# Notes on the GSW function gsw_SA_from_Sstar

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 ($\delta S_{\mathrm{A}}$) data set using the gsw function gsw_delta_SA to the (p, long, lat) location and then uses this interpolated value to calculate Absolute Salinity $S_{\mathrm{A}}$ according to

$$S_{\mathrm{A}} \;=\; S_* + \left(1+r_1\right)\delta S_{\mathrm{A}}\,. \tag{1}$$

where $r_1$ is taken to be the constant 0.35 based on the work of Pawlowicz *et al.* (2010).

If the observation is from the Baltic Sea, Absolute Salinity $S_{\mathrm{A}}$ is simply put equal to Preformed Salinity $S_*$ ($S_{\mathrm{A}} = S_*$) and returned. 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.

In summary, the gsw_SA_from_Sstar function returns Eqn. (1) whether or not the observation is in the Baltic Sea, since in the case of the Baltic we have put $\delta S_{\mathrm{A}}$ equal to zero.

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, $\delta S_{\mathrm{A}}$ is set equal to zero and gsw_SA_from_Sstar returns $S_{\mathrm{A}} = S_*$ in accordance with Eqn. (1).

References

IOC, SCOR and IAPSO, 2010: *The international thermodynamic equation of seawater – 2010: Calculation and use of thermodynamic properties*. Intergovernmental Oceanographic Commission, Manuals and Guides No. 56, UNESCO (English), 196 pp. Available from http://www.TEOS-10.org

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

Pawlowicz, R., D. G. Wright and F. J. Millero, 2010: The effects of biogeochemical processes on oceanic conductivity/salinity/density relationships and the characterization of real seawater. *Ocean Science Discussions*, **7**, 773–836.

Below is appendix A.20 of the TEOS-10 Manual (IOC *et al*. (2010)) which discusses the conservative nature of Preformed Salinity $S_*$ and its use in numerical ocean models.

## 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 derivatives for use in the hydrostatic relationship and frequently 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.4.5) and (A.4.6) between the salinity variables $S_{\mathrm{R}}$, $S_*$ and $S_{\mathrm{A}} = S_{\mathrm{A}}^{\mathrm{dens}}$ that were discussed in section A.4. 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 restating Eqns. (A.4.5) and (A.4.6), namely

$$S_{\mathrm{R}} - S_* \;\approx\; r_1\, \delta S_{\mathrm{R}}^{\mathrm{dens}}, \tag{A.20.1}$$

$$S_{\mathrm{A}}^{\mathrm{dens}} - S_* \;\approx\; (1 + r_1)\, \delta S_{\mathrm{R}}^{\mathrm{dens}}, \tag{A.20.2}$$

where $r_1$ will be taken to be the constant 0.35 based on the work of Pawlowicz *et al.* (2010), and in this section these approximate relations will be taken to be exact. The Absolute Salinity Anomaly $\delta S_{\mathrm{R}}^{\mathrm{dens}} \equiv S_{\mathrm{A}}^{\mathrm{dens}} - S_{\mathrm{R}}$ is the salinity difference that can be directly measured from seawater samples using a vibrating beam densimeter and knowledge of the sample's Practical Salinity, and a global look-up table exists for this quantity (McDougall *et al.* (2010a)). Because this particular salinity difference is based on direct measurements, it is the natural measure of the anomalous composition of seawater to use in developing the following options for numerical modeling of composition anomalies.

### *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)),

$$\frac{\mathrm{d}\hat{S}_*}{\mathrm{d}t} \;=\; \tfrac{1}{h}\nabla_n \cdot \left( hK\nabla_n \hat{S}_* \right) \;+\; \left( D\frac{\partial \hat{S}_*}{\partial z} \right)_z . \tag{A.20.3}$$

