PARAMETERIZING MIXING IN INVERSE MODELS

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ABSTRACT

The conservation equations for scalars are developed in forms that are suitable for use in inverse models and with emphasis on the ways in which mixing processes are represented. The difference between the lateral Lagrangian and Eulerian velocity vectors is discussed and a suitable parameterization for the difference velocity (the Stokes drift) is proposed. The conservation equation for potential density is developed and is shown to be much more complicated than the normal diapycnal advective-diffusive balance. The extra terms that have not previously been included are often as large as the more obvious terms that have been retained in the past. In order to be able to draw comparisons with previous inverse models, the scalar conservation equations are developed with respect to potential-density surfaces rather than neutral surfaces. The differences that arise here are due to the lateral mixing being directed along neutral surfaces rather than along potential-density surfaces, and again the extra terms can be surprisingly large. The conservation statements for spiciness and Veronicity have their own set of problems since these variables are as nonlinear as is potential density.

The special problems that can beset box inversions are then described, including the need to include vertical diffusion as well as interfacial advection. For the purpose of deducing information about vertical mixing, perhaps the most serious failing of previous box-model inversions has been the masking of the information contained in the scalar conservation equations (particularly the salinity equation) by noise in the continuity equation. This has led previous workers in this field to conclude that vertical mixing was not needed by their inversions even when the results had strong diapycnal advection. A solution is suggested to overcome this problem with the divergence form of the conservation statements.

INTRODUCTION

Due to increasing societal pressure to predict the impact of the Greenhouse Effect on future climate, the role of the ocean in climate change is becoming more widely acknowledged and the subject of greater study. On the timescales of decades to centuries, the intermediate and deep waters of the ocean play a crucial role in the complicated feedbacks between the ocean and the atmosphere, and the circulation at these depths is intimately linked to the existence of vertical mixing processes (Bryan, 1987). We do not yet know how the strength of this mixing is regulated nor whether it is widely distributed in space or localized in small regions such as near topography. For these reasons it is increasingly important to use all methods at our disposal to deduce the strength of vertical mixing processes. One such method is to apply inverse procedures to hydrographic and tracer data to infer the strength of mixing processes that must have been present to cause the observed three-dimensional tracer patterns.

Much of the effort on oceanographic inverse models has been directed to determining the time-averaged circulation of the ocean, and so the models have concentrated on using the thermal wind relation in

conjunction with the continuity equation or the conservation of potential vorticity to solve for the lateral velocity vector for every station-pair at some (deep) reference level. Much less effort has been spent on using these techniques to deduce the magnitude of mixing processes in general, and the vertical diffusivity in particular. Three recent papers that have made substantial progress in this direction are Olbers, Wenzel and Willebrand (1985) and Hogg (1987) that have both been based on the β-spiral technique, and Schlitzer (1988) that has used the box-inverse technique. Another paper that was not only successful in detecting oceanic mixing, but was also able to distinguish between two different types of vertical mixing processes (salt-fingering and vertical eddy diffusion), is that by Bauer and Siedler (1988). This paper used the form of the conservation equations that did not explicitly include dianeutral advection, and so ensured that there could be no confusion in their model between dianeutral advection and dianeutral diffusion. While their work is not a full inversion in the sense that it did not solve for the velocity components simultaneously with the mixing parameters, I hope that it is typical of the results we can expect when inverse models are set up specifically with mixing processes in mind.

There is a distinct advantage in determining vertical diffusivities from hydrographic data as compared with determining the strength of lateral mixing processes. This advantage is due to the large separation of vertical scales between the small vertical scale at which the mixing processes act (of order 1 m), and the large vertical scale on which either an inverse model or a forward model is constructed (of order 100 m). Because of this large separation of scales we can expect that any answer that we believe for the vertical diffusivity from an inverse model will also apply to a forward model since the vertical scales in both models are so much larger than the scales of the mixing processes. A similar favorable ratio of relevant scales does not apply to lateral mixing processes so that one cannot be sure that a lateral eddy diffusivity that one obtains from an inversion using data at a certain horizontal spacing will be applicable to a forward model that has its grid points at a different horizontal resolution.

The paper begins with a review of the conservation equations for scalars in the neutral surface framework and goes on to derive a parameterization for the lateral bolus transport or Stokes velocity. Then, in order to compare what has been done by previous inverse modellers, the conservation equations for scalars are derived when mixing is performed with respect to potential-density surfaces. Many extra terms arise due to the different slopes and curvatures (in x,y,z space) of potential-density surfaces and neutral surfaces. These terms are often not negligible. An additional set of problems can arise when using the divergence form of the conservation equations, as is necessary in box-model inversions. The straightforward use of a salinity conservation equation in these box models seldom finds mixing processes to be important, even though the β-spiral techniques, using data from the same region, are able to detect the influence of ocean mixing. We show that this is most likely because the salinity conservation equation is dominated by uncertainty in the net volume flux into or out of the box. A suggestion is offered to overcome this problem, thereby increasing the rank of the solution and allowing mixing information to be recovered from the inversion.

A REVIEW OF SUITABLE CONSERVATION EQUATIONS FOR INVERSE MODELS

Since the lateral mixing by mesoscale eddies is believed to occur along neutral surfaces, it is convenient to develop the conservation equations in this reference frame. The vertical turbulent property fluxes are then parameterized by a vertical diffusivity, D, acting on the vertical property gradients, but the lateral turbulent fluxes are parameterized separately on the basis of a further Reynolds decomposition performed in this section. The continuity equation, $\nabla \cdot \mathbf{u} = 0$, and the divergence form of the conservation statement for a tracer, C, are integrated over the thickness, h, between two neutral surfaces (see Figure 1), to obtain

$$\frac{\partial h}{\partial t} + \nabla_n \cdot (h\mathbf{V}) + e^u - e^\ell = 0 \tag{1}$$

and

$$\frac{\partial (hC)|_n}{\partial t} + \nabla_n \cdot (h\mathbf{V}C) + [eC]_\ell^u = [DC_z]_\ell^u. \tag{2}$$

Here C is any conservative scalar variable (including S and θ), e is the vertical velocity of fluid through the neutral surface (henceforth called the dianeutral velocity), $\mathbf{V}$ is the instantaneous two-dimensional horizontal velocity vector, and ∇_n is the two-dimensional lateral gradient operator for properties measured in the neutral surface. The exact nature of the geometrical transformation between the Cartesian and neutral surface reference frames is explained in McDougall (1987a). The superscripts u and ℓ refer to the upper and lower neutral surfaces, as in Figure 1.
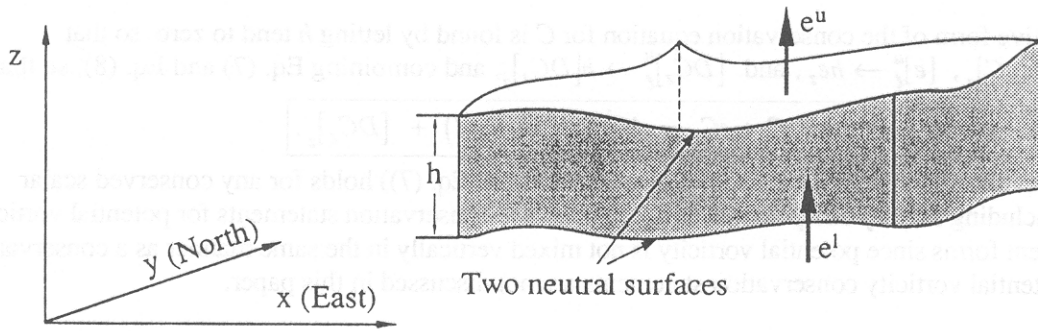

Fig. 1. Sketch showing two neutral surfaces separated by a height $h(x,y)$. Mixing processes can cause fluid to flow vertically through these neutral surfaces with the velocities e^u and e^ℓ.

Now we specifically allow for the lateral eddy motions by performing a Reynolds decomposition on the lateral velocity vector and on the scalar fields. The quasi-Lagrangian velocity vector is defined as

$$\overline{\mathbf{V}}^L \equiv \overline{\mathbf{V}}^E + \frac{\overline{h'\mathbf{V}'}}{\overline{h}}, \tag{3}$$

(called "quasi-Lagrangian" because, while $\overline{\mathbf{V}}^L$ follows the average position of marked fluid parcels along a neutral surface, it doesn't follow the dianeutral motion). $\overline{\mathbf{V}}^E$ is the usual Eulerian average velocity vector as would be measured by a current meter at a fixed position. Reynolds decomposing all the variables in (1) and (2) and averaging yields

$$\frac{\partial \overline{h}}{\partial t} + \nabla_n \cdot (\overline{h}\,\overline{\mathbf{V}}^L) + e^u - e^\ell = 0 \tag{4}$$

and

$$\frac{\partial (\overline{h}\overline{C})|_n}{\partial t} + \frac{\partial (\overline{h'C'})|_n}{\partial t} + \nabla_n \cdot (\overline{h}\,\overline{\mathbf{V}}^L\overline{C}) + [e\overline{C}]_\ell^u = -\nabla_n \cdot \left\{ \overline{h}\,\overline{C'\mathbf{V}'} + \overline{h'C'}\,\overline{\mathbf{V}}^E + \overline{h'C'\mathbf{V}'} \right\}$$
$$+ [D\overline{C}_z]_\ell^u. \tag{5}$$

Note that the mean value of C that appears in Eq. (5) is the Eulerian average value, not the quasi-Lagrangian value that would be defined in a similar way to Eq. (3). We are very likely to be justified in

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assuming that the triple correlation term on the right-hand side of Eq. (5) is quite small, and probably also $\overline{h'C'}\,\overline{\nabla}^E \ll \overline{C'\nabla'h}$ (Rhines, 1982) but in any case, we will assume that the lateral diffusivity, K, of a scalar is defined by

$$-\overline{h}K\nabla_n\overline{C} \equiv \left\{\overline{h}\,\overline{C'\nabla'} + \overline{h'C'}\,\overline{\nabla}^E + \overline{h'C'\nabla'}\right\}.$$ (6)

If the term $\partial\left[\overline{h'C'}|_n\right]\big/\partial t$ is taken to be zero, the divergence form, Eq. (5) simplifies to

$$\boxed{\frac{\partial(hC)|_n}{\partial t} + \nabla_n\cdot\left(h\nabla^L C\right) + [eC]_\ell^u = \nabla_n\cdot\left(hK\nabla_n C\right) + [DC_z]_\ell^u,}$$ (7)

where the overbars have been dropped from all the variables, while the continuity equation is

$$\boxed{\frac{\partial h}{\partial t} + \nabla_n\cdot\left(h\nabla^L\right) + [e]_\ell^u = 0.}$$ (8)

The advective form of the conservation equation for C is found by letting h tend to zero so that $[eC]_\ell^u \to h[eC]_z$, $[e]_\ell^u \to he_z$, and $[DC_z]_\ell^u \to h[DC_z]_z$, and combining Eq. (7) and Eq. (8), so that

$$\boxed{C_t|_n + \nabla^L\cdot\nabla_n C + eC_z = h^{-1}\nabla_n\cdot\left(hK\nabla_n C\right) + [DC_z]_z.}$$ (9)

This conservation statement (and also the divergence form, Eq. (7)) holds for any conserved scalar quantity including salinity and potential temperature. The conservation statements for potential vorticity take different forms since potential vorticity is not mixed vertically in the same manner as a conservative tracer. Potential vorticity conservation statements are not discussed in this paper.

The spatial gradients of θ and S along a neutral surface and also their temporal derivatives on a neutral surface are related through the thermal expansion coefficient, α, and the saline contraction coefficient, β, so that

$$\alpha\theta_t|_n = \beta S_t|_n, \quad\text{and}\quad \alpha\nabla_n\theta = \beta\nabla_n S.$$ (10)

Using these relations and the advective conservation statements for S and θ, Eq. (9), one finds

$$\boxed{\begin{aligned}\theta_t|_n + \left[\nabla^L - h^{-1}\nabla_n(hK)\right]\cdot\nabla_n\theta &= K\nabla_n^2\theta + DgN^{-2}\theta_z^3\beta\frac{d^2S}{d\theta^2}\\ &\quad + KgN^{-2}\theta_z\left\{C_b\nabla_n\theta\cdot\nabla_n\theta + T_b\nabla_n\theta\cdot\nabla_n p\right\},\end{aligned}}$$ (11)

and

$$\boxed{[e - D_z]\left[\alpha\theta_z - \beta S_z\right] = D\left[\alpha\theta_{zz} - \beta S_{zz}\right] - K\left\{C_b\nabla_n\theta\cdot\nabla_n\theta + T_b\nabla_n\theta\cdot\nabla_n p\right\},}$$ (12)

where C_b and T_b are the cabbeling and thermobaric parameters respectively, defined by

$$C_b = \left[\frac{\partial\alpha}{\partial\theta} + 2\frac{\alpha}{\beta}\frac{\partial\alpha}{\partial S} - \frac{\alpha^2}{\beta^2}\frac{\partial\beta}{\partial S}\right] \quad\text{and}\quad T_b = \left[\frac{\partial\alpha}{\partial p} - \frac{\alpha}{\beta}\frac{\partial\beta}{\partial p}\right].$$

Typical values are $10^{-5}\,K^{-2}$ for the cabbeling parameter and $2.6\times10^{-8}\,K^{-1}\,(db)^{-1}$ for the thermobaric parameter.

If one were able to measure the Lagrangian rate of change of a fluid property, say potential temperature, following a fluid parcel, vertical mixing with diffusivity D would cause the parcel's potential temperature to change at the rate $[D\theta_z]_z$. However, since we are only able to observe the ocean after a series of mixing processes has occurred, this Lagrangian approach cannot be pursued. By using the neutral surface reference frame, the vertical advection caused by vertical mixing can be accurately identified (Eq. 12) and then eliminated from the conservation equations in the form of Eq. (11).

Vertical mixing processes affect the conservation statement both through the non-advective diffusion of tracer and also through dianeutral advection. The ratio of dianeutral diffusion to dianeutral advection is, in general, different for different tracers.

It is important to realize that the dianeutral advection, e, is not a separate mixing process in its own right. Rather, e occurs simply because of the vertical diffusivity, D, and also due to cabbeling and thermobaricity. Once these physical mixing processes are specified and the hydrographic fields are known, e follows directly from Eq. (12). Eq. (11) is the appropriate form of the θ conservation equation for water-mass analysis since such studies are performed in property-property space and are inherently not fully Lagrangian. Vertical mixing by small-scale (isotropic) turbulence causes observable changes of fluid properties only if the relevant property-property plots are curved. Eq. (11) is sometimes called a water-mass transformation equation, since the temporal change of potential temperature on a neutral surface is equivalent to a change of the S-θ curve of a water-mass.

