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Conservative Tracers and the Ocean Circulation

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Conservative tracers and the ocean circulation

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Inclusion of chemical tracers in inverse schemes for calculating the ocean circulation leads to a better determined system of constraints to the flow and may result in increased knowledge about mixing processes as well as current systems. A type of tracer suggested by Broecker, namely a conservative combination of nitrates or phosphates and oxygen ('NO' or 'PO') uses standard observed quantities. It is shown that although these tracers do add information to more conventional inverse schemes, the present sampling strategy is inadequate for determining the ocean circulation quantitatively. The principal reasons for this are the variability of the ocean and the limited spatial coverage of present hydrographic surveys.

1. Introduction

One of the reasons for interest in chemical tracers in the ocean is the hope that they may provide orthogonal information to the more traditional tracers of density, temperature and salinity when investigating the general circulation. Much qualitative insight and a degree of quantitative data has been gained from analysis of various chemical species' distribution, detailed well in Broecker & Peng (1982). In this paper we will investigate the degree of success with which one of the most comprehensive oceanic chemical surveys, GEOSECS (see references in Broecker & Peng, pp. 670–672), can be integrated into the methodology of inverse methods of determining the ocean circulation. Two different inverse methods will be used, namely the β-spiral method (Schott & Stommel 1978) and the Bernoulli method (Killworth 1986), and in addition to the conventional conservative tracer, density, we will consider potential vorticity and the chemical combinations of oxygen, nitrates and phosphates suggested by Broecker (1974).

2. The data

The GEOSECS data are far from ideal for use with many inverse methods for determining the general circulation of the ocean, as they provide information mostly along long sections, making estimation of the full set of derivatives required by the inverse methods difficult. The box-type inverse technique pioneered by Wunsch (1978), which we will not be considering, partly does away with this problem. It still, however, requires the sections to enclose a region of ocean and the GEOSECS cruises, shown in figure 1, do not generally meet this requirement except on very large scales. Nonetheless, we have been able to consider three regions for this paper, marked on figure 1. They include a point in the central North Atlantic (station 30)