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.20.3) 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, Density Salinity must be evaluated. This can be done from Eqn. (A.20.2) as the sum of the model's salinity variable $\hat{S}_*$ and $(1 + r_1)\, \delta S_{\mathrm{R}}^{\mathrm{dens}}$. This could be done by simply adding to the model's salinity variable $(1 + r_1)$ times the fixed spatial map of $\delta S_{\mathrm{R}}^{\mathrm{dens}}(\mathrm{obs})$ as observed today (and as is available from the computer algorithm of McDougall *et al.* (2010a)). 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 Absolute Salinity Anomalies $\delta S_{\mathrm{R}}^{\mathrm{dens}}(x,y,p)$ while not permitting them to develop large differences from the observed values $\delta S_{\mathrm{R}}^{\mathrm{dens}}(\mathrm{obs})$, we recommend carrying an evolution equation for $\delta S_{\mathrm{R}}^{\mathrm{dens}}$ so that it becomes an extra model variable which evolves according to

$$\frac{\mathrm{d}\delta S_{\mathrm{R}}^{\mathrm{dens}}}{\mathrm{d}t} = \tfrac{1}{h}\nabla_n \cdot \left( hK\nabla_n \delta S_{\mathrm{R}}^{\mathrm{dens}} \right) + \left( D\frac{\partial \delta S_{\mathrm{R}}^{\mathrm{dens}}}{\partial z} \right)_z + \tau^{-1}\left( \delta S_{\mathrm{R}}^{\mathrm{dens}}(\mathrm{obs}) - \delta S_{\mathrm{R}}^{\mathrm{dens}} \right). \qquad (\mathrm{A.20.4})$$

Here the model variable $\delta S_{\mathrm{R}}^{\mathrm{dens}}$ would be initialized based on observations, $\delta S_{\mathrm{R}}^{\mathrm{dens}}(\mathrm{obs})$, and advected and diffused like any other tracer, but in addition, there is a non-conservative source term $\tau^{-1}\left( \delta S_{\mathrm{R}}^{\mathrm{dens}}(\mathrm{obs}) - \delta S_{\mathrm{R}}^{\mathrm{dens}} \right)$ which serves to restore the model variable $\delta S_{\mathrm{R}}^{\mathrm{dens}}$ towards the observed value with a restoring time $\tau$ 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 of Eqn. (A.20.4) provides a way forward. An indication of how this approach might be improved in the future can be gleaned from looking at Eqn. (A.4.14) for $S_{\mathrm{A}}^{\mathrm{dens}} - S_*$ (taken from Pawlowicz *et al.* (2010)). 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 included biogeochemical processes on the model's density and its circulation.

In summary, the approach suggested here carries the evolution Eqns. (A.20.3) and (A.20.4) for $\hat{S}_*$ and $\delta S_{\mathrm{R}}^{\mathrm{dens}}$, while $\hat{S}_{\mathrm{A}}^{\mathrm{dens}}$ is calculated by the model at each time step according to

$$\hat{S}_{\mathrm{A}}^{\mathrm{dens}} = \hat{S}_* + (1 + r_1)\, \delta S_{\mathrm{R}}^{\mathrm{dens}}, \qquad (\mathrm{A.20.5})$$

with our best present estimate of $(1 + r_1)$ being $1.35$. The model is initialized with values of Preformed Salinity using Eqn. (A.20.1) (namely $\hat{S}_* = \hat{S}_{\mathrm{R}} - r_1\, \delta S_{\mathrm{R}}^{\mathrm{dens}}$) based on observations of Reference Salinity and on the global data base of $\delta S_{\mathrm{R}}^{\mathrm{dens}}(\mathrm{obs})$ from McDougall *et al.* (2010a).

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

An equivalent procedure is to carry the following evolution equation (A.20.6) for Absolute Salinity, which more specifically, is called Density Salinity, $S_{\mathrm{A}} \equiv S_{\mathrm{A}}^{\mathrm{dens}}$. On inspection of Eqn. (A.20.2), $S_{\mathrm{A}}^{\mathrm{dens}} - S_* \approx (1 + r_1)\, \delta S_{\mathrm{R}}^{\mathrm{dens}}$, and recognizing that $S_*$ is a conservative variable, it is clear that the non-conservative production of $S_{\mathrm{A}}^{\mathrm{dens}}$ must occur at the rate $(1 + r_1)$ times the rate at which the same non-conservative processes affect the Absolute Salinity