The reason for concentrating on the advective form of the conservation equations in neutral surfaces is because scalar properties are usually measured with high precision and so one can detect quite small changes in property-property diagrams (like the S-θ curves), and a change in such a property-property diagram is equivalent to a change on some kind of density horizon such as a neutral surface. In their divergence forms, the conservation equations contain not only the information of how mixing processes change properties along neutral surfaces, but they are also affected by the temporal change of the volume of the control volume, and the uncertainty in the volume fluxes into and out of a control volume bounded by two neutral surfaces. This volume is never well known in oceanographic observations because internal waves and mesoscale eddies cause large vertical excursions of neutral surfaces and so cause a large temporal variability of the height between neutral surfaces. However, these same wave-like processes do not change the property-property diagrams at all, and so these diagrams and the advective conservation equations in the neutral surface framework contain information that is sensitive to mixing processes and insensitive to the vertical heaving motions caused by internal waves and the like.

A simple scale analysis of the potential temperature conservation equation, Eq. (11), can reveal the magnitude of cabbeling and thermobaricity in relation to the epineutral mixing of θ by the lateral Laplacian term. At a thermoclinic front the magnitude of the epineutral Laplacian scales as the lateral gradient divided by the half-width of the front, L, that is, $\left|\nabla_n^2\theta\right| \approx \left|\nabla_n\theta\right|/L$. Setting half the epineutral θ and p contrasts across the front equal to $\Delta\theta$ and Δp respectively ($\Delta\theta = L\left|\nabla_n\theta\right|$ and $\Delta S = L\left|\nabla_n S\right|$), we find from Eq. (11) that

$$KgN^{-2}\theta_z\left\{C_b\nabla_n\theta\cdot\nabla_n\theta + T_b\,\nabla_n\theta\cdot\nabla_n p\right\}/\left(K\nabla_n^2\theta\right) = \frac{R_\rho}{[R_\rho-1]}\left\{\frac{C_b}{\alpha}\Delta\theta \pm \frac{T_b}{\alpha}\Delta p\right\}$$

$$\approx \frac{R_\rho}{[R_\rho-1]}\left\{0.1\Delta\theta \pm 3x10^{-4}\Delta p\right\}. \qquad (13)$$

In the Antarctic Circumpolar Current where $R\rho$ is about 2, $\Delta\theta$ is about 1 K, and Δp is about 500 db (and in the same sense as $\Delta\theta$), Eq. (13) is about 0.5, implying that the peak contribution of thermobaricity and cabbeling to water-mass conversion is 50% of the peak contribution of the epineutral Laplacian term. However thermobaricity and cabbeling are much more important than this comparison suggests because the epineutral Laplacian term changes sign across the front and so averages to zero in the frontal region, while cabbeling and thermobaricity contribute a term of the same sign across the whole front.

SUGGESTED PARAMETERIZATION FOR THE BOLUS TRANSPORT

The conservation equations that have been developed above have all included the bolus transport, $\overline{h'\mathbf{V}'}$, of volume along neutral surfaces. This is equivalent to recognizing that in both the advective and divergence forms of tracer conservation statements, the relevant velocity vector is the Lagrangian-mean velocity, not the Eulerian-mean velocity (Rhines, 1986, p 121). The difference between Lagrangian and Eulerian velocities in the dianeutral direction does not arise since the coordinate frame is already quasi-Lagrangian in this direction. The prefix quasi- is used to indicate that the coordinate frame does not quite move with the fluid: the difference being the dianeutral velocity, e. This means that the dianeutral velocity, e, is inherently a Lagrangian velocity component with respect to neutral surface coordinates. The lateral velocity vector that a current meter would measure at a fixed point is the Eulerian lateral velocity, $\mathbf{V}^E$, whereas the mean lateral velocity of a patch of dye or a cluster of floats is the Lagrangian velocity, $\mathbf{V}^L$, which is the sum of the Eulerian velocity and the Stokes drift, $h^{-1}\overline{h'\mathbf{V}'}$. In Cartesian coordinates, this bolus transport arises as a skew diffusion tensor when the diffusion tensor contains antisymmetric terms (Haidvogel and Rhines (1983), Rhines (1986), and Middleton and Loder (1989)).

The geostrophic and thermal wind equations relate the Eulerian velocity to the pressure and in-situ density fields, while the above equations show that it is the Lagrangian velocity vector that appears in the continuity and tracer equations (in both the advective and the divergence forms). To date inverse models have not distinguished between the Eulerian and Lagrangian lateral velocity vectors, and we do not yet know whether the distinction between these velocity vectors is significant in the ocean. In this section a parameterization is suggested for the difference velocity, the Stokes drift, $\mathbf{V}^S = \mathbf{V}^L - \mathbf{V}^E$. By trying this parameterization in inverse models we may be able to deduce the importance of the Stokes drift in the conservation of tracers.

In a quasi-geostrophic layered eddy-resolving model, Holland and Rhines (1980) have found that the eddy flux of potential vorticity is directed down the lateral gradient of mean potential vorticity, and that this eddy flux is dominated by the thickness flux. The only exception to this was in the western boundary current where the eddy relative vorticity flux was larger than that due to the bolus transport. The eddy flux of relative vorticity was much smaller, had smaller spatial scales and was both up and down-gradient at different locations. Brown, Owens and Bryden (1986) have used the LDE (Local Dynamics Experiment) current meter data of POLYMODE to determine both the eddy flux of relative vorticity and the thickness flux of potential vorticity at depth of about 600 m.. They found that the thickness flux of potential vorticity was an order of magnitude larger than the eddy flux of relative vorticity, and that the thickness flux of potential vorticity was directed almost exactly down the large-scale lateral gradient of potential vorticity (i.e. in the sense of a positive diffusivity, that is, in the direction of $-\nabla_\sigma\left(f/h^\sigma\right)$). The lateral diffusivity of potential vorticity that is implied by their measurements is about 2600 m² s⁻¹. Since $\overline{q'\mathbf{V}'} \approx -qh^{-1}\overline{h'\mathbf{V}'}$, the Stokes velocity, $h^{-1}\overline{h'\mathbf{V}'}$, was directed up the epineutral gradient of potential vorticity. Their observed thickness flux of potential vorticity is equivalent to a Stokes velocity, $h^{-1}\overline{h'\mathbf{V}'}$, of about 1.5 mm s⁻¹.

The observation from both quasi-geostrophic ocean models and from the LDE measurements of Brown et al (1986) that the thickness flux of potential vorticity is directed down the lateral q gradient suggests a parameterization for the eddy flux of potential vorticity as being minus a diffusivity times the epineutral gradient of potential vorticity. Because of the difficulty in Reynolds decomposing $q = f/h$, (since h is in the denominator), and because $\bar{h}$ and h' do arise unavoidably in the continuity equation, I denote the reciprocal of q as a new variable, r, and assert that the thickness flux of r is directed down its lateral gradient, so that

$$\overline{r'\mathbf{V}'} = -B\nabla_n\bar{r} = -B\nabla_n[\bar{h}/f], \text{ where } r \equiv h/f, \ \bar{r} = \bar{h}/f, \text{ and } r' = h'/f. \tag{14}$$

For small amplitude perturbations, this is equivalent to the more obvious $\overline{q'\mathbf{V}'} = -B\nabla_n\bar{q}$ parameterization, but at large amplitude when $h'/\bar{h}$ is not small, it is not clear how to link q' and $\bar{q}$ to h' and $\bar{h}$. With this parameterization of the epineutral flux of r due to eddies, the bolus flux is given by

$$\boxed{\mathbf{V}^S = \mathbf{V}^L - \mathbf{V}^E = \bar{h}^{-1}\overline{h'\mathbf{V}'} = B\nabla_n[\ell n\ \breve{q}] = -B\nabla_n[\ell n\ \bar{h}] + [\beta/f]B\mathbf{j},} \tag{15}$$

where $\breve{q} \equiv \bar{r}^{-1} = f/\bar{h}$. The overbars will henceforth be omitted from averaged variables. Since the magnitude of the neutral-surface potential vorticity generally increases towards the poles, the Stokes velocity will often be directed poleward.

The lateral advection term in the scalar conservation equations contains the combination of terms, $\mathbf{V}^L - h^{-1}\nabla_n(hK)$, and this can be most readily expressed as (using the geometrical identity $\nabla_n[\ell n h] = \partial[\nabla_n\mathcal{N}]/\partial z$ where $\mathcal{N}[x, y]$ is the height of a neutral surface)

$$\mathbf{V}^L - h^{-1}\nabla_n(hK) = \mathbf{V}^E - [B + K]\partial[\nabla_n\mathcal{N}]/\partial z - \nabla_n K + [\beta/f]B\mathbf{j}. \tag{16}$$

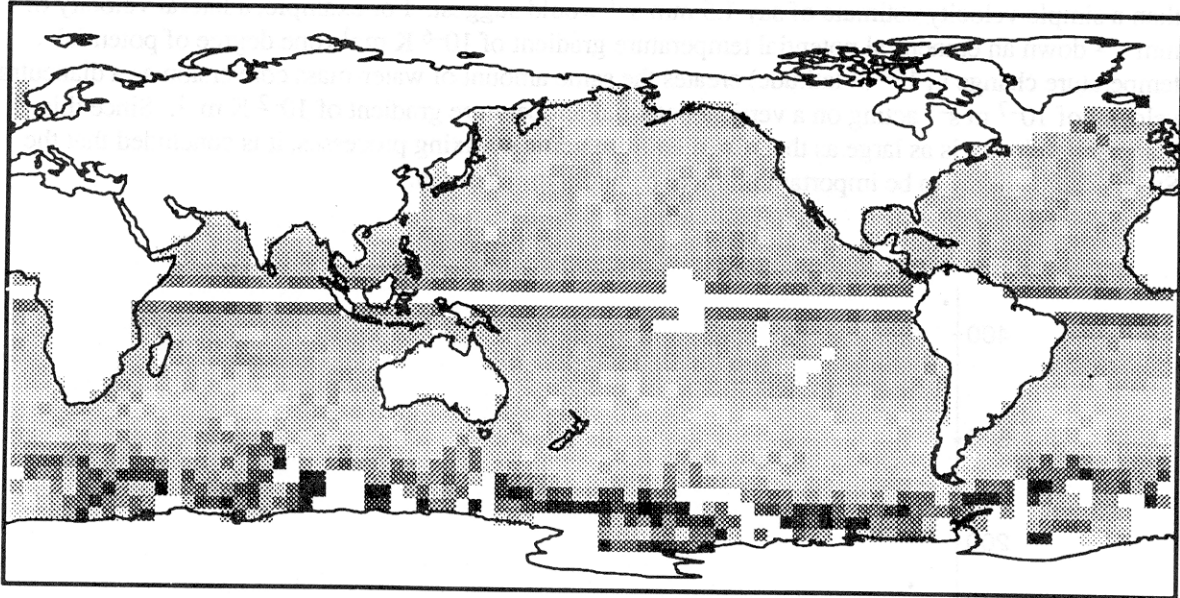| 0. | 0.36 | 0.86 | 1.5 | 2.5 | 3.7 | 5.4 | 7.8 | 11. | 15. |

Fig. 2. Map of the magnitude of the lateral Stokes velocity, $\mathbf{V}^S$, as given by Eq. (15), on a neutral surface that lies at about 1200 m in the equatorial Pacific (where σ_θ is about 27.5), and with the lateral diffusivity, B, equal to 1000 m^2 s^{-1}. The grey-scale covers the range from 0-15 mm s^{-1} and is evenly spaced in $\ell n(1 + |\mathbf{V}^S|)$.

Following Rhines and Holland (1979) we take the lateral diffusivity of potential vorticity to be equal to that of passive scalars, that is, $B = K$, so that

$$\left[\mathbf{V}^L - h^{-1}\nabla_n(hK)\right] = \mathbf{V}^E - 2K\,\partial[\nabla_n\mathcal{X}]/\partial z - \nabla_n K + [\beta/f]K\mathbf{j}. \tag{17}$$

This is the effective lateral velocity that advects tracers, whereas $\mathbf{V}^E$ is the lateral velocity that is evaluated from the thermal wind equation plus the reference level velocity.

The difference between Lagrangian and Eulerian lateral velocity vectors has not yet been incorporated into any inverse model of the ocean circulation. Rather, inverse models to date have assumed that the same lateral velocity vector appears in the tracer conservation equations as in the thermal wind equation. In fact, we have very little insight from either oceanographic theory or observations about the magnitude of the bolus transport. The deduction of a Stokes drift of 1.5 mm s^{-1} from the work of Brown et al (1986) is a rare insight into the importance of this process.

Since the contours of potential vorticity and of other tracers are often nearly parallel (although with the gradients often pointing in opposite directions), the Stokes drift or bolus transport can be expected to have a substantial component *across* the mean epineutral gradients of other tracers (including S and θ), and its direction will be up the epineutral tracer gradients as often as down them. Because the lateral velocity vector generally points almost along epineutral isolines of tracers rather than down the epineutral tracer gradients, the Stokes drift will be much more important for the conservation of tracers than a simple velocity estimate of say 1.5 mm s^{-1} would suggest. For example, a lateral velocity of 1 mm s^{-1} down an epineutral potential temperature gradient of 10^{-6} K m^{-1} (one degree of potential temperature change in $10°$ of latitude) creates the same amount of water-mass conversion as a dianeutral velocity of 10^{-7} m s^{-1} acting on a vertical potential temperature gradient of 10^{-2} K m^{-1}. Since this dianeutral velocity is as large as that expected from vertical mixing processes, it is concluded that the Stokes drift is likely to be important in tracer balances in the ocean.
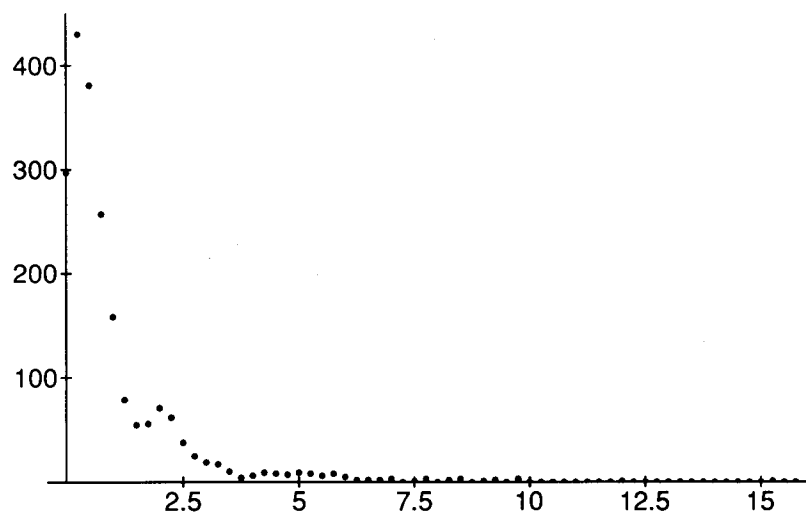

Fig. 3. Histogram of the number of occurrences of various magnitudes of the Stokes velocity (from 0 to 15 mm s^{-1}) in the map of Figure 2.