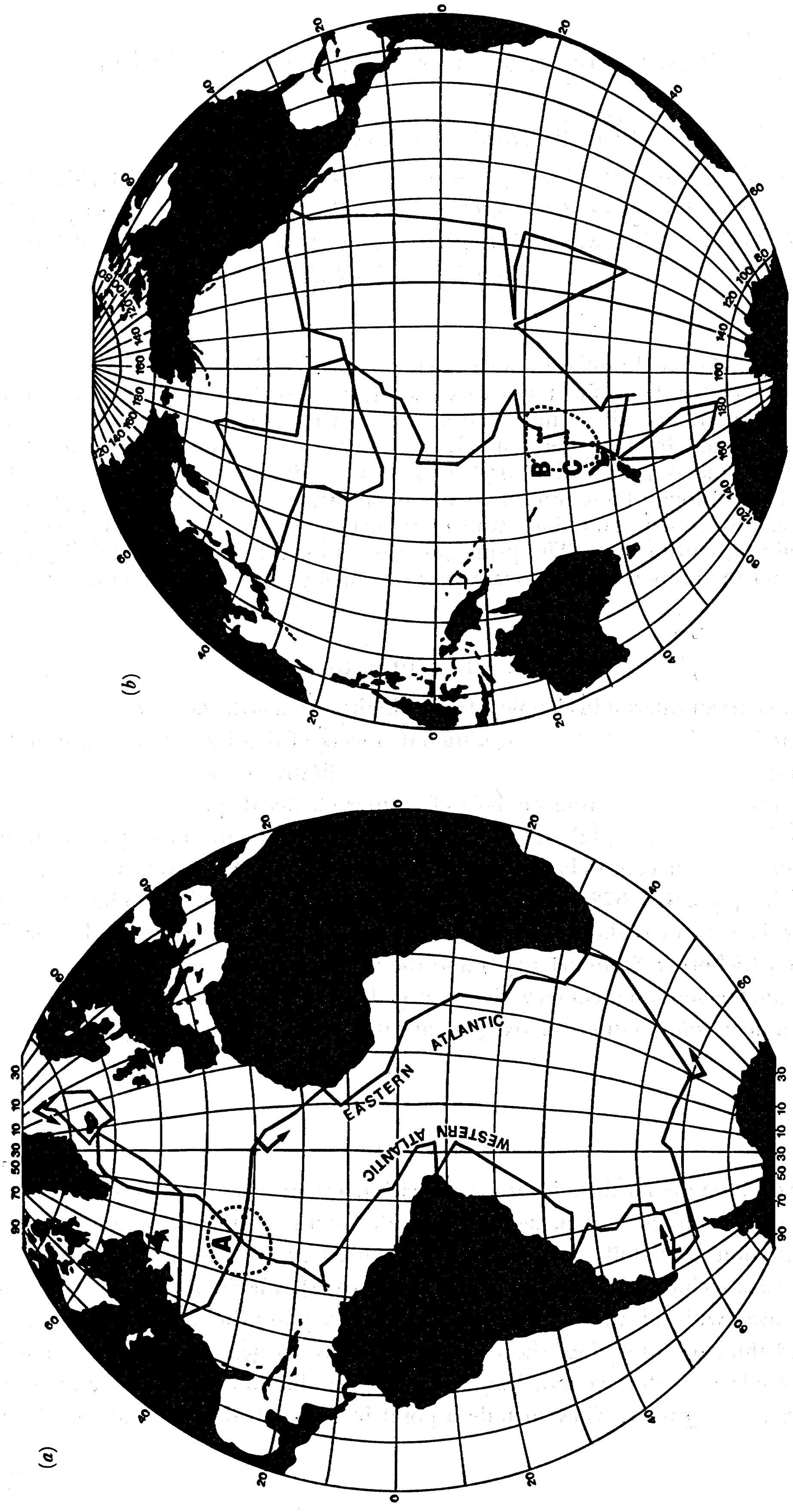

FIGURE 1. GEOSECS (*a*) Atlantic and (*b*) Pacific sections. A, station 30; B, Tongan Trench section; C, Kermadec Trench section. The ends of the sections shown in figure 2 are marked on (*a*).

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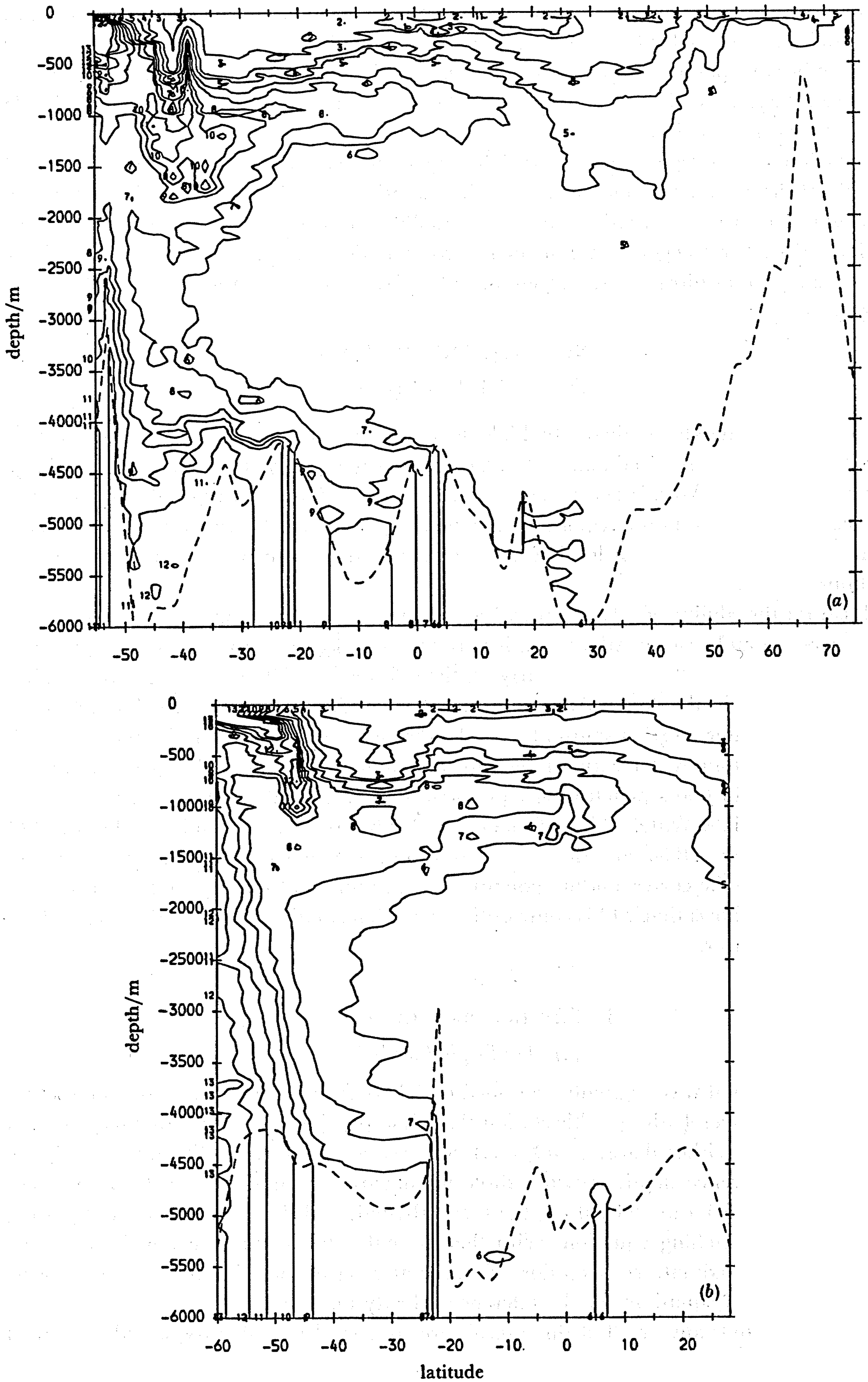