Anomaly $\delta S_R^{\text{dens}}$. Since (from Eqn. (A.20.4)) the non-conservative source term for $\delta S_R^{\text{dens}}$ is $\tau^{-1}\left(\delta S_R^{\text{dens}}(\text{obs}) - \delta S_R^{\text{dens}}\right)$, we find that the evolution equation for Density Salinity to be

$$\begin{aligned}
\frac{d\hat{S}_A^{\text{dens}}}{dt} &= \tfrac{1}{h}\nabla_n \cdot \left(hK\nabla_n \hat{S}_A^{\text{dens}}\right) + \left(D\frac{\partial \hat{S}_A^{\text{dens}}}{\partial z}\right)_z + (1+r_1)\tau^{-1}\left(\delta S_R^{\text{dens}}(\text{obs}) - \delta S_R^{\text{dens}}\right) \\
&= \tfrac{1}{h}\nabla_n \cdot \left(hK\nabla_n \hat{S}_A^{\text{dens}}\right) + \left(D\frac{\partial \hat{S}_A^{\text{dens}}}{\partial z}\right)_z + \hat{\mathcal{S}}^{S_A}
\end{aligned} \tag{A.20.6}$$

Alternatively, this equation can be derived by summing Eqn. (A.20.3) plus $(1 + r_1)$ times Eqn. (A.20.4). Here the non-conservative source term in the evolution equation for Density Salinity has been given the label $\hat{\mathcal{S}}^{S_A}$ for later use.

In this approach the evolution equation (A.20.4) for $\delta S_R^{\text{dens}}$ is also carried and the model's salinity variable, $\hat{S}_A^{\text{dens}}$, 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 Density Salinity using Eqn. (A.4.2) (namely $\hat{S}_A^{\text{dens}} = \hat{S}_R + \delta S_R^{\text{dens}}$) based on observations of Reference Salinity and on the global data base of $\delta S_R^{\text{dens}}(\text{obs})$ from McDougall *et al.* (2010a).

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.20.6) 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 Density Salinity. Such air-sea fluxes do not affect Preformed Salinity.

### *A.20.3 Including a source term in the evolution equation for Reference Salinity*

An equivalent procedure is to carry the following evolution equation (A.20.7) for Reference Salinity. On inspection of Eqn. (A.20.1), $S_R - S_* \approx r_1\,\delta S_R^{\text{dens}}$, and recognizing that $S_*$ is a conservative variable, it is clear that the non-conservative production of $S_R$ must occur at the rate $r_1$ times the rate at which the same non-conservative processes affect the Absolute Salinity Anomaly $\delta S_R^{\text{dens}}$. Since (from Eqn. (A.20.4)) the non-conservative source term for $\delta S_R^{\text{dens}}$ is $\tau^{-1}\left(\delta S_R^{\text{dens}}(\text{obs}) - \delta S_R^{\text{dens}}\right)$, the evolution equation for Reference Salinity is

$$\begin{aligned}
\frac{d\hat{S}_R}{dt} &= \tfrac{1}{h}\nabla_n \cdot \left(hK\nabla_n \hat{S}_R\right) + \left(D\frac{\partial \hat{S}_R}{\partial z}\right)_z + r_1\tau^{-1}\left(\delta S_R^{\text{dens}}(\text{obs}) - \delta S_R^{\text{dens}}\right) \\
&= \tfrac{1}{h}\nabla_n \cdot \left(hK\nabla_n \hat{S}_R\right) + \left(D\frac{\partial \hat{S}_R}{\partial z}\right)_z + \frac{r_1}{(1+r_1)}\hat{\mathcal{S}}^{S_A}
\end{aligned}\quad, \tag{A.20.7}$$

where the non-conservative source term is $r_1/(1+r_1)$ times the corresponding source term in the evolution equation for Density Salinity in Eqn. (A.20.6).