The Levitus (1982) atlas has been used to generate two neutral surfaces throughout the world ocean that were at depths of 1100 m and 1200 m respectively in the equatorial Pacific. The height, h, between them was used in Eq. (15) to estimate the Stokes velocity using 1000 m^2 s^{-1} for the lateral diffusivity. The magnitude of this estimate of the Stokes drift is shown in Figure 2 and the distribution of these estimates is shown in the histogram of Figure 3 where it is seen that a value of order 1 mm s^{-1} is typical. It remains to be seen whether the incorporation into inverse models of the difference between the lateral velocity vectors in the tracer equations and in the thermal wind equation, using the above parameterization Eq. (15) for the Stokes drift, makes any significant differences.

MIXING PRESCRIPTIONS IN β-SPIRAL INVERSIONS: The Advective Forms of Conservation Statements in Potential-Density Surfaces

Inversions of the β-spiral type are local in nature, in that a solution is found for the reference-level lateral velocity components and the mixing coefficients from the information at just one location. The inversion procedure can be cast in terms of the slopes of the surfaces of the conserved quantity (Schott and Stommel, 1978) or in terms of the conservation equation of this scalar quantity (e.g. Olbers et al., 1985). In either case a conservation statement is written in the advective form as opposed to the flux, or divergence, form. Here the equation for the conservation of potential density is derived and compared with that used by previous researchers. Important differences are found. Then the conservation equations of potential temperature and spiciness will be discussed.

The Potential Density "Conservation" Equation

In a potential-density surface the temporal and lateral gradients of salinity and potential temperature are related by (McDougall, 1987b)

$$\tilde{\alpha}\theta_t\big|_\sigma = \tilde{\beta}S_t\big|_\sigma, \text{ and } \tilde{\alpha}\nabla_\sigma\theta = \tilde{\beta}\nabla_\sigma S,$$

(18)

where $\tilde{\alpha}$ and $\tilde{\beta}$ are the values of the thermal expansion and saline contraction coefficients evaluated at the reference pressure of the potential density variable, that is, $\tilde{\alpha} = \alpha(S, \theta, p_r)$ and $\tilde{\beta} = \beta(S, \theta, p_r)$. The material derivative in the advective form, Eq. (9), of the tracer conservation equation can be written with respect to either neutral surfaces or potential-density surfaces, so that

$$C_t\big|_n + \mathbf{V}^L \cdot \nabla_n C + eC_z = C_t\big|_\sigma + \mathbf{V}^L \cdot \nabla_\sigma C + w^d C_z = h^{-1}\nabla_n \cdot (hK\nabla_n C) + [DC_z]_z,$$

(19)

where w^d is the vertical velocity of fluid through the potential-density surface (henceforth called the diapycnal velocity). This equation applies for both potential temperature and salinity, and these equations can be multiplied by $\tilde{\alpha}$ and $\tilde{\beta}$ respectively and then subtracted so as to eliminate the temporal and isopycnal advective terms, obtaining (after rearrangement) the following equation for the diapycnal velocity, (since $\tilde{\beta}S_t\big|_\sigma = \tilde{\alpha}\theta_t\big|_\sigma$, $\tilde{\beta}\nabla_\sigma S = \tilde{\alpha}\nabla_\sigma\theta$, and $(\rho_\theta)^{-1}(\rho_\theta)_z = \tilde{\beta}S_z - \tilde{\alpha}\theta_z$, see McDougall, 1987b),

$$w^d \left[\frac{1}{\rho_\theta}\frac{\partial\rho_\theta}{\partial z}\right] = \left[D\frac{1}{\rho_\theta}\frac{\partial\rho_\theta}{\partial z}\right]_z$$
$$+ D\frac{\partial\tilde{\alpha}}{\partial\theta}\theta_z^2$$
$$+ \tilde{\alpha}(c-1)\frac{1}{h}\nabla_n \cdot (hK\nabla_n\theta) + \frac{\tilde{\beta}}{\beta}K\{C_b\nabla_n\theta \cdot \nabla_n\theta + T_b\nabla_n\theta \cdot \nabla_n P\}.$$

(20)

This is the full conservation equation for potential density. The first term on the right-hand side is the only one that would occur if potential density were a conservative variable. If so desired, the left-hand side can be written with respect to Cartesian coordinates (as in Olbers et al (1985)) as

$$\left.\frac{\partial \rho_\theta}{\partial t}\right|_z + \mathbf{V}^L \cdot \nabla_2 \rho_\theta + w\left.\frac{\partial \rho_\theta}{\partial z}\right|_{x,y} = w^d \left.\frac{\partial \rho_\theta}{\partial z}\right|_{x,y}. \tag{21}$$

The usual approach with the potential-density equation is to equate the diapycnal advection of potential density, $w^d(\partial\rho_\theta/\partial z)$, to (minus) the diapycnal flux divergence, $\partial[D\,\partial\rho_\theta/\partial z]/\partial z$. That is, normally one sees the left-hand side of Eq. (20) being balanced by only the first term on the right. Here we investigate the magnitudes of the other terms that are usually neglected. The second term on the right of Eq. (20) arises because while the vertical gradient of potential density is given by $-(\rho_\theta)^{-1}(\rho_\theta)_z = \tilde\alpha\theta_z - \tilde\beta S_z$, when casting the right-hand side of Eq. (20) in terms of $(\rho_\theta)_{zz}$, the extra term, $D(\partial\tilde\alpha/\partial\theta)\theta_z^2$ appears. (The relatively small variation of $\tilde\alpha$ with S and the variation of $\tilde\beta$ with both θ and S have been ignored.) McDougall and You (1990) have shown that this extra term is larger than the correct term, $-D\left[\tilde\alpha\theta_{zz} - \tilde\beta S_{zz}\right]$, in much of the subtropical thermoclines of each of the world's ocean basins (see their Figure 9). This is illustrated in Figures 4-6 which show three different combinations of terms mapped on a neutral surface in each of the three major oceans. On much of the neutral surface of Figure 4 in the North Atlantic, the correction term in Eq. (20), $D\frac{\partial\tilde\alpha}{\partial\theta}\theta_z^2$, is larger than the sum of the first two terms in Eq. (20), $-D\left[\tilde\alpha\theta_{zz} - \tilde\beta S_{zz}\right]$, (ignoring D_z), implying that the straightforward term in Eq. (20), $D\left[(\rho_\theta)^{-1}\partial\rho_\theta/\partial z\right]$, has the opposite sign to the correct right-hand side of Eq. (20) in these places. In the Pacific in Figure 5 the nonlinear term is up to 40% of the correct term, while in the Indian Ocean in Figure 6 it is as large as 30% of the correct term. It is concluded that serious errors have occurred in the conservation equation of potential density in present inverse models. From these figures it can be seen that in Hogg's (1987) study of the circulation and mixing in the central North Atlantic, the second term in Eq. (20), $D(\partial\tilde\alpha/\partial\theta)\theta_z^2$, which Hogg omitted, was 50% of the correct term, $D\left[\tilde\alpha\theta_{zz} - \tilde\beta S_{zz}\right]$, on the upper of the two σ_1 surfaces he considered. In parts of the North Atlantic, the relative error is more than 100%, and this type of error was built into the Olbers et al (1985) model.

In the third term in Eq. (20), the parameter c is defined by $c = [\alpha/\beta]\left[\tilde\alpha/\tilde\beta\right]^{-1}$ and is unity at the reference pressure, p_r, of the potential density. This third term in the equation scales as $K\tilde\alpha[c-1]\nabla_n^2\theta$ and the magnitude of this term can be estimated as follows. Consider the use of potential density (referenced to the sea surface) down to a depth of 2000 m (as in Olbers et al., 1985). At that depth, c is about 1.5 and $K\nabla_n^2\theta$ can be taken to be the same order as $e\theta_z$ where the dianeutral velocity is 1×10^{-7} m s^{-1} and the vertical gradient of potential temperature is 3×10^{-3} K m^{-1}. When divided by the vertical gradient of potential density at 2000 m in the North Atlantic, this third term in Eq. (20) amounts to a contribution of 0.3×10^{-7} m s^{-1} to the diapycnal velocity. Again, this is not an insignificant diapycnal velocity, although it is rather unusual these days to find researchers using potential-density surfaces as far as 2000 m away from their reference pressure.

The last term in Eq. (20) is due to thermobaricity and cabbeling, (see the corresponding terms in the dianeutral velocity equation, Eq. (12)). Because the buoyancy frequency is related to the vertical gradient of potential density by $N^2 = \mu\left(\beta/\tilde\beta\right)\left[-(g/\rho_\theta)(\partial\rho_\theta/\partial z)\right] \approx \mu\left[-(g/\rho_\theta)(\partial\rho_\theta/\partial z)\right]$, (see McDougall, 1987b and Eq. (23) below for a definition of μ) the *diapycnal* velocity induced by cabbeling and thermobaricity will in fact be larger by the factor μ than the *dianeutral* velocity, e, caused by these processes. McDougall and You (1990) assumed a lateral diffusivity, K, of 1000 m^2 s^{-1} and have shown that in parts of the North Atlantic and in the Southern Ocean, cabbeling causes a downward dianeutral velocity as large as -1×10^{-7} m s^{-1}, so that the contribution of the last term in
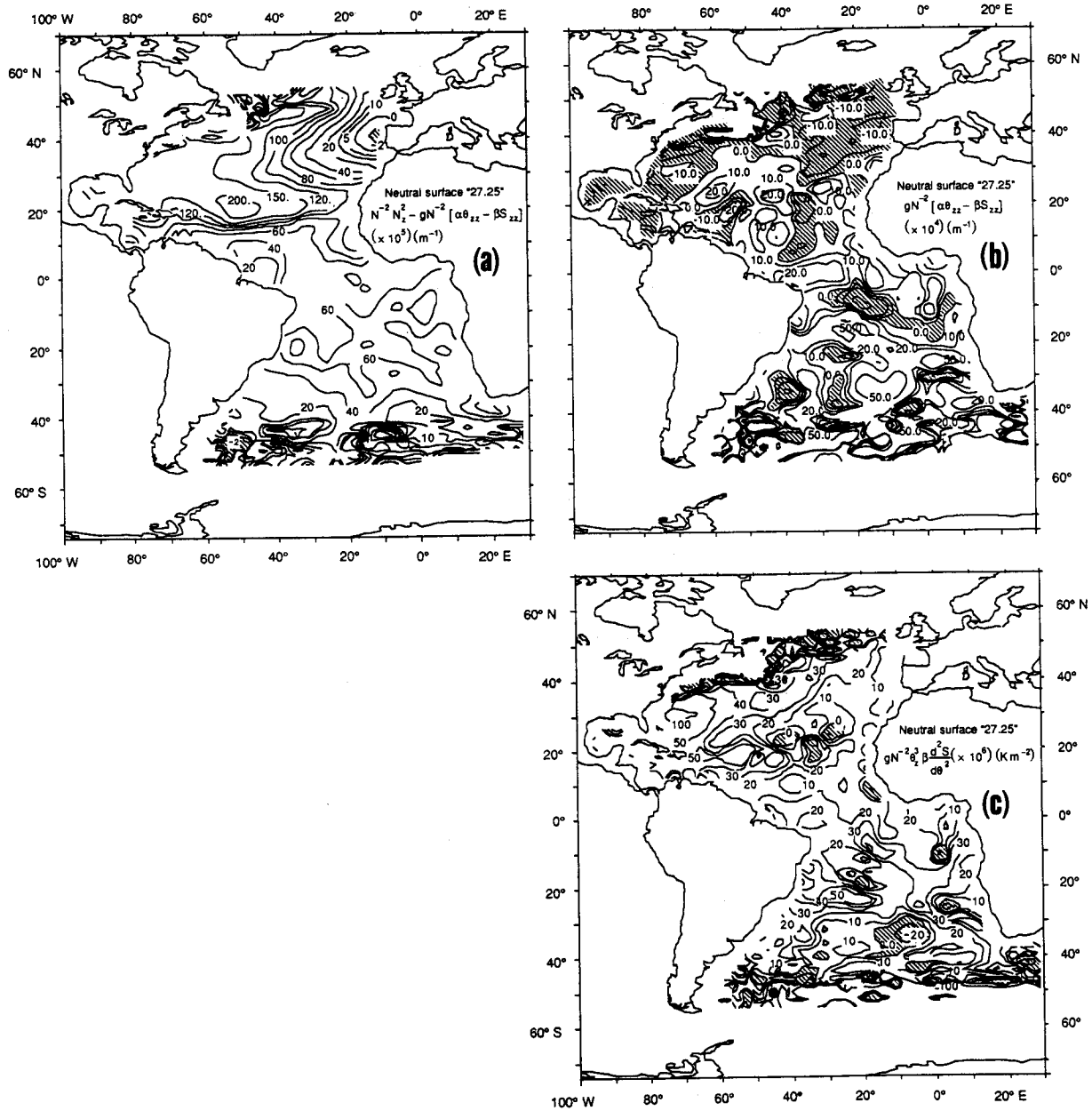
Fig. 4. Graphs of various terms on a neutral surface in the Atlantic at a depth of approximately 800 m in mid-latitudes. (a) The term plotted here, $N^{-2}N_z^2 - gN^{-2}\{\alpha\theta_{zz} - \beta S_{zz}\}$, is approximately equal to $gN^{-2}\frac{\partial\alpha}{\partial\theta}\theta_z^3$ in the upper 1000 m of the ocean. (b) When multiplied by the vertical diffusivity, D, this term, $gN^{-2}\{\alpha\theta_{zz} - \beta S_{zz}\}$, is the rate at which vertical mixing contributes to the dianeutral velocity. (c) When multiplied by the vertical diffusivity, D, this term, $gN^{-2}\theta_z^3\beta\frac{d^2S}{d\theta^2}$, is the rate at which vertical turbulent mixing causes potential temperature to change on a neutral surface. (From McDougall and You (1990) Figure 1).
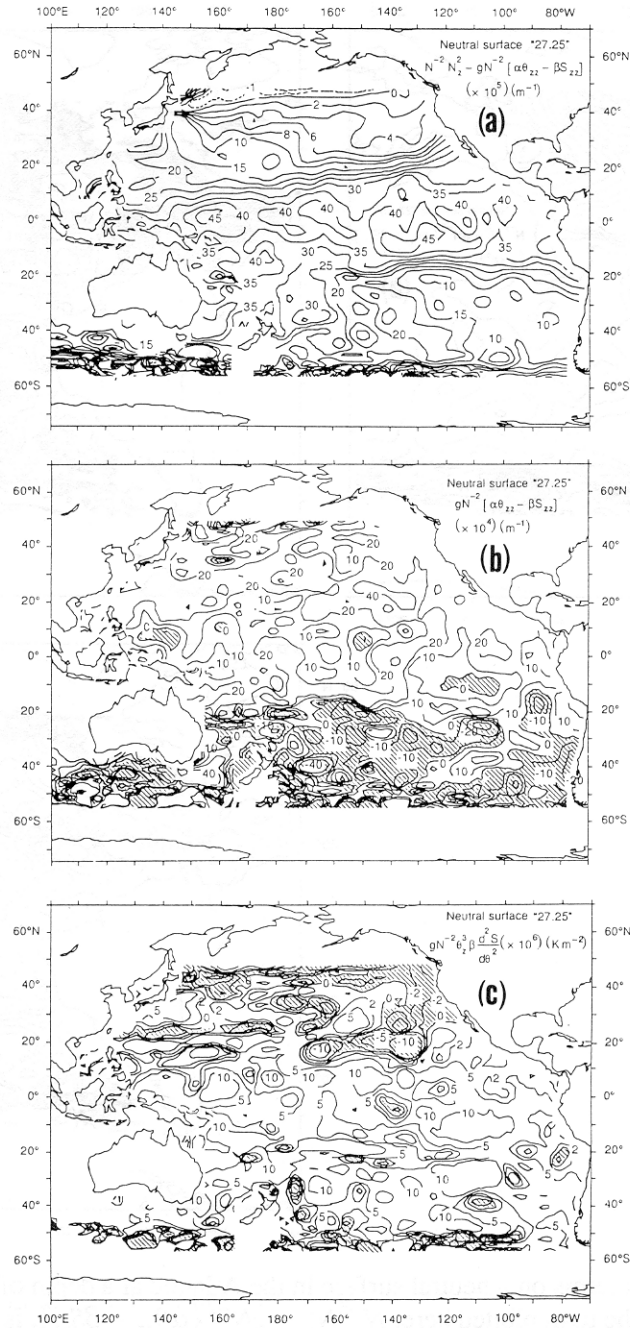
365