FIGURE 2. NO sections in (a) the western Atlantic and (b) the eastern Atlantic. The sections are marked on figure 1. The contour intervals are n micromoles per kilogram: 1–4, $n \times 100$; 5–6, $400+(n-4)\times 50$; 7–8, $500+(n-6)\times 25$; 9–13, $550+(n-8)\times 10$. The broken line follows the deepest sampling depth.

where two sections intersect, and two short sections in the South Pacific across the Tongan (station 269) and Kermadec (station 273) Trenches. It should be emphasized that these areas were chosen because of the possibility of evaluating both horizontal derivatives and not because of their scientific interest. Indeed, the layout of the data points generally possesses undesirable features for inverse modelling.

In each of these three regions the potential density σ_θ and potential vorticity q were calculated at each depth horizon as, in addition, were the quantities 'NO' and 'PO'. The latter two, derived, variables are conservative tracers essentially representing preformed nutrient concentrations (Broecker 1974) and are defined as combinations of the concentrations in micromoles per kilogram of nitrate and oxygen and phosphate and oxygen respectively (Broecker *et al.* 1985) as

$$\left.\begin{aligned} NO &= 11[NO_3]+[O_2], \\ PO &= 175[PO_4]+[O_2]. \end{aligned}\right\} \quad (1)$$

The two quantities are closely linked by biological processes that tend to maintain a constant ratio of N:P in the ocean (Goldman 1980). Correlating the values of NO and PO over large regions of each of the World's oceans leads to Pearson correlations of typically greater than 98%, except in water formation regions such as the Greenland Sea. There are subtle differences between the two variables on a local scale, however, and so both were used in the inverse calculations.

To illustrate the ability of NO to 'trace' water masses, sections from the GEOSECS cruises along the western and eastern Atlantic basins are shown in figure 2. In both, but particularly the western basin (figure 2*a*), we can clearly see the intermediate NO waters (high oxygen but low nitrate) formed in the North Atlantic north of Iceland, and subducted below relatively NO-poor surface water, moving south at most depths below 2000 m. Similarly, the very cold, dense Antarctic Bottom Water with a large nutrient content and thus still higher NO values, is seen on both basin floors penetrating equatorwards, as, around 1000 m, is the less dense Antarctic Intermediate Water. The effect of the North Atlantic Gyre mixing the low-NO surface waters into the NO-richer deep water is also evident north of 20° N. Comparison of these diagrams with the corresponding potential temperature and salinity sections of GEOSECS (Bainbridge 1980) shows that NO is contributing extra information and should therefore be a useful additional tracer.

3. The inverse methods

(*a*) *The β-spiral method*

The β-spiral method was originally described in Schott & Stommel (1978). It assumes that in the locality of a given hydrographic station there is approximate steady-state thermal-wind balance and tracer (either density, NO, etc.) conservation. The three-dimensional velocity vector at some reference depth provides three unknowns. The horizontal velocity at other depths is computed from these by using the thermal wind, and the vertical velocity by using the linear vortex stretching equation. With the thermal wind linking the velocities at each depth horizon, approximate conservation of tracer at each of these levels leads to an overdetermined system of equations for the reference velocity (u, v, w).

If it is assumed that any or all of three terms are conserved (e.g. density, q and NO) then we can combine all the resulting equations for the reference-level velocity to give a highly over-determined problem. This enables us to allow horizontal and vertical diffusion coefficients to be introduced as unknowns at each level and still retain an over-determined problem. In essentially all calculations with diffusion coefficients the unknowns were found to be not significantly different from zero by using the error analysis intrinsic to least-squares problems (Press *et al.* 1986).