In this approach the evolution Eqns. (A.20.7) and (A.20.4) for $\hat{S}_R$ and $\delta S_R^{\text{dens}}$ are carried by the ocean model, while $\hat{S}_A^{\text{dens}}$ is calculated by the model at each time step according to Eqn. (A.4.2), namely

$$\hat{S}_A^{\text{dens}} = \hat{S}_R + \delta S_R^{\text{dens}}. \tag{A.20.8}$$

This approach, like that of section A.20.2 should give identical results to that described in section A.20.1 using Preformed Salinity except for the more complicated air-sea flux boundary condition for Reference Salinity than for Preformed Salinity. It does seem that the conservative nature of Eqn. (A.20.3) for Preformed Salinity is a significant advantage, and so this approach is likely to be preferred by ocean modelers.

### *A.20.4 Discussion of the consequences if remineralization is ignored*

If an ocean model does not carry the evolution equation for Absolute Salinity Anomaly (Eqn. (A.20.4)) 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.20.3). In this approach there is still a choice of how to initialize 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.20.3) contains no non-conservative source terms. In this approach the equation of state will be called with $\hat{S}_*$ rather than $\hat{S}_{\mathrm{A}}^{\mathrm{dens}}$, and these salinities differ by approximately $(1 + r_1)\,\delta S_{\mathrm{R}}^{\mathrm{dens}}$. 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 $\hat{S}_{\mathrm{A}}^{\mathrm{dens}}$ and with $\hat{S}_{\mathrm{R}}$. The figure shows that when using $\hat{S}_{\mathrm{R}}$, for all the data in the world ocean below a depth of $1000\ \mathrm{m}$, 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 $\hat{S}_{\mathrm{R}}$, the errors would be larger in the ratio $(1 + r_1) \approx 1.35$. That is, for 58% of the data in the world ocean deeper than 1000 $\mathrm{m}$, the "thermal wind" relation would be misestimated by $\approx 2.7\%$ if $\hat{S}_*$ is used in place of $\hat{S}_{\mathrm{A}}^{\mathrm{dens}}$ as the salinity argument to 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 $\hat{S}_{\mathrm{A}}^{\mathrm{dens}}$. 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 term in Eqn. (A.20.6) 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 Density Salinity to begin to be important. This is not to suggest that the relaxation time scale $\tau$ 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 $\mathcal{S}^{\hat{S}_{\mathrm{A}}}$ in Eqn. (A.20.6) to become significant.

A third choice is to initialize the model with Reference Salinity, $\hat{S}_{\mathrm{R}}$. 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 that represent the effects of biogeochemistry on conductivity and $\hat{S}_{\mathrm{R}}$. 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 studies since we have routinely initialized models with observations of Practical Salinity and have treated it as though it were a conservative variable and have used it as the salinity argument for the equation of state.

In principle, there are other combinations of options where the evolution equation for Absolute Salinity Anomaly (A.20.4) is carried by an ocean model, but some option other than those discussed in subsections A.20.1 – A.20.3 is pursued. We do not consider these various options here, since if one goes to the trouble of carrying the evolution equation for Absolute Salinity Anomaly, then one should be sufficiently careful to implement one of the options discussed in subsections A.20.1 – A.20.3.

### *A.20.5 Discussion of the options for including remineralization*

The approaches of subsections A.20.1 – A.20.3 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.20.3) with no source term on the right-hand side. Since $S_*$ is designed to be a conservative salinity variable, it would appear to be the most appropriate salinity variable for having as an axis of the traditional "$S-\theta$ diagram", which would then become the $S_*-\Theta$ diagram. Similarly, $\hat{S}_*$ would also be the best choice for the salinity variable in an inverse study.

If an ocean model were to be run without carrying the evolution equation for Absolute Salinity Anomaly (A.20.4) 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 Density 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.

It should be noted that each of the modelling approaches described in subsections A.20.1 – A.20.3 are related to today's estimate of the $\delta S_{\mathrm{R}}^{\mathrm{dens}}(\mathrm{obs})$ field. This field will change not only as the observational data base improves but also as the ocean composition evolves with time.