Fig. 5. Graphs of various terms on a neutral surface in the Pacific at a depth of approximately 900 m in mid-latitudes. (a) The term plotted here, $N^{-2}N_z^2 - gN^{-2}\{\alpha\theta_{zz} - \beta S_{zz}\}$, is approximately equal to $gN^{-2}\frac{\partial\tilde{\alpha}}{\partial\theta}\theta_z^3$ in the upper 1000 m of the ocean. (b) When multiplied by the vertical diffusivity, D, this term, $gN^{-2}\{\alpha\theta_{zz} - \beta S_{zz}\}$, is the rate at which vertical mixing contributes to the dianeutral velocity. (c) When multiplied by the vertical diffusivity, D, this term, $gN^{-2}\theta_z^3\beta\frac{d^2S}{d\theta^2}$, is the rate at which vertical turbulent mixing causes potential temperature to change on a neutral surface. (From McDougall and You (1990) Figure 4).
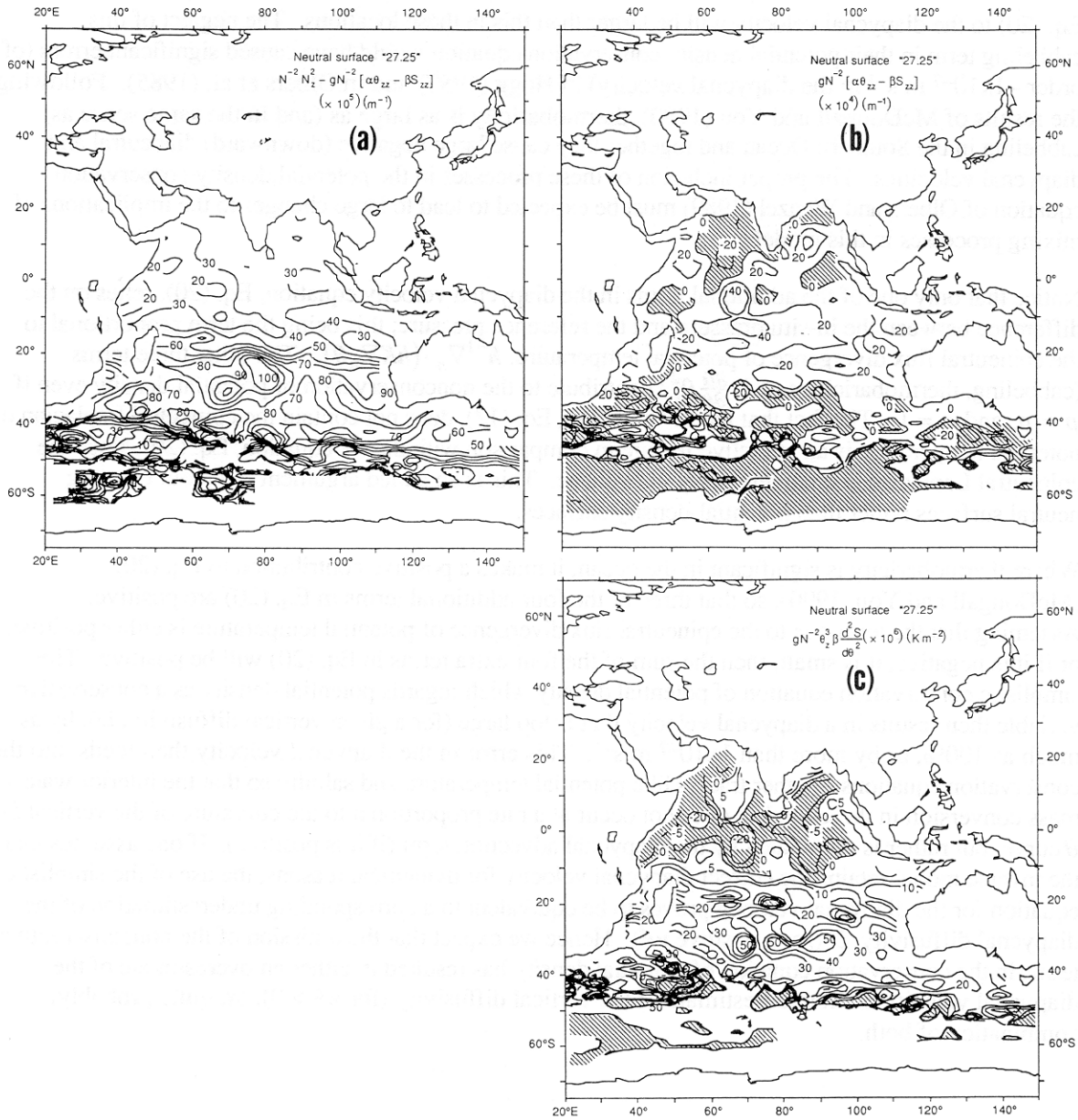
366

Fig. 6. Graphs of various terms on a neutral surface in the Indian at a depth of approximately 950 m in mid-latitudes. (a) The term plotted here, $N^{-2}N_z^2 - gN^{-2}\{\alpha\theta_{zz} - \beta S_{zz}\}$, is approximately equal to $gN^{-2}\frac{\partial\bar{\alpha}}{\partial\theta}\theta_z^3$ in the upper 1000 m of the ocean. (b) When multiplied by the vertical diffusivity, D, this term, $gN^{-2}\{\alpha\theta_{zz} - \beta S_{zz}\}$, is the rate at which vertical mixing contributes to the dianeutral velocity. (c) When multiplied by the vertical diffusivity, D, this term, $gN^{-2}\theta_z^3\beta\frac{d^2S}{d\theta^2}$, is the rate at which vertical turbulent mixing causes potential temperature to change on a neutral surface. (From McDougall and You (1990) Figure 6).

Eq. (20) to the diapycnal velocity will be larger than this in these locations. The neglect of this cabbeling term in their potential density conservation equation would have caused significant errors (of order -1×10^{-7} m s^{-1} in the diapycnal velocity) in Hogg (1987) and in Olbers et al. (1985). Following the results of McDougall and You (1990), thermobaricity is as large as (and in the same sense as) cabbeling in the Southern Ocean and together they cause large negative (downward) dianeutral and diapycnal velocities. The proper inclusion of these processes in the potential density conservation equation of Olbers and Wenzel (1989) must be expected to lead to large changes to the implications of mixing processes in this model.

Notice that only one of the additional terms in the diapycnal velocity equation, Eq. (20), relies on the difference between the in-situ pressure and the reference pressure; this being the term proportional to the epineutral flux divergence of potential temperature, $h^{-1}\nabla_n \cdot (hK\nabla_n\theta)$. The other three terms (cabbeling, thermobaricity and $D\frac{\partial \tilde{\alpha}}{\partial \theta}\theta_z^2$) contribute to the nonconservation of potential density even if $p = p_r$ and $c = 1$. The fact that the "e" equation, Eq. (12), does not contain the epineutral Laplacian of potential temperature is an attractive feature in comparison with the w^d equation, Eq. (20), since the epineutral Laplacian is relatively noisy to evaluate. This is an added argument in favour of using neutral surfaces rather than potential-density surfaces.

Where thermobaricity is significant in the ocean, it makes a positive contribution to Eq. (20) (McDougall and You, 1990), so that three of the four additional terms in Eq. (20) are positive. Assuming that the term due to the epineutral flux divergence of potential temperature is either positive, or if it is negative, it is small, then the sum of the four extra terms in Eq. (20) will be positive. The simplistic conservation equation of potential density which regards potential density as a conservative variable then results in a diapycnal velocity that is too large (for a given vertical diffusivity, D), by as much as 100%, or by more than 1×10^{-7} m s^{-1}. This error in the diapycnal velocity then feeds into the conservation equations of other tracers like potential temperature and salinity so that the interior water-mass conversion in these models does not occur at a rate proportional to the curvature of the vertical S-θ curve, but rather is dominated by the diapycnal advection term (if it is positive). If one assumes that the inverse model retains the correct diapycnal velocity for dynamical reasons, the use of the simplistic equation for the diapycnal velocity proves to be equivalent to a corresponding underestimation of the diapycnal diffusivity, D (for a positive w^d). Hence we expect that the omission of the nonconservative terms in the conservation equation of potential density has resulted in either an overestimate of the diapycnal velocity or an underestimate of the vertical diffusivity (for $w^d > 0$), or, quite probably, a combination of both.

The Potential Temperature Conservation Equation

The conservation equation of potential temperature with the total material derivative written with respect to potential-density surfaces is (from Eq. (19))

$$\theta_t\big|_\sigma + \mathbf{V}^L \cdot \nabla_\sigma\theta + w^d\theta_z = \frac{1}{h}\nabla_n \cdot (hK\nabla_n\theta) + [D\theta_z]_z$$
$$\neq \frac{1}{h^\sigma}\nabla_\sigma \cdot (h^\sigma K\nabla_\sigma\theta) + [D\theta_z]_z .$$

(22)

The lateral flux divergence of potential temperature in a neutral surface framework is not the same as that in a potential density framework, and here we derive the differences.

The lateral gradient of potential temperature in a neutral surface, $\nabla_n \theta$, is related to the lateral gradient in the intersecting potential-density surface, $\nabla_\sigma \theta$, by the simple expression (McDougall, 1987b)

$$\boxed{\nabla_\sigma\theta = \mu\nabla_n\theta,} \qquad \text{where} \qquad \boxed{\mu = c\left[R_\rho - 1\right]/\left[R_\rho - c\right],} \tag{23}$$

c is defined by $c = \left[\alpha/\beta\right]\left[\tilde\alpha/\tilde\beta\right]^{-1}$ and R_ρ is the density ratio $\alpha\theta_z / \beta S_z$. The same multiplying factor, μ, applies to the temporal derivatives of potential temperature in the two reference frames. In order to find the relationship between the lateral mixing terms in the two different reference frames in Eq. (22), the following relationship between the lateral differential operators is used (McDougall and Jackett, 1988)

$$\nabla_\sigma = \nabla_n + \left[\nabla_\sigma\mathcal{R} - \nabla_n\mathcal{N}\right]\frac{\partial}{\partial z}\Big|_{x,y}, \tag{24}$$

where $\mathcal{R}[x,y]$ and $\mathcal{N}[x,y]$ are the heights of a particular potential-density surface and the intersecting neutral surface respectively, so that $\nabla_\sigma\mathcal{R} = \left[\mathcal{R}_x,\mathcal{R}_y\right]$ and $\nabla_n\mathcal{N} = \left[\mathcal{N}_x,\mathcal{N}_y\right]$. Applying the differential operator, Eq. (24), to $\nabla_\sigma\theta$ ($= \mu\nabla_n\theta$) we find that

$$\nabla_\sigma^2\theta = \mu\nabla_n^2\theta + \nabla_n\mu\cdot\nabla_n\theta + \left[\nabla_\sigma\mathcal{R} - \nabla_n\mathcal{N}\right]\cdot\left(\nabla_\sigma\theta\right)_z, \tag{25}$$

and the potential temperature conservation equation can be rewritten in the form

$$\boxed{\begin{aligned}
\theta_t\big|_\sigma + \mathbf{V}^L\cdot\nabla_\sigma\theta + w^d\theta_z &= \tfrac{1}{h^\sigma}\nabla_\sigma\cdot\left(h^\sigma K\nabla_\sigma\theta\right) + \left[D\theta_z\right]_z \\
&\quad - \left[\mu - 1\right]\tfrac{1}{h}\nabla_n\cdot\left(hK\nabla_n\theta\right) - K\nabla_n\mu\cdot\nabla_n\theta \\
&\quad - K\left(\left[\mu^2 - \mu\right]\theta_z^{-1}\nabla_n\theta\cdot\nabla_n\theta\right)_z + \mu\nabla_n\theta\cdot\left(\nabla_n K - \nabla_\sigma K\right),
\end{aligned}} \tag{26}$$

where the following geometrical relationships between the slopes of potential-density surfaces and neutral surfaces have been used (McDougall, 1988),

$$\left[\nabla_\sigma\mathcal{R} - \nabla_n\mathcal{N}\right] = \left[\mu - 1\right]\nabla_n\theta/\theta_z, \tag{27}$$

$$\left[\nabla_\sigma\mathcal{R} - \nabla_n\mathcal{N}\right]_z = \tfrac{1}{h^\sigma}\nabla_\sigma h^\sigma - \tfrac{1}{h}\nabla_n h. \tag{28}$$

The usual conservation equation of potential temperature in a potential density framework involves just the terms on the first line of Eq. (26). The additional terms on the second and third lines arise because of the different lateral gradients of potential temperature in the two coordinate frames and because of the different slopes of potential-density surfaces and neutral surfaces. As an example of the importance of the first term on the second line, consider the use of potential-density surfaces down to a depth of 2000 m in the North Atlantic, as in the inversion of Olbers et al (1985). At 1500 m in the North Atlantic, μ is generally greater than 1.5 so this term, $-\left[\mu - 1\right]\tfrac{1}{h}\nabla_n\cdot\left(hK\nabla_n\theta\right)$, represents a correction of 50% of the correct lateral mixing term that appears on the right of this equation (see Eq. (22)). In addition, the next term, $-K\nabla_n\mu\cdot\nabla_n\theta$, is of similar magnitude at this depth in frontal regions of the North Atlantic.

