part of the ocean that is deeper than $1000\,\text{m}$ through the adoption of TEOS-10 but ignoring the influence of compositional variations. By comparing Figs. A.5.1 and A.5.2 it is seen that the main benefit that TEOS-10 delivers to the evaluation of the "thermal wind" is through the incorporation of spatial variations in seawater composition; the greater accuracy of TEOS-10 over EOS-80 for Standard Seawater is only 18% as large as the improvement gained by the incorporation of compositional variations into TEOS-10 (i. e. the rms value of the vertical axis in Fig. A.5.2 is 18% of that of the vertical axis of Fig. A.5.1). If the Atlantic were excluded from this comparison, the relative importance of compositional variations would be even larger.
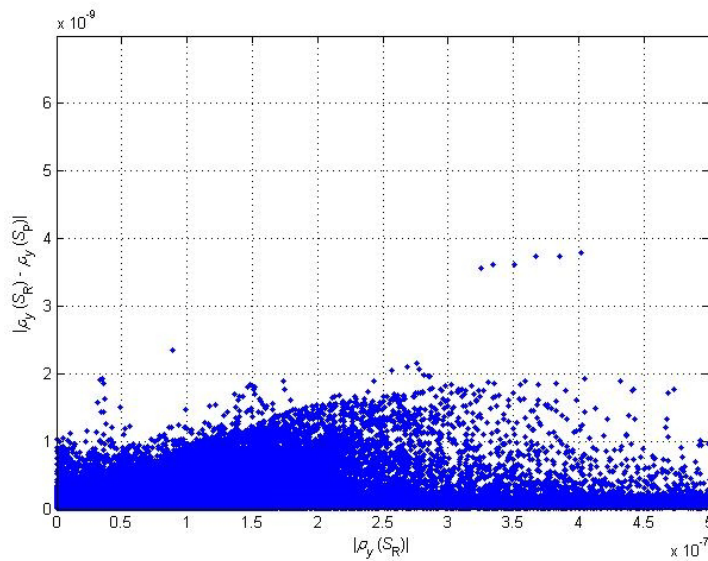

Figure A.5.2. The northward density gradient at constant pressure (the horizontal axis) for data in the global ocean atlas of Gouretski and Koltermann (2004) for $p > 1000\ \text{dbar}$. The vertical axis is the magnitude of the difference between evaluating the density gradient using S_R as the salinity argument in the TEOS-10 expression for density compared with using S_P in the EOS-80 algorithm for density.

The thermodynamic description of seawater and of ice Ih as defined in IAPWS-08 and IAPWS-06 has been adopted as the official description of seawater and of ice Ih by the Intergovernmental Oceanographic Commission in June 2009. The adoption of TEOS-10 has recognized that this technique of estimating Absolute Salinity from readily measured quantities is perhaps the least mature aspect of the TEOS-10 thermodynamic description of seawater. The present computer software, in both FORTRAN and MATLAB, which evaluates Absolute Salinity S_A given the input variables Practical Salinity S_P, longitude λ, latitude ϕ and sea pressure p is available at www.TEOS-10.org. It is expected, as new data (particularly density data) become available, that the determination of Absolute Salinity will improve over the coming decades, and the algorithm for evaluating Absolute Salinity in terms of Practical Salinity, latitude, longitude and pressure, will be updated from time to time, after relevant appropriately peer-reviewed publications have appeared, and such an updated algorithm will appear on the www.TEOS-10.org web site. Users of this software should state in their published work which version of the software was used to calculate Absolute Salinity.

A.20 The representation of salinity in numerical ocean models

Ocean models need to evaluate salinity at every time step as a necessary prelude to using the equation of state to determine density and its partial derivatives for use in the hydrostatic relationship and in neutral mixing algorithms. The current practice in numerical models is to treat salinity as a perfectly conserved quantity in the interior of the ocean; salinity changes at the surface and at coastal boundaries due to evaporation, precipitation, brine rejection, ice melt and river runoff, and satisfies an advection-diffusion equation away from these boundaries. The inclusion of composition anomalies necessitates several changes to this approach. These changes can be divided into two broad categories. First, in addition to fresh water inputs and brine rejection, all sources of dissolved material entering through the surface and coastal boundaries of the model should be considered as possible sources of composition anomalies. Second, within the interior of the model, changes due to the growth, decay and remineralization of biological material must be considered. Here, we focus on this second issue. While the ultimate resolution of these issues will involve biogeochemical models, in this appendix we discuss some practical ways forward based on the approximate relations (A.5.7) - (A.5.12) between the salinity variables S_R, S_* and $S_A = S_A^{dens}$. At the time of writing, the suggested approaches here have not been tested, so it must be acknowledged that the treatment of seawater composition anomalies in ocean models is currently a work in progress.