(*b*) *The Bernoulli method*

This method is developed in Killworth (1986). It assumes a steady-state ocean in approximate geostrophic and hydrostatic balance that conserves mass, density and chemical tracer. Linear vorticity $q = f\rho_z$ is thus conserved (Welander 1971), where f is the Coriolis parameter, ρ the density and z a coordinate vertically upwards. The Bernoulli function $B = P + \rho g z$ is also conserved, where P is the pressure and g is the acceleration due to gravity. With several quantities all being approximately conserved we can consider one (e.g. B) as being a function of others. So we have considered $B = F(\rho, q)$ (as in Killworth 1986) or $B = F(\rho, \mathrm{NO})$. In both these systems it is B that is not uniquely defined as the surface pressure is not known. Once B is known the horizontal velocity may be evaluated from the pressure field.

The problem then is to find B. To do this we take a set of stations and examine them pairwise, seeking for a depth (below the mixed layer) at one station at which ρ and q (or ρ and NO) match the values at some depth at the other station. As B must also match, this gives a linear equation connecting the differences in surface pressure at the two stations. With there being typically a number of matches between any pair of stations a large over-determined system of equations for the surface pressure is produced that can be solved by singular-value decomposition in the least-squares manner (as in the β-spiral method).

(*c*) *Gauging the success of inverse methods*

One of the biggest problems with the use of inverse methods to infer the ocean circulation is to estimate how well they capture the desired flow. Many different oceanic locations have been examined in the literature but it is rare to have velocity measurements with which to compare the inversions. One way around this problem is to seek bounds to the flow rather than its actual value. Wunsch (1984) has had some success with this approach.

In previous work (Killworth & Bigg 1987) we have addressed this problem by examining the performance of the two techniques used here, plus a simple version of Wunsch's (1978) box-type inverse method, on data obtained from an eddy-resolving general circulation model of Cox (1985). We therefore had the 'real' velocities with which to compare the inversions of that study. The reader is referred to Killworth & Bigg (1988) for a full description; it suffices here to say that in general the Bernoulli and box methods performed well, whereas the β-spiral method was to a large degree unsatisfactory, producing large residuals to its composite equations. The β-spiral method has been retained for this investigation because of the different quantities (e.g. NO) used in the present study and because the model and real oceans are perforce not identical in their dynamics. Another result of Killworth & Bigg (1988) worth reporting here is that for accurate thermal winds (i.e. well within 1 cm s^{-1} top-to-bottom of the model values) horizontal derivatives needed to be evaluated over distances of less than 100 km. This has important implications for most oceanographic surveys.

Apart from the error estimates accompanying least-squares problems there are two means (or northern section, B) in the Pacific and the North Atlantic site (A). The σ_θ and geopotential finite difference derivative cases are similar at all three locations, with the geopotential thermal wind always being noisier, because of the level-by-level method of calculation (as opposed to the depth-integrated form of calculation for σ_θ estimates). However, the least-squares σ_θ estimate, although roughly similar to the others at the Atlantic location, is wildly different for both Pacific sites. This is largely because of the special nature of the Pacific sites. The zonal sections are much shorter than the meridional scale, and including both zonal sections in a calculation seriously distorts the x-derivative fit.

So it is found that calculating the thermal wind, before trying to apply any inverse methods, does not lead to a unique answer. Instead, it is strongly dependent on the method, and site, of calculation. Fortunately, the inverse methods are robust to the significant noise level of the geopotential thermal wind and give similar results to the equivalent σ_θ estimate. Use of this thermal wind will therefore not be considered further. It remains now to examine the degree of internal consistency of the inverse methods.

(*b*) *Inverse calculations*

At each location we carried out three inversions from both methods. These were for different depth ranges: a 'full depth' calculation (400–3500 m), an upper range (400–1500 m) and a lower range calculation (1600–3500 m). The GEOSECS data were interpolated to give σ_θ, etc., at every 100 m so that the least over-determined β-spiral inversion had eleven equations and three unknowns. The three velocity components were always resolved but the addition of unknown mixing coefficients raised the rank only slightly and so these components were not resolved. The Bernoulli inversions were characteristically an order of magnitude more over-determined with well over 100 $\rho - q$ (or $\rho -$NO) crossings and five unknown surface pressures. For consistency, only the results for the finite difference σ_θ estimates of thermal wind are shown, except for the North Atlantic Bernoulli runs that used the least-squares fits (see the previous section for comments). In all the following diagrams, the velocity at 1500 m only will be examined. The thermal-wind profiles of figure 3 enable the reader to gauge the ramifications of the discussion for other depths.

In figure 4, the 1500 m Bernoulli velocities for all three depth ranges and the two variable combinations (ρ and q, ρ and NO) are shown for each of the three locations. Comparing the magnitudes of the scatter in the solutions with the thermal wind of figure 3 shows that the variability in the inverse velocity profile is considerable. There tends to be grouping of the