The third line of Eq. (26) contains the term $-K\mu_z\left[2\mu - 1\right]\theta_z^{-1}\nabla_n\theta\cdot\nabla_n\theta$, which does not go to zero as μ tends to 1; that is, as the in-situ pressure tends to the reference pressure. Neither does the $-K\nabla_n\mu\cdot\nabla_n\theta$ term go to zero as p tends to p_r. These terms arise because while the two types of surface are tangent where μ is 1, they do not have the same curvature in space. Even though Hogg's (1987) study used σ_1 surfaces rather than σ_θ surfaces so that μ was close to unity, the $-K\mu_z\left[2\mu - 1\right]\theta_z^{-1}\nabla_n\theta\cdot\nabla_n\theta$ term is estimated to contribute 10^{-9} K s^{-1} to the rate of change of potential temperature in the southern part of his western box; a magnitude that is as large as that of any of his mixing or advection terms. In the Antarctic Circumpolar Current $-K\nabla_n\mu\cdot\nabla_n\theta$ is as large as any other term in (26) even if $p_r = p$, due to the pressure dependence of c through the term $-K\frac{\partial\mu}{\partial c}\frac{1}{\tilde\alpha}T_b\nabla_n\theta\cdot\nabla_n p$.

When the diapycnal velocity is estimated using just the first line of Eq. (20), the constraint that the potential temperature conservation equation places on the temporal and epipycnal changes of θ, $\theta_t|_\sigma + \mathbf{V}^L \cdot \nabla_\sigma \theta$, is not due to the (correct) mixing terms that would result from inserting the full expression Eq. (20) for w^d into the correct conservation equation for θ, (the top line of Eq. (22) or all of Eq. (26)), but has additional terms due to the errors made in estimating the diapycnal velocity. Using Eq. (20) and Eq. (26), it can be shown that

$$
\begin{aligned}
\theta_t|_\sigma + \mathbf{V}^L \cdot \nabla_\sigma \theta \;=\;& \tfrac{1}{h^\sigma} \nabla_\sigma \cdot \left(h^\sigma K \nabla_\sigma \theta \right) + \left[D\theta_z \right]_z - \theta_z \left[\tilde{\alpha}\theta_z - \tilde{\beta} S_z \right]^{-1} \left[D \left(\tilde{\alpha}\theta_z - \tilde{\beta} S_z \right) \right]_z \\
&+ \tfrac{\beta}{\tilde{\beta}} \mu g N^{-2} D \tfrac{\partial \tilde{\alpha}}{\partial \theta} \theta_z^3 \\
&- K \nabla_n \mu \cdot \nabla_n \theta - K \left(\left[\mu^2 - \mu \right] \theta_z^{-1} \nabla_n \theta \cdot \nabla_n \theta \right)_z + \mu \nabla_n \theta \cdot \left(\nabla_n K - \nabla_\sigma K \right) \\
&+ \mu K g N^{-2} \theta_z \left\{ C_b \nabla_n \theta \cdot \nabla_n \theta + T_b \nabla_n \theta \cdot \nabla_n p \right\}.
\end{aligned}
\tag{29}
$$

The top line of the right-hand side of this equation represents the way in which the mixing processes parameterized by D and K affect the temporal and epipycnal changes of potential temperature in such a truncated model, while the additional terms are corrections that result partially from the fact that θ has been mixed along potential-density surfaces rather than along neutral surfaces (the many error terms in Eq. (26)) and partially due to the inaccurate estimation of the diapycnal velocity from just the first term in Eq. (20), that is, as $\left[\tilde{\alpha}\theta_z - \tilde{\beta} S_z \right]^{-1} \left[D(\tilde{\alpha}\theta_z - \tilde{\beta} S_z) \right]_z$ rather than using the full Eq. (20). Note that the divergence of the epineutral flux of potential temperature terms that appear in both Eq. (20) and Eq. (26) have cancelled and do not appear in Eq. (29). The $\beta\tilde{\beta}^{-1}\mu g N^{-2} D \tfrac{\partial \tilde{\alpha}}{\partial \theta} \theta_z^3$ term in Eq. (29) is important in the upper ocean, while thermobaricity and cabbeling tend to be larger at thermoclinic fronts deeper in the water column, and the other terms involving the lateral diffusivity, K, have been illustrated following Eq. (26). The discussion following Eq. (13) above indicates how serious the omission of thermobaricity and cabbeling is in the water-mass conversion equation, Eq. (11) or Eq. (29), at a thermoclinic front such as the Antarctic Circumpolar Current (cf Olbers and Wenzel, 1989).

This section has shown that even though potential temperature, θ, is a conservative variable, the use of a potential density rather than a neutral surface reference frame for the lateral mixing process results in many additional terms in the conservation equation (see Eq. (26)). None of these terms have previously been included in inverse models. Two of these terms, $- K \nabla_n \mu \cdot \nabla_n \theta$, and $- K\mu_z [2\mu - 1] \theta_z^{-1} \nabla_n \theta \cdot \nabla_n \theta$ remain even when the reference pressure of the potential density is equal to the in-situ pressure. We have also seen how a mistaken estimate of the diapycnal velocity feeds through into the tracer conservation statements so that these equations represent an incorrect balance between epipycnal advection (LHS) and mixing (RHS). This leads to an error in the estimated lateral flow field. A similar misestimate of the lateral velocity field occurs in the linear vorticity equation through the vortex stretching term, part of which is due to the difference of the diapycnal velocity through neighboring potential-density surfaces.

The ρ_θ "Conservation" Equation as a Linear Combination of the θ and S Equations

Rather than carrying a conservation equation for potential density in an inverse model, one can instead carry conservation equations for both potential temperature, θ, and salinity, S. The linear combination of these equations using the multiplying coefficients, $\tilde{\alpha}$ and $\tilde{\beta}$ is the potential density equation. It would actually be desirable to replace either the θ or the S equation with this linear combination of the S and θ equations because it is independent of any errors in the lateral velocity vector and so yields a more direct link (better signal to noise) between the mixing processes and the consequent diapycnal

advection (see the discussion around Eq. (41) below). Another real advantage of approaching the potential density equation by using the θ and S equations is that one does not leave out the nonlinear term due to vertical mixing, $D\frac{\partial\tilde\alpha}{\partial\theta}\theta_z^2$ that is commonly omitted from Eq. (20). Also, the nonlinear terms due to lateral mixing are smaller (at least when at the reference pressure). To see this we need to first derive the conservation equation for salinity that is analogous to Eq. (26) for potential temperature. This is done by applying the differential operator, Eq. (24), to $\nabla_\sigma S = \frac{\mu}{c}\nabla_n S$, obtaining

$$
S_t\big|_\sigma + \mathbf{V}^L\cdot\nabla_\sigma S + w^d S_z = \frac{1}{h^\sigma}\nabla_\sigma\cdot\left(h^\sigma K\nabla_\sigma S\right) + [DS_z]_z
$$
$$
- \left[\frac{\mu}{c}-1\right]\frac{1}{h}\nabla_n\cdot\left(hK\nabla_n S\right) - K\nabla_n\!\left(\frac{\mu}{c}\right)\cdot\nabla_n S \tag{30}
$$
$$
- K\left(\frac{\tilde\alpha}{\tilde\beta}\left[\mu^2-\mu\right]\theta_z^{-1}\nabla_n\theta\cdot\nabla_n\theta\right)_z + \frac{\mu}{c}\nabla_n S\cdot\left(\nabla_n K-\nabla_\sigma K\right).
$$

Multiplying this equation by $\tilde\beta$ and subtracting $\tilde\alpha$ times Eq. (26) we find

$$
\boxed{
\begin{aligned}
w^d\left[\frac{1}{\rho_\theta}\frac{\partial\rho_\theta}{\partial z}\right] &= \frac{\tilde\beta}{h^\sigma}\nabla_\sigma\cdot\left(h^\sigma K\nabla_\sigma S\right) - \frac{\tilde\alpha}{h^\sigma}\nabla_\sigma\cdot\left(h^\sigma K\nabla_\sigma\theta\right) + \tilde\beta[DS_z]_z - \tilde\alpha[D\theta_z]_z \\
&\quad + \tilde\alpha(c-1)\frac{1}{h}\nabla_n\cdot\left(hK\nabla_n\theta\right) + \tilde\alpha\frac{\mu}{c}K\nabla_n c\cdot\nabla_n\theta \\
&\quad - K\frac{\partial\tilde\alpha}{\partial\theta}\left[\mu^2-\mu\right]\nabla_n\theta\cdot\nabla_n\theta - \frac{\tilde\beta}{\tilde\beta}\left[\frac{\mu}{c}-1\right]K\{C_b\nabla_n\theta\cdot\nabla_n\theta + T_b\nabla_n\theta\cdot\nabla_n p\}.
\end{aligned}
}
\tag{31}
$$

The terms in the second and third lines of this equation are due to having assumed that the lateral diffusion occurs along potential-density surfaces rather than along neutral surfaces. In contrast to the ρ_θ equation, Eq. (20), there are no correction terms in Eq. (31) due to vertical mixing. If the reference pressure is equal to the in-situ pressure, the only error term in Eq. (31) comes from the $\tilde\alpha\frac{\mu}{c}K\nabla_n c\cdot\nabla_n\theta$ term and is $KT_b\nabla_n\theta\cdot\nabla_n p$, that is, thermobaricity, whereas in Eq. (20) there is also the cabbeling term, $KC_b\nabla_n\theta\cdot\nabla_n\theta$, in this situation. Of course, if the lateral mixing had been parameterized as being epineutral there would be no correction terms in Eq. (31). It is concluded that carrying both the θ and S conservation statements, even in their truncated forms (i.e. the top lines of Eq. (24) and Eq. (30)), is more desirable than using the top line of the conservation equation for potential density, Eq. (20). As noted above, signal-to-noise considerations mean that it is preferable to carry either the S or the θ equations, and the linear combination $\tilde\beta$ times Eq. (30) minus $\tilde\alpha$ times Eq. (26).

The Spiciness "Conservation" Equation

Olbers et al., (1985) and Olbers and Wenzel (1989) chose to use Veronicity, τ^V, instead of salinity or potential temperature in their beta-spiral inversions of the North Atlantic and Southern Ocean. Here it is shown that just as potential density is not a conservative variable, neither is Veronicity, and the non-conservative nature of Veronicity has introduced significant errors in these inversions. The non-conservative nature of Veronicity can be noted from the fact that contours of constant τ^V are not straight lines on the S-θ diagram (see Figure 7) so that mixing between two water parcels that have the same Veronicity will produce a parcel with a different value of Veronicity. The curvature of the τ^V isolines on this diagram is similar to that of the σ_θ isolines, so nonlinear effects of a similar magnitude may be expected. For a given (and arbitrary) value of the relative scaling of the two axes, Veronicity has the property that its isolines are orthogonal to lines of constant potential density on the S-θ diagram. Jackett and McDougall (1985) have proposed a different definition of orthogonality that does not depend on the scaling of the axes of the S-θ diagram, and here a conservation equation is developed for their variable, spiciness, τ.
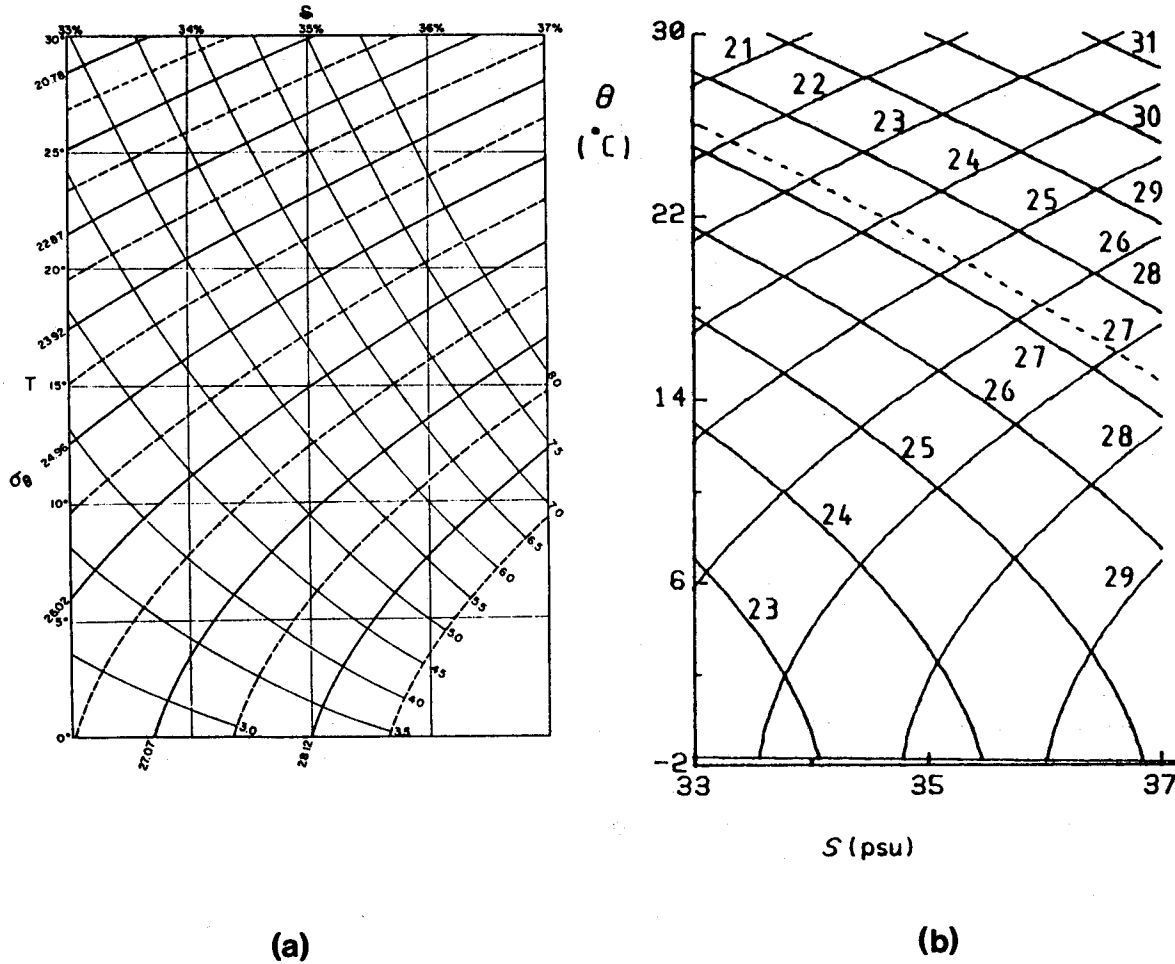
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(a) **(b)**

Fig. 7. Contour plots of, (a) Veronicity, τ^V and (b), spiciness, τ, on the S-θ diagram. The other lines shown are of potential density referenced to the sea-surface.