   We begin by repeating Eqns. (A.5.11) and (A.5.12), namely

$$S_* = S_R\left(1 - r_1 R^\delta\right), \qquad (A.20.1)$$

$$S_A = S_*\left(1 + F^\delta\right), \qquad (A.20.2)$$

where

$$R^\delta \equiv \frac{\delta S_A^{ref}}{S_R^{ref}} \quad \text{and} \quad F^\delta = \frac{\left[1 + r_1\right]R^\delta}{\left(1 - r_1 R^\delta\right)} . \qquad (A.20.3)$$

Recall that $R^\delta \equiv \delta S_A^{ref} / S_R^{ref}$ is the ratio of the reference (ref) values of Absolute Salinity Anomaly and Reference Salinity. The stored values of R^δ are interpolated onto the latitude, longitude and pressure of an oceanographic observation and R^δ takes values no larger than 0.001 in the global ocean. With r_1 taken to be 0.35 we have the approximate expression $F^\delta \approx 1.35 R^\delta$.

A.20.1 Using Preformed Salinity S_* as the conservative salinity variable

Because Preformed Absolute Salinity S_* (henceforth referred to by the shortened name, Preformed Salinity) is designed to be a conservative salinity variable, blind to the effects of biogeochemical processes, its evolution equation will be in the conservative form (A.8.1). When this type of conservation equation is averaged in the appropriate manner (see appendix A.21) the conservation equation for Preformed Salinity becomes (from Eqn. (A.21.7)),

$$\frac{d\hat{S}_*}{dt} = h^{-1}\nabla_n \cdot \left(hK\nabla_n\hat{S}_*\right) + \left(D\frac{\partial\hat{S}_*}{\partial z}\right)_z . \qquad (A.20.4)$$

As explained in appendix A.21, the over-tilde of $\hat{S}_*$ indicates that this variable is the thickness-weighted average Preformed Salinity, having been averaged between a pair of closely spaced neutral tangent planes. The material derivative on the left-hand side of Eqn. (A.20.4) is with respect to the sum of the Eulerian and quasi-Stokes velocities of height coordinates (equivalent to the description in appendix A.21 in terms of the thickness-weighted average horizontal velocity and the mean dianeutral velocity), while the right-hand side of this equation is the standard notation indicating that $\hat{S}_*$ is being

diffused along neutral tangent planes with the diffusivity K and in the vertical direction with the diapycnal diffusivity D (and h here is the average thickness between two closely spaced neutral tangent planes).

In order to evaluate density during the running of an ocean model, Absolute Salinity $S_A = S_A^{\text{dens}}$ must be evaluated. This can be done from Eqn. (A.20.2) as the product of the model's salinity variable $\hat{S}_*$ and $(1 + F^\delta)$. This could be done by simply multiplying the model's salinity by the fixed spatial map of $(1 + F^\delta)$ as observed today (using $r_1 = 0.35$ and the value of R^δ obtained from the computer algorithm of McDougall *et al.* (2011a)). However experience has shown that even a smooth field of density errors can result in significant anomalies in diagnostic model calculations, primarily due to the misalignment of the density errors and the model bottom topography. Indeed, even if the correct mean density could somehow be determined, approximations associated with the specification of the model bottom topography would result in significant errors in bottom pressure torques that can degrade the model solution. One way to minimize such errors is to allow some dynamical adjustment of the specified density field so that, for example, density contours tend to align with bottom depth contours where the flow is constrained to follow bottom topography. This simple idea is the key to the success of the robust diagnostic approach (Sarmiento and Bryan (1982)). To allow dynamical adjustment of the salinity difference $S_A - S_*$ while not permitting $S_A - S_*$ to drift too far from the observed values, we recommend carrying an evolution equation for F^δ so that it becomes an extra model variable which evolves according to

$$\frac{\mathrm{d}F^\delta}{\mathrm{d}t} = h^{-1}\nabla_n \cdot \left(hK\nabla_n F^\delta \right) + \left(D\frac{\partial F^\delta}{\partial z} \right)_z + \tau^{-1}\left(F^{\delta\,\text{obs}} - F^\delta \right). \qquad (A.20.5)$$

Here the model variable F^δ would be initialized based on observations, $F^{\delta\,\text{obs}}$ (using Eqn. (A.20.3) with $r_1 = 0.35$ and the interpolated values of R^δ from McDougall *et al.* (2011a)), and advected and diffused like any other tracer, but in addition, there is a non-conservative source term $\tau^{-1}\left(F^{\delta\,\text{obs}} - F^\delta \right)$ which serves to restore the model variable F^δ towards the observed value with a restoring time τ that can be chosen to suit particular modeling needs. It should be at least 30 days to permit significant adjustment, but it might prove appropriate to allow a much longer adjustment period (up to several years) if drift from observations is sufficiently slow. The lower bound is based on a very rough estimate of the time required for the density field to be aligned with topography by advective processes. The upper bound is set by the requirement to have the restoring time relatively short compared to vertical and basin-scale horizontal redistribution times.

Ideally one would like the non-conservative source term to reflect the actual physical and chemical processes responsible for remineralization in the ocean interior, but until our knowledge of these processes improves such that this is possible, the approach based on Eqn. (A.20.5) provides a way forward. An indication of how an approach based on modeled biogeochemical processes might be implemented in the future can be gleaned from looking at Eqn. (A.4.14) for $S_A - S_*$. If a biogeochemical model produced estimates of the quantities on the right-hand side of this equation, it could be immediately integrated into an ocean model to diagnose the effects of the biogeochemical processes on the model's density and its circulation.

In summary, the approach suggested here carries the evolution Eqns. (A.20.4) and (A.20.5) for $\hat{S}_*$ and F^δ, while $\hat{S}_A$ is calculated by the model at each time step according to

$$\hat{S}_A = \hat{S}_*\left(1 + F^\delta \right). \qquad (A.20.6)$$

The model is initialized with values of Preformed Salinity using Eqn. (A.20.1) based on observations of Reference Salinity and on the interpolated global data base of R^δ from McDougall *et al.* (2011a) using $r_1 = 0.35$.

A.20.2 Including a source term in the evolution equation for Absolute Salinity

An alternative procedure would be to carry an evolution equation for Absolute Salinity rather than for Preformed Salinity in an ocean model. Using Eqns. (A.20.4) - (A.20.6), the following evolution equation for Absolute Salinity can be constructed,

$$\frac{\mathrm{d}\hat{S}_A}{\mathrm{d}t} = h^{-1}\nabla_n \cdot \left(hK\nabla_n \hat{S}_A \right) + \left(D\frac{\partial \hat{S}_A}{\partial z} \right)_z - 2K\nabla_n \hat{S}_* \cdot \nabla_n F^\delta - 2DF_z^\delta \frac{\partial \hat{S}_*}{\partial z} + \frac{\hat{S}_*}{\tau}\left(F^{\delta\,\mathrm{obs}} - F^\delta \right)$$

(A.20.7)

$$= h^{-1}\nabla_n \cdot \left(hK\nabla_n \hat{S}_A \right) + \left(D\frac{\partial \hat{S}_A}{\partial z} \right)_z + \hat{\mathcal{S}}^{S_A} .$$

Here the non-conservative source term in the evolution equation for Absolute Salinity has been given the label $\hat{\mathcal{S}}^{S_A}$ for later use. If the ocean model resolves mesoscale eddies then the term $-2K\nabla_n \hat{S}_* \cdot \nabla_n F^\delta$ in Eqn. (A.20.7) becomes the scalar product of $\nabla_n F^\delta$ and the epineutral flux of S_* plus the scalar product of $\nabla_n \hat{S}_*$ and the epineutral flux of F^δ . In this approach the evolution equation (A.20.5) for F^δ is also carried and the model's salinity variable, $\hat{S}_A$, is used directly as the argument of the equation of state and other thermodynamic functions in the model. The model would be initialized with values of Absolute Salinity using Eqn. (A.5.10) (namely $S_A = S_R\left(1 + R^\delta\right)$) based on observations of Reference Salinity and on the global data base of R^δ from McDougall *et al.* (2011a). The production terms involving $\hat{S}_*$ in Eqn. (A.20.7) would need to be evaluated in terms of the model's salinity variable $\hat{S}_A$ using Eqn. (A.20.6).

This approach should give identical results to that described in section A.20.1 using Preformed Salinity. One disadvantage of having Density Salinity as the model's salinity variable is that its evolution equation (A.20.7) is not in the conservative form so that, for example, it is not possible to perform easy global budgets of salinity to test for the numerical integrity of the model code. Another disadvantage is that the air-sea flux of carbon dioxide and other gases may need to be taken into account as the surface boundary condition of Absolute Salinity. Such air-sea fluxes do not affect Preformed Salinity. But perhaps the largest disadvantage of this approach is the difficulty in evaluating the non-conservative terms $-2K\nabla_n \hat{S}_* \cdot \nabla_n F^\delta - 2DF_z^\delta \,\partial\hat{S}_*/\partial z$ in Eqn. (A.20.7), especially when meso-scale eddies are present, as discussed above.

A.20.3 Discussion of the consequences if remineralization is ignored

If an ocean model does not carry the evolution equation for F^δ (Eqn. (A.20.5)) and the model's salinity evolution equation does not contain the appropriate non-conservative source term, is there then any preference to initializing and interpreting the model's salinity variable as either Preformed Salinity, Absolute Salinity or Reference Salinity? That is, the simplest method of dealing with these salinity issues is to continue the general approach that has been taken for the past several decades of simply taking one type of salinity in the model, and that salinity is taken to be conservative. Under this approximation the salinity that is used in the equation of state to calculate density in the model is the same as the salinity that obeys a normal conservation equation of the form Eqn. (A.20.4). In this approach there is still a choice of how to initialize and to interpret the salinity in a model, and here we discuss the relative virtues of these options.