To a good approximation, variations of spiciness are related to those of potential temperature and salinity by

$$d\tau = \tilde{\beta}dS + \tilde{\alpha}d\theta. \tag{32}$$

For this total differential to define a path-independent function, τ, one needs $\partial\tilde{\beta}/\partial\theta = \partial\tilde{\alpha}/\partial S$ which is not true of the real equation of state of seawater. One can imagine an equation of state that did satisfy this constraint (by for example, having $\partial^2\rho/\partial\theta\partial S = 0$), and then a linear combination of the conservation statements of potential temperature and salinity can be taken to arrive at the following conservation equation for τ

$$\tau_t\big|_z + \mathbf{V}^L \cdot \nabla_2 \tau + w\tau_z = \tau_t\big|_\sigma + \mathbf{V}^L \cdot \nabla_\sigma \tau + w^d\tau_z = h^{-1}\nabla_n \cdot (hK\nabla_n\tau) + [D\tau_z]_z \\ - K\tfrac{\partial\tilde{\alpha}}{\partial\theta}\nabla_n\theta \cdot \nabla_n\theta - D\tfrac{\partial\tilde{\alpha}}{\partial\theta}\theta_z^2 . \tag{33}$$

Just as in Eq. (20) above where the nonlinear mixing terms in the potential density conservation equation were found to be large in the thermoclines of many ocean basins, so too in these regions will the above terms, $-D\frac{\partial\tilde\alpha}{\partial\theta}\theta_z^2$ and $-K\frac{\partial\tilde\alpha}{\partial\theta}\nabla_n\theta\cdot\nabla_n\theta$ be important in Eq. (33).

In practice, the lateral mixing of τ in previous inverse models has been along potential-density surfaces, rather than along neutral surfaces, and the differences can be found by applying the differential operator, Eq. (24) to $\nabla_\sigma\tau$ $(=2\tilde\alpha\nabla_\sigma\theta)$ so that Eq. (33) can be written as

$$
\begin{aligned}
\tau_t\big|_\sigma + \mathbf{V}^L\cdot\nabla_\sigma\tau + w^d\tau_z &= \tfrac{1}{h^\sigma}\nabla_\sigma\cdot\left(h^\sigma K\nabla_\sigma\tau\right) + [D\tau_z]_z \\
&\quad - D\frac{\partial\tilde\alpha}{\partial\theta}\theta_z^2 \\
&\quad - \tilde\alpha[2(\mu-1)-(c-1)]\tfrac{1}{h}\nabla_n\cdot\left(hK\nabla_n\theta\right) - 2\tilde\alpha K\nabla_n\mu\cdot\nabla_n\theta \\
&\quad - 2\tilde\alpha K\left(\left[\mu^2-\mu\right]\theta_z^{-1}\nabla_n\theta\cdot\nabla_n\theta\right)_z + 2\tilde\alpha\mu\nabla_n\theta\cdot\left(\nabla_n K-\nabla_\sigma K\right) \\
&\quad - 2\mu^2\frac{\partial\tilde\alpha}{\partial\theta}K\nabla_n\theta\cdot\nabla_n\theta + \frac{\tilde\beta}{\beta}K\left\{C_b\nabla_n\theta\cdot\nabla_n\theta + T_b\nabla_n\theta\cdot\nabla_n p\right\}.
\end{aligned}
$$

(34)

The mixing terms that were included by Olbers et al (1985) and Olbers and Wenzel (1989) were the first two, on the top line of this equation; all the other terms are due to the nonconservative nature of both potential density and spiciness. There are now five terms that do not disappear when p_r is equal to p (i.e. when $c=\mu=1$). These are $-2\tilde\alpha K\nabla_n\mu\cdot\nabla_n\theta$, $-2\tilde\alpha K\mu_z[2\mu-1]\theta_z^{-1}\nabla_n\theta\cdot\nabla_n\theta$, and the three terms on the last line of the equation. Since $C_b\approx\frac{\partial\tilde\alpha}{\partial\theta}$, cabbeling will effectively appear as $-\left[2\mu^2-1\right]KC_b\nabla_n\theta\cdot\nabla_n\theta$. All of these terms have been discussed above and they were found to each be large in different parts of the ocean, notably at thermoclinic fronts where either $\nabla_n\theta\cdot\nabla_n\theta$ or $\nabla_n\theta\cdot\nabla_n p$ is large.

Since the diapycnal velocity is commonly estimated with a truncated conservation equation, the effective constraint that the spiciness conservation equation would maintain between the epipycnal advection of τ and the mixing processes is illustrated better by the following τ conservation equation,

$$
\begin{aligned}
\tau_t\big|_\sigma + \mathbf{V}^L\cdot\nabla_\sigma\tau &= \tfrac{1}{h^\sigma}\nabla_\sigma\cdot\left(h^\sigma K\nabla_\sigma\tau\right) + [D\tau_z]_z - \tau_z\left[\tilde\alpha\theta_z - \tilde\beta S_z\right]^{-1}\left[D\left(\tilde\alpha\theta_z - \tilde\beta S_z\right)\right]_z \\
&\quad + \frac{2\mu}{(R_\rho-1)}D\frac{\partial\tilde\alpha}{\partial\theta}\theta_z^2 - 2\tilde\alpha K\nabla_n\mu\cdot\nabla_n\theta \\
&\quad - 2\tilde\alpha K\left(\left[\mu^2-\mu\right]\theta_z^{-1}\nabla_n\theta\cdot\nabla_n\theta\right)_z + 2\tilde\alpha\mu\nabla_n\theta\cdot\left(\nabla_n K-\nabla_\sigma K\right) \\
&\quad - 2\mu^2\frac{\partial\tilde\alpha}{\partial\theta}K\nabla_n\theta\cdot\nabla_n\theta + \frac{2R_\rho}{(R_\rho-c)}\frac{\tilde\beta}{\beta}K\left\{C_b\nabla_n\theta\cdot\nabla_n\theta + T_b\nabla_n\theta\cdot\nabla_n p\right\}
\end{aligned}
$$

(35)

Again, only the top line was included in the previous inversions. Notice that the $h^{-1}\nabla_n\cdot\left(hK\nabla_n\theta\right)$ term has again cancelled from this equation. The nonlinear mixing term due to vertical diffusion has changed sign between Eq. (34) and Eq. (35) and has increased in magnitude by the factor $2\mu(R_\rho-1)^{-1}=2c(R_\rho-c)^{-1}$. At 1500 m in the North Atlantic this factor is about 3. Similarly, cabbeling and thermobaricity has a different multiplying factor, $2R_\rho(R_\rho-c)^{-1}$, and this is about 5 in the North Atlantic at 1500 m. These multiplying factors increase the magnitude of these nonlinear terms which were already as large as the physically correct terms in the conservation statements that have been considered above. It is the compounding of the errors from the potential density conservation statement, and the assumption that spiciness is a conservative variable that has led to these large multiplying factors.

The simple lesson for us to learn here is that just as potential density is not a conservative variable, neither is Veronicity, τ^V, or spiciness, τ, and so conservation statements for these variables must take this into account. What many will find surprising is the magnitude of the many nonconservative terms in relation to the traditional terms in the conservation statements, and also the fact that the difference between epipycnal and epineutral mixing remains even when the potential density's reference pressure is equal to the in-situ pressure.

MIXING PRESCRIPTIONS IN BOX MODEL INVERSIONS: The Divergence Forms of Conservation Statements in Potential-Density Surfaces

The Nonconservative Production Terms in the Divergence Forms of the Conservation Equations

As far as the conservation equations are concerned, the distinguishing feature between β-spiral inversion methods and box-inverse methods is that the β-spiral methods use advective conservation statements while box-model methods use divergence (or flux) conservation statements. In addition, the β-spiral method is often used with data that have been laterally smoothed in some way, whereas the box models are generally used with unsmoothed data. The β-spiral method examines the balance of terms at a point while the box-inverse method is concerned with the balance of fluxes through the six faces of a box. The streamfunction method is a sub-set of the box-model approach that expresses the Eulerian lateral velocity vector in terms of a geostrophic streamfunction. Note that the Lagrangian lateral velocity vector does not satisfy the required relationship to be expressible as the derivative of a streamfunction. However, since inverse methods have not yet addressed this question of the difference between the Lagrangian and Eulerian mean flows, this aspect has not yet been an issue. Some models can be a little hard to classify as a box inversion or as a β-spiral inversion. For example, Hogg (1987) used a divergence form for the lateral gradient operator (using a streamfunction) but evaluated the vertical derivatives on a potential-density surface rather than between a pair of surfaces. In this way his model is like a β-spiral method in the vertical while being like a box model in the lateral directions.

In neutral surface coordinates, the divergence form of the general conservation statement for a conservative tracer, C, is given by Eq. (7), and when integrated over the sides of a box of volume V and lateral area A, is

$$V\frac{\partial(hC)|_n}{\partial t} + \left[L_{NS}hu^LC\right]_W^E + \left[L_{EW}hv^LC\right]_S^N + [AeC]_\ell^u = \left[L_{NS}hKC_x\right]_W^E + \left[L_{EW}hKC_y\right]_S^N + [ADC_z]_\ell^u, \qquad (36)$$

where L_{EW} and L_{NS} are the horizontal length scales of a face of the box in the east-west and north-south directions respectively, and the lateral derivatives of C are evaluated in neutral surfaces. Here u^L and v^L are the x and y components of the Lagrangian-mean velocity vector

To date, box models have used potential-density surfaces as their upper and lower boundaries rather than neutral surfaces, and here we examine the errors so introduced in the lateral transport of properties. To do so, divergence forms of conservation statements are needed in the potential-density surface coordinate frame. These are obtained by noting that the continuity equation can be written with respect to potential-density surfaces as (cf Eq. (8)),

$$\frac{\partial h^\sigma}{\partial t} + \nabla_\sigma \cdot \left(h^\sigma \mathbf{V}^L\right) + \left[w^d\right]_{\sigma_\ell}^{\sigma_u} = 0, \qquad (37)$$

and taking C times this equation plus h^σ times the advective form of the C conservation equation, (Eq. (9) with the advection terms on the left-hand side written with respect to potential-density surfaces), one finds

$$
\frac{\partial(h^\sigma C)|_\sigma}{\partial t} + \nabla_\sigma \cdot \left(h^\sigma \mathbf{V}^L C\right) + \left[w^d C\right]_{\sigma_\ell}^{\sigma_u} = \nabla_\sigma \cdot \left(h^\sigma K \nabla_\sigma C\right) + \left[DC_z\right]_{\sigma_\ell}^{\sigma_u}
$$
$$
+ h^\sigma \left\{ \frac{1}{h} \nabla_n \cdot \left(hK\nabla_n C\right) - \frac{1}{h^\sigma} \nabla_\sigma \cdot \left(h^\sigma K\nabla_\sigma C\right) \right\}.
$$

(38)

The extra terms due to the different coordinate frames appear in the second line of this equation and exactly correspond to the extra terms in the advective forms of the equation, for example, in Eq. (22) and Eq. (26) in the case of potential temperature, and in Eq. (30) for salinity. The extra terms in the conservation equations for potential density (Eqs. 20 or 31) and spiciness (Eq. 34) due to the non-conservative nature of these variables also carry directly across to the divergence forms. We conclude that all the extra terms due to the non conservative nature of potential density and spiciness that have been found in the previous section of this paper for the advective forms apply equally to the divergence forms of these conservation equations. For this reason we do not need to repeat the error analysis for these extra terms. Suffice it to say that these terms that have been missing from previous inverse studies are often as large as the straightforward mixing terms in various parts of the model domains.

The Impact of Uncertainty in the Continuity Equation on the Tracer Equations

The single most important aspect of many past box-inverse models that has precluded them from being influenced by and detecting oceanic mixing processes is the overwhelming effect of errors in the continuity equation (the incompressibility equation) on the tracer conservation equations. In order to demonstrate this, the left-hand side of Eq. (38) is rewritten as the linear combination of Eq. (9) and Eq. (37) as

$$
C \left\{ \frac{\partial h^\sigma}{\partial t} + \nabla_\sigma \cdot \left(h^\sigma \mathbf{V}^L\right) + \left[w^d\right]_{\sigma_\ell}^{\sigma_u} \right\}
$$
$$
+ h^\sigma \left\{ C_t |_\sigma + \mathbf{V}^L \cdot \nabla_\sigma C + w^d C_z \right\} = \frac{h^\sigma}{h} \nabla_n \cdot \left(hK\nabla_n C\right) + \left[DC_z\right]_{\sigma_\ell}^{\sigma_u}.
$$

(39)

The physical constraint that we wish to glean from this equation is the connection between the mixing of tracer C (the right-hand side) and the Lagrangian advection of C (the second curly bracket on the left). The first curly bracket is included so as to be able to write the left-hand side of Eq. (38) in a divergence form. When integrated over the sides of a box of a typical oceanic box model, the uncertainty in the continuity equation (first bracket in Eq. (39)) is typically 1 Sv (10^6 m^3 s^{-1}) and this is so large as to swamp any signal that represents the physically interesting "advective-diffusive" balance of C-stuff. As an example, consider the conservation of salinity in box 11 of Wunsch and Minster (1982). From their Figures 1c and 3a the epipycnal and vertical advection of salt amount to only 1% of the mean salinity (35 psu) times the volume flux imbalance into the box. That is, the solution has the left-hand sides of our Eq. (38) and Eq. (39) being dominated, by a factor of a hundred, by the error in the continuity equation. The consequence of this is that the signature of mixing processes and the balancing advection of C are simply small terms in the equation so that even when the mixing and advection are modelled correctly, the variance of the salt equation can only decrease by two percent. Effectively, the salt conservation equation becomes simply another continuity equation and consequently (i) the rank of the system of equations suffers because of the nearly collinear nature of the equations, (ii) the information that is contained in the salinity contours in three-dimensional space is not

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imposed as a constraint on the solution, and (iii) no information on the mixing processes can be obtained from the inversion.