If the model is initialized with a data set of estimated Preformed Salinity S_*, then S_* should evolve correctly, since S_* is a conservative variable and its evolution equation Eqn. (A.20.4) contains no non-conservative source terms. In this approach the equation of state will be called with $\hat{S}_*$ rather than $\hat{S}_A$, and these salinities differ by approximately $(1 + r_1)\,\delta S_A$. The likely errors with this approach can be estimated using the simple example of Figure A.5.1. The vertical axis in this figure is the difference between the northward density gradient at constant pressure when the equation of state is called with $\hat{S}_A$ and with $\hat{S}_R$. The figure shows that when using $\hat{S}_R$, for all the data in the world

ocean below a depth of 1000 m, 58% of this data is in error by more than 2%. If this graph were re-done with $\hat{S}_*$ as the salinity argument rather than $\hat{S}_R$, the errors would be larger by the ratio $(1 + r_1) \approx 1.35$. That is, for 58% of the data in the world ocean deeper than 1000 m, the "thermal wind" relation would be misestimated by $\approx 2.7\%$ if $\hat{S}_*$ is used in place of $\hat{S}_A$ as the salinity argument of the equation of state. Also, these percentage errors in "thermal wind" are larger in the Pacific Ocean.

Another choice of the salinity data to initialize the model is $\hat{S}_A$. This choice has the advantage that for an initial period of time after initialization the equation of state is called with the correct salinity variable. However at later times, the neglect of the non-conservative source terms in Eqn. (A.20.7) means that the model's salinity variable will depart from reality and errors will creep in due to the lack of these legitimate non-conservative source terms. How long might it be acceptable to integrate such a model before the errors approached those described in the previous paragraph? One could imagine that in the upper ocean the influence of these different salinity variables is dwarfed by other physics such as air sea interaction and active gyral motions. If one considered a depth of 1000m as being a depth where the influence of the different salinities would be both apparent and would make a significant impact on the thermal wind equation, then one might guess that it would take several decades for the neglect of the non-conservative source terms in the evolution equation for Absolute Salinity to begin to be important. This is not to suggest that the relaxation time scale τ should be chosen to be as long as this, rather this is an estimate of how long it would take for the neglect of the non-conservative source term $\hat{\mathscr{S}}^{S_A}$ in Eqn. (A.20.7) to become significant.

A third choice is to initialize the model with Reference Salinity, $\hat{S}_R$. This choice incurs the errors displayed in Figure A.5.1 right from the start of any numerical simulation. Thereafter, on some unknown timescale, further errors will arise because the conservation equation for Reference Salinity is missing the legitimate non-conservative source terms representing the effects of biogeochemistry on conductivity and $\hat{S}_R$. Hence this choice is the least desired of the three considered in this subsection. Note that this choice is basically the approach that has been used to date in ocean modeling since we have routinely initialized models with observations of Practical Salinity and have treated it as a conservative variable and have used it as the salinity argument for the equation of state.

To summarize, the approaches of both subsections A.20.1 and A.20.2 of this appendix can each account for the non-conservative effects of remineralization if r_1 is a constant and so long as the appropriate boundary conditions are imposed. The advantage of using $\hat{S}_*$ is that it obeys a standard conservative evolution equation (A.20.4) with no source term on the right-hand side. If an ocean model were to be run without carrying the evolution equation for F^δ and hence without the ability to incorporate the appropriate non-conservative source terms in either Eqns. (A.20.6) or (A.20.7), then the model must resort to carrying only one salinity variable, and this salinity variable must be treated as a conservative variable in the ocean model. In this circumstance, we advise that the ocean's salinity variable be interpreted as Absolute Salinity, and initialized as such. In this way, the errors in the thermal wind equation will develop only slowly over a time scale of several decades or more in the deep ocean.

Since S_* is designed to be a conservative salinity variable, it would appear to also be the best choice for the salinity variable in inverse models. An argument can also be made that S_* should be the salinity variable that is used as an axis of the traditional "$S - \theta$ diagram", which would then become the $S_* - \Theta$ diagram. However, this argument is resisted because potential density contours cannot be drawn on the $S_* - \Theta$ diagram because density is a function of Absolute Salinity, not of Preformed Salinity.

Note that the modelling approaches described in subsections A.20.1 and A.20.2 are related to today's estimate of the observed field of δS_{A} . This field will change not only as the observational data base improves but also as the ocean composition evolves with time.