The same comments apply to many other box-inverse papers including Wunsch (1984), Joyce Wunsch and Pierce (1986), and Wunsch, Hu and Grant (1983). In all of these papers, the balancing advective-diffusive terms in the salinity conservation equations were typically 1% of the residual error left in the salt conservation equation by the fact that the continuity equation was not satisfied identically. Similar comments apply to other conservation statements (e.g. potential temperature, dissolved oxygen or silicate) but the situation is worst for salinity simply because its mean value is quite large in relation to its variations in the ocean.

The Wunsch and Minster (1982) paper is especially interesting in this regard because it carried both epipycnal and diapycnal diffusivities, and surprisingly, the lateral diffusivities of the model were of order 1-10 $m^2 s^{-1}$, or a factor of between a hundred and a thousand less than what we believe for the ocean. One would think that any inconsistencies in a model's data or its equations would cause the magnitude of its parameters to increase so as to soak up some of the noise. Why then were the lateral diffusivities close to zero? I believe the answer is again related to the volume flux imbalances in the continuity equation. When using all the eigenvectors, in addition to satisfying the equations identically, the SVD solution procedure also minimizes the norm of the solution vector. When some of the eigenvectors are discarded (the ones with the smallest eigenvalues) the solution norm becomes even smaller and the equations are no longer satisfied exactly. The method then represents a tension between satisfying the equations while also having a small solution vector. This competition between minimizing the equation errors and the solution norm is more mathematically obvious in the ridge regression or tapered least squares procedure. Because the error in the salinity conservation statement is dominated by the error in the continuity equation for each box, a respectable value of the lateral diffusivity (of order 1000 $m^2 s^{-1}$) would only reduce the error variance in the salinity equation by 2% so the solution procedure chooses instead to have a small solution vector, and in particular, to have small lateral diffusivities. In this situation, the solution will be sensitive to the column weighting, and presumably a different choice of column weights could also have yielded very small vertical diffusivities as well. This explanation of the unrealistically small values of the lateral diffusivity found by Wunsch and Minster (1982) is due to the combination of (i) the signature of mixing and advection of salinity being well below the allowable error in the salinity conservation equation, combined with (ii), a solution procedure that prefers small values of the diffusivities.

The inverse model of Wunsch, Hu and Grant (1983) is, I believe, another example of a study that has been unwittingly plagued by the salt equation being effectively another continuity equation. The paper concludes that there is no need for vertical mixing in their model, even though the downward diapycnal velocities were of order 10^{-7} m s^{-1} (see their Figure 11a). The necessity for diapycnal advection but not for vertical diffusion was argued because the imbalances in the tracer conservation equations (notably salinity) were almost completely explained (a posteriori) by interfacial advection with little apparent need for vertical diffusion. However 99% of the interfacial advection that was added into the salt conservation equation went into correcting the first curly bracket in Eq. (39) by adding the vertical part of the volume flux divergence, leaving a comparatively small salt residual (called ε_2 by the authors) that resembles the physically interesting Lagrangian advection of salinity. From Figure 5b, one finds a value of $gN^{-2}\{\alpha\theta_{zz} - \beta S_{zz}\}$ of about -1×10^{-3} m^{-1} in the region of the South Pacific between the two Scorpio sections at a depth of about 1000 m. At this depth Wunsch et al (1983) find a (downward) diapycnal velocity of about -0.7×10^{-7} m^2 s^{-1}, which is consistent with a vertical diffusivity of 0.7×10^{-4} m^2 s^{-1} acting on the above value of $gN^{-2}\{\alpha\theta_{zz} - \beta S_{zz}\}$. However, deeper in the water column at 1400 m in this region, McDougall and You's (1990) figure 5 shows that $gN^{-2}\{\alpha\theta_{zz} - \beta S_{zz}\}$ is positive so that a positive vertical diffusivity would not be consistent with the downward diapycnal

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velocity found by Wunsch et al (1983) at this depth. Since the salinity equations in Wunsch et al (1983) were functionally linearly dependent with the continuity equations, the reference level velocity vectors that came out of the inversion were effectively not influenced by the advective-diffusive salt balances. Only by allowing this advection of salinity to emerge as signal in a conservation equation, rather than being hidden in the last few percent of an equation's noise, and at the same time balancing this advection of salt with a parameterized mixing term, will we be able to say whether mixing processes are required by the data.

Is there a procedure by which mixing processes can be made to stand out above the noise in tracer equations in box inverse models? The answer is yes, and the key is to minimize the influence of the first curly bracket in Eq. (39) by writing a conservation equation, not for the tracer itself, but for the tracer anomaly, C', from some fixed value, $\overline{C}$. The reason why this procedure works is that the advective form of the conservation statement applies equally well to C' as to C, since it involves only various derivatives of the tracer. Hence in forming Eq. (38) and Eq. (39) we can multiply Eq. (37) by the primed tracer variable instead of by C, and Eq. (38) and Eq. (39) become exactly the same equations with C replaced by C'. This procedure has in fact been used to good effect by several researchers, including Hogg (1987), and Lee and Veronis (1991). This procedure is easiest to justify if the same mean tracer value is subtracted from every box, but in the last subsection of this paper it is argued that it may be beneficial to subtract a different mean tracer value for each box.

Memery and Wunsch (1990) were able to balance the volume fluxes into and out of their boxes to within about 0.02 Sv without having an excessively large solution norm. This was most likely due to the fact that they used the Levitus (1982) data set that is that is temporally and horizontally averaged and so does not contain the complicating features such as internal waves and mesoscale eddies that are found in real cruise data. Presumably the salinity conservation equations were not unduly correlated with the continuity equations in the Memery and Wunsch (1990) study, and that if vertical diffusivities were added to the model, the inversion would have found them to be necessary. Conservation equations for potential temperature should also be added to the system in order to provide added information on the mixing processes (see the section below). Schlitzer (1987, 1988) also used the Levitus data set and was able to specify the volume flux imbalances to as little as 0.001 Sv, and he resolved both diapycnal advection and diapycnal diffusivities. This lends support to the present claim that the errors in the continuity equation are what have been precluding most box-inverse models from resolving mixing processes.

Many box-inverse models of the Atlantic and Indian Oceans (e.g. Wunsch and Grant (1982), Rintoul and Wunsch (1991) and Fu (1986)), have found that salinity conservation did not add any information to their inversions. Since these oceans contain substantial variations of salinity along neutral surfaces, some of which information has previously been used to determine flow directions of water types by the Wüstian tongue method, it would be quite incredible if the salinity field contained no information on mixing and advection: the challenge is to extract this information.

The Need for Vertical Diffusion as well as Interfacial Advection

It has been quite common in box inversions to include a diapycnal flux of volume but not to have any diffusive flux of tracers such as potential temperature or salinity. Since diapycnal advection occurs only in response to mixing processes (see Eq. (20)), it is clearly dangerous to include one part of the effect of mixing processes (the advection of tracer) without at the same time carrying the other part (the diffusion of tracer). For example, in the solutions for the North Atlantic circulation presented by Wunsch and Grant (1982) and by Wunsch (1984), many of the isopycnal interfaces had diapycnal

velocities of more than 10×10^{-7} m s^{-1} passing through them. That is, the diapycnal velocity was more than ten times the canonical value of the upwelling velocity in the deep ocean. On the face of it, this implies that the vertical diffusivity must be about ten times its canonical value, or about 10×10^{-4} m^2 s^{-1} in order to fuel this seemingly large (but probably not impossibly large) diapycnal flow. Wunsch (1984) has obviously wrestled with this aspect of his model, as the discussion around his equation (18) shows (and the corresponding discussion in Wunsch, Hu and Grant (1983)). There it was proposed to regard the model's interfacial velocity as a combination of a true interfacial velocity and a diffusive flux of density. But a scale analysis shows that the eddy diffusion of density is a very small fraction (less than 0.3%) of the advection of density (i.e. $D \partial \rho_\theta / \partial z \ll \rho_\theta w^d$). We are obviously never going to be able to account for terms in conservation equations to this accuracy.

Many of the box-inversion papers write conservation equations for "density" or "mass", however, in the divergence form, a conservation equation for "density" is almost the same as a conservation statement for volume transport. This is apparent from a scale analysis of the two curly brackets on the left of Eq. (39), using the in-situ density (or indeed any other kind of density) for C. Since the imbalance in the volume transport in and out of a box is allowed to be say 0.3 Sv, the second curly bracket in Eq. (39) (the advection of density) amounts to only 0.3% of the first bracket, hence the "density" conservation equation is equivalent to the incompressibility condition. There is an extra pedantic twist to this issue in that McDougall and Garrett (1991) have shown that while the divergence of the instantaneous velocity vector, $\nabla \cdot \mathbf{u}$, is directly related to the instantaneous Lagrangian change of density, the divergence of the mean velocity vector, $\nabla \cdot \bar{\mathbf{u}}$, is unaffected by the divergence of the turbulent fluxes of heat and salt (even though the molecular flux divergences of heat and salt do contribute to $\nabla \cdot \bar{\mathbf{u}}$!). In this way, $\nabla \cdot \bar{\mathbf{u}} = 0$ is actually a better embodiment of the continuity equation in a turbulent ocean than is $\nabla \cdot (\bar{\rho} \, \bar{\mathbf{u}}) = 0$, although, as we have just shown, the differences are of order 0.3% and so are quite negligible.

The separate roles of dianeutral advection and dianeutral mixing in causing water-mass conversion have been illustrated by maps of the relevant vertical derivatives of hydrographic variables on some neutral surfaces from each of the world's oceans in McDougall and You (1990). Maps of the dianeutral advection caused by small-scale mixing, $gN^{-2} \{ \alpha \theta_{zz} - \beta S_{zz} \}$, and the rate at which vertical mixing changes the potential temperature on a neutral surface, $gN^{-2} \theta_z^3 \beta \frac{d^2 S}{d\theta^2}$, (both terms are normalized by the vertical diffusivity, D), are plotted in Figures 4-6. These maps show well-defined patterns in the magnitude and sign of these terms and there are many regions where the terms have the same sign. In these locations the rate of water-mass conversion achieved by vertical mixing is of opposite sign to that caused by the dianeutral advection alone. An inverse model that carries only vertical advection in the salinity or potential temperature conservation equation will tend to force the dianeutral advection to be the opposite sign to reality. This is explained in more detail by McDougall and You (1990) and will not be repeated here.

I wish to emphasize that there is no problem at all with the neglect of eddy diffusion terms from the continuity equation (called by Wunsch the "mass" or the "density" conservation equation), rather it is the omission of vertical diffusive terms from the tracer conservation equations that causes concern. In particular, if an inverse model carries just thermal wind equations and continuity equations, without considering any tracer conservation equations, then there can be no argument with the interpretation of the diapycnal velocities that one obtains from the model. One realizes that there must be some vertical mixing going on to cause this diapycnal flow, but since the diapycnal diffusivity does not appear in the two types of equations in one's model (thermal wind and incompressibility) the model is quite consistent without having to include the diapycnal diffusion. The problems referred to in the previous paragraph and described more fully in McDougall and You (1990) arise when a tracer or several tracers

are carried by the model. Then one has no choice but to include both interfacial diffusion and advection in order to construct a physically consistent model.

When is it Redundant to Carry both S and θ Conservation Equations?

One has a tendency to think that since the epineutral (and epipycnal) gradients of salinity and potential temperature are related, the conservation equations of S and θ must be linearly dependent. This is not the case, as can be readily appreciated by inspecting the form of Eq. (9). While the temporal and epineutral derivatives of S and θ are proportional (through the ratio α/β) the dianeutral advection terms are in the different ratio S_z/θ_z and the dianeutral diffusion terms are related by a third different ratio. It is only when the dianeutral advection is eliminated from the S and θ conservation statements to arrive at the form Eq. (11) that the S and θ equations are redundant. Another way in which a real redundancy can arise is if some kind of density conservation equation is used together with both the θ and S equations in the form of Eq. (9). Since density conservation equations (such as the "e" equation, Eq. (12)), are simply a linear combination of the S and θ equations, it is obvious how the linear dependance arises when all three equations are carried.

Wunsch and Minster (1982) carried a continuity equation and both S and θ equations and found that all three types of equations were effectively linearly dependent. As explained above, such linear dependence should not have been expected since their model carried both diapycnal advection and diapycnal diffusion. The reason for the near collinearly in their case would have been the dominance of both the S and θ equations by the same imbalances in the continuity equation:- both the S and θ equations were essentially repeated continuity equations with the mixing information buried in the noise. I believe that the simple procedure of subtracting a suitable mean salinity and a suitable mean potential temperature of each box before writing down the divergence forms of the conservation statements would have yielded very different results in their study: the rank of the model would have risen substantially, the lateral diffusivities would have been much larger, and quite possibly, the vertical diffusivities and diapycnal advection would have been better-determined.

Why use a neutral surface coordinate scheme rather than Cartesian coordinates?

The issue of the surfaces in which one assumes the lateral mixing to occur has been addressed earlier in this paper, and will not be repeated here. Rather, here some observations are offered on the advantages of casting the left-hand sides of the conservation statements in the neutral surface framework. These remarks will apply equally well to the advective and the divergence forms of the conservation statements and so apply to both the β-spiral and box inversions. Consider the steady-state conservation statement for say potential temperature, θ, in a region where the epineutral gradient of potential temperature is small in relation to the horizontal gradient, $\nabla_2\theta = \theta_x \mathbf{i} + \theta_y \mathbf{j}$, and where the neutral surface slopes significantly. The three-dimensional advection of θ is the same in both coordinate frames so that (from Eq. (9))

$$\left\{ \mathbf{V}^L \cdot [\nabla_2 C - \nabla_n C] + [w - e]C_z \right\} + \mathbf{V}^L \cdot \nabla_n C + eC_z = h^{-1}\nabla_n \cdot (hK\nabla_n C) + [DC_z]_z. \quad (40)$$

The terms in the curly brackets here sum to zero exactly, but if the neutral surface is significantly sloped, this cancellation can, and often does, represent the difference between two large numbers. In this situation, any uncertainty in the lateral velocity components will cause an unnecessarily large uncertainty in the left-hand side of this equation and so potentially upset the desired balance between advection (LHS) and diffusion (RHS) in Eq. (40). When the equations are weighted by their row-

norms, the equation error that is allowed in the inversion procedure will be unnecessarily large in the Cartesian formulation.

This is especially obvious in the linear combination of the S and θ conservation equations that is the 'e' equation, Eq. (12) (in loose terminology, this is the advective form of the 'density' conservation equation). In neutral surface coordinates, this represents a very direct relationship between the dianeutral advection, e, and mixing processes. Since the lateral velocity vector does not appear in this equation in the neutral surface framework, the inherent uncertainty in the inversion's lateral velocity vector can neither upset this balance nor can it contribute to the expected error of the equation. In this way the 'density' or 'e' equation is almost guaranteed to contain separate information to the other conservation statements that contain the lateral velocity vector. However, in the Cartesian framework this same equation does contain large balancing terms that do involve the lateral velocity vector, as in the curly bracket below,

$$\left\{ \mathbf{V}^L \cdot \left[\alpha\nabla_2\theta - \beta\nabla_2 S\right] + \left[w-e\right]\left(\alpha\theta_z - \beta S_z\right) \right\} + e\left(\alpha\theta_z - \beta S_z\right) =$$
$$\left[D_z\left(\alpha\theta_z - \beta S_z\right)\right]_z - K\left\{C_b\nabla_n\theta\cdot\nabla_n\theta + T_b\nabla_n\theta\cdot\nabla_n p\right\}. \tag{41}$$

The terms in the curly brackets on the left of this equation sum to exactly zero. The individual terms in this bracket are frequently much larger than the other term on the left, namely, $e\left(\alpha\theta_z - \beta S_z\right)$, as the magnitude of $[w - e]$ is frequently much larger than that of e. The same point can be made regarding the equation for the diapycnal velocity, w^d, in the potential density framework compared with the Cartesian framework in that Eq. (20) does not involve the lateral velocity components whereas in the Cartesian form, Eq. (21), it does contain the do-nothing combination of terms, $\left\{\mathbf{V}^L \cdot \nabla_2\rho_\theta + \left[w - w^d\right]\frac{\partial\rho_\theta}{\partial z}\right\}$. Another appealing feature of the e equation in the neutral surface framework is that it does not contain the lateral Laplacian of any property. Since the lateral Laplacian is a relatively noisy quantity to estimate from data, this feature of the e equation, Eq. (12), augments the absence of the lateral velocity vector to suggest that the equation is a relatively noise-free connection between dianeutral advection and (mainly vertical) diffusion.

The above discussion of the merits of performing inversions in neutral surface coordinates has been focused on the implications for determining the strength of mixing processes. But even in models without mixing the different slopes of various surfaces affects the reference level velocities and other outputs. For example, Schott and Zantopp (1979) showed that the β-spiral technique gave reference level velocities at 1000 m that differed by 5 mm s^{-1} depending on whether potential density or steric anomaly (specific volume anomaly) was conserved by the inversion. In a box model inversion of sections in the North Atlantic, Rintoul and Wunsch (1991) have compared their model which used interfaces that were a close approximation to neutral surfaces with a previous model that used surfaces that were a coarser approximation to neutral surfaces. They found that the differences between the surfaces caused the poleward flow of intermediate water to decrease by 2.4 Sv and the equatorward flow of deep water to be reduced by the same amount. The poleward heat flux changed by 0.1×10^{15} W.

Some recommendations for box inversions

The above issues for box inversions are all intimately linked because (i) the tracer (especially salinity) conservation statements have been dominated by noise from the "mass" conservation equation (really the incompressibility equation), (ii) diapycnal diffusion coefficients have not been resolvable from the models and hence (iii) it has been pointless to add a conservation equation for potential temperature

since this would also have been linearly dependent with the existing two sets of equations. It is to be hoped that the above recommendation of forming divergence conservation statements for (a) volume and (b) for the deviations of tracer concentrations from suitable average values, will cure all three problems simultaneously. This simple procedure should make the tracer conservation statements become linearly independent of the continuity equations, giving the advective-diffusive balance of say salinity a chance of constraining both diffusivity coefficients and the mean velocity field. This will also result in an increase in the rank of the system of equations. Conservation equations of potential temperature and of other tracers should also be included in the inversions so as to extract the further independent information on mixing processes that these equations contain.

The interfaces that separate the boxes should be neutral surfaces in order to avoid the many error terms in Eq. (26) and Eq. (30) that arise due to mixing laterally along potential-density surfaces rather than along neutral surfaces. The previous subsection also shows that the neutral surface framework should be superior from the signal-to-noise viewpoint. In particular, the direct relationship between dianeutral advection and mixing processes can be obtained by taking the linear combination of α times Eq. (36) with the anomaly of potential temperature as the tracer, minus β times Eq. (36) with the salinity anomaly as the tracer.

Previous box inverse models have carried continuity equations for each box (despite the different labels of these equations as "density" or "mass" conservation statements), whereas β-spiral methods do not enforce the continuity equation. Perhaps this is the key difference between the two methods. Box models should continue to carry the volume conservation equations for each box (in the form of Eq. (36) with $C = 1$), and it may be necessary to recognize that the Lagrangian velocity components that appear in this equation contain the Stokes drift (Eq. (15)) in addition to the Eulerian-mean velocity that is obtained from thermal wind.

On the choice of mean tracer value for each box

Consider forming the salinity anomaly for each box by subtracting a mean salinity (say 35 psu) from all the salinities in all the boxes of a box model. The maximum value of S' for any particular box may be say 1 psu so that the uncertainty in the salinity conservation equation due to the continuity imbalance is improved by a factor of 35. However, this may not be enough of an improvement to guarantee that the salinity conservation statement enforces an advective-diffusive salinity balance. In the examples quoted above, the advective-diffusive salt balance would improve from being 1% of the residual equation error to being 35%. If this proved to be not enough of an improvement, then one would need to use tracer anomaly values that were referenced to a mean tracer value that is closer to the average tracer value of each box. In order to extract the advective-diffusive tracer balance from the divergence form of the conservation equations, the most appropriate mean value of the tracer, $\overline{C}$, to subtract from C to form the new variable, C', is the mean value along all six faces of the box. The diffusive terms on the right-hand sides of Eqs. (36), (38) or (39) would still be evaluated with the original values of the tracer variable since there is no gain in accuracy to be had by changing variables here, but the left-hand sides of these equations would be evaluated using the refined tracer anomaly variable. In the case of salinity, the variation of the salinity over the six sides of a box may be 0.1 psu so that the influence of the continuity equation in the salinity balance will be reduced by a further factor of ten or more, so that instead of the continuity uncertainty accounting for 99% of the error in this equation, it could account for no more than 20% of the error. In this way the salinity conservation statement will tend to represent the desired advective-diffusive balance.

By choosing the box-average tracer value as the mean that is subtracted from each box, one has essentially forced the divergence form of the conservation statements to have the same balance that is present in β-spiral methods, namely the advective-diffusive balance. Unlike the β-spiral methods however, this proposed box-inverse method also carries the continuity equation (Eq. (36) with $C = 1$). In this way, the method recommended above can be interpreted as a β-spiral method, but with the inclusion of the continuity constraint. One could of course add the normal β-spiral equations to a box inverse method, but the grids on which the velocity components are evaluated are different for an advective and a divergence grid. The above procedure achieves the same physical balances in the equations as would a combined β-spiral and box inverse model, but without any complications due to the different grids, since one uses the box-model grid throughout.

When using anomalies from box-averaged data rather than from a single constant value, the sum of the tracer conservation equations over more than one box does not have a physical interpretation (Rintoul and Bindoff, personal communications, 1991). Using salinity as an example, if a single mean salinity of say 35 psu is used to form the salinity anomaly variable for the left-hand side of the conservation equations, the sum of these equations over many boxes does not amount to the conservation of salt over the boxes, but it does represent the conservation of a different variable, namely $(S - 35 \text{ psu})$. But with a mean salinity that varies from box to box, there is no such interpretation. Should one worry about this? I think that this is not a concern for the following two reasons. First, by regarding the above procedure as a β-spiral method with the added continuity constraint, the issue of what the sum of the salinity conservation statements represents does not seem so pressing since this has not been part of past β-spiral methods. Second, if after performing an inversion one calculates the total salt imbalance (not salt anomaly imbalance) summed over all the boxes, the answer will be dominated by the errors in the continuity equation for each box multiplied by the mean salinity of that box. This will be very close to the global-averaged salinity times the global-averaged volume flux imbalance, no matter what mean salinity is chosen for the mean value of each box in the inversion. For these reasons I believe that using a salinity anomaly that is defined differently for each box is a viable procedure. Of course, proof of the pudding will be in the eating.

CONCLUSIONS

This paper has derived the conservation equations for scalars (including potential density and spiciness) with respect to both neutral surfaces and potential-density surfaces, and in both the advective form which is applicable to the β-spiral method, and in the divergence form that is used in box-model inversions. In the limited space available, conservation statements for potential vorticity were not addressed. The salient findings of the paper are listed below.

• Scalars are advected by the Lagrangian-mean velocity vector rather than the Eulerian-mean velocity that appears in the geostrophic and thermal wind relations, and it may well be important to recognize the distinction between these velocities. A simple parameterization for the difference velocity (the Stokes drift) is proposed and this should be easy to implement in inverse models. Even when this Stokes drift is relatively small, it may well be significant for the lateral advection of tracers because it will be much more closely aligned with the epineutral tracer gradient than will be the Eulerian-mean lateral velocity vector. The magnitude of the estimated Stokes drift is displayed in Figures 2 and 3 for a single neutral surface in the world ocean, and values in excess of 1 mm s^{-1} are common. A lateral velocity of this magnitude down the epineutral tracer gradient causes as much water-mass conversion as vertical mixing

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processes. This highlights the importance of the distinction between Lagrangian and Eulerian velocities.

• The nonlinear nature of the equation of state has been shown to cause significant errors in the diapycnal velocity when it is deduced from the commonly used advection-diffusion balance for potential density. The potential density variable is significantly nonconservative and more care must be taken when writing a conservation equation for potential density. The terms that have been omitted from the potential density conservation equation in the past are (see Eq. (20)), (i) a term proportional to the vertical diffusivity that is largest in the upper 1000 m of the water column, (ii) a term that depends on the epineutral flux divergence of potential temperature and arises because potential density varies along neutral surfaces, (iii) cabbeling and (iv), thermobaricity. Each of these terms are too large to be ignored in various regions of the ocean.

• The omission of the nonconservative terms in the conservation equation of potential density results in either an overestimate of the diapycnal velocity or an underestimate of the vertical diffusivity (for $w^d > 0$), or, quite probably, a combination of both. The use of a simplistic potential density equation also affects the way mixing processes are extracted from the potential temperature or salinity conservation equations, as is illustrated in Eq. (29).

• Thermobaricity and cabbeling were found to be quite strong in the North Atlantic and Southern Oceans, causing contributions to the dianeutral downwelling velocity of order -1×10^{-7} m s^{-1}. These in turn make a large impact on the conservation equations of scalars in these regions and probably also cause significant vortex stretching in the conservation equation for potential vorticity. Of the two processes, thermobaricity is rather smaller than cabbeling except in the Antarctic Circumpolar Current where it is at least as large as cabbeling and also of the same sign.

• The contributions of both thermobaricity and cabbeling to water-mass conversion at a thermoclinic front have been compared with the epineutral mixing of potential temperature. The ratios of these processes were found to be significant and to be proportional to the changes in potential temperature and pressure across the front (see Eq. 13). In the Antarctic Circumpolar Current each of these three processes were found to be equally important, especially because the net water-mass conversion achieved by the lateral diffusion term averages to zero whereas cabbeling and thermobaricity have a consistent sign across the front.

• Many of the pitfalls with forming a potential density conservation equation are avoided if one uses the S and θ equations separately rather than attempting to form a "density" conservation equation. The remaining differences are due to the difference between the epineutral flux divergences and the epipycnal flux divergences of S and θ, as in Eq. (31).

• Conservation equations for conservative variables (like potential temperature and salinity) are affected by the nonlinear nature of the equation of state when a model's lateral mixing is directed along potential-density surfaces rather than along neutral surfaces. The differences between these two lateral mixing parameterizations are explored and are documented in Eqs. (26) and (30). Several terms arise that are significant when the reference pressure of the potential density is significantly different to the in-situ pressure, and two terms remain even when this pressure difference is zero. The difference between epineutral and epipycnal mixing of tracers is important at regions of large epineutral gradient of potential temperature (i.e. at thermoclinic fronts).

• The 'orthogonal' variables on the S-θ diagram, spiciness and Veronicity, are significantly nonconservative variables and the nonlinear terms that appear in their conservation equations are of similar magnitude to those that appear in the potential density equation. It has been shown that one cannot afford to write conservation equations for either potential density or spiciness as though they were conservative variables.

• Box inverse models need their conservation equations cast in the divergence (or flux) form, and it is shown that in this form, the conservation equation for 'density' or 'mass' is really simply a volume integral of the incompressibility equation.

• One often reads that a box inverse model has not required vertical mixing in order to explain the data. Here it has been argued that these models have been set up in such a way that the signatures of all types of mixing processes are well hidden behind the noise due to errors in the continuity equation. The imbalance in the continuity equation is directly reflected in the tracer conservation equations, and is a consequence of the need to write the conservation equations in the divergence form. This causes the tracer equations, and particularly the salinity equation, to be linearly dependent with the continuity equation, so causing a reduced rank in the system of equations. This is similar to the well known problem that, if the mass flux across an ocean section is not zero, the heat flux across the section is different if the temperatures are measured in Kelvins rather than in degrees Celsius.

• A very simple solution to this deficiency of present box-inverse models is proposed: it is to subtract a suitable mean value from the values of a tracer before the conservation equations are evaluated. This should have the effect of (i), increasing the rank of the solution, (ii), extracting information on the advection and diffusion of salinity, thereby constraining both the interfacial advection and diffusion, and (iii), making the conservation equation of potential temperature independent of that of salinity.

• It is argued that the neutral surface framework provides the best link between advection and diffusion of tracers in that the individual terms that comprise the advection of tracer are not large in comparison with the total advection of tracer. In this way, uncertainties in the lateral velocity vector do not introduce as much uncertainty into the left-hand side of these conservation equations as they do in Cartesian coordinates. This is especially true of the e equation, Eq. (12) that is totally independent of the lateral velocity vector. This e equation has the added advantage that it does not have a lateral Laplacian term (which is relatively noisy) on the right-hand side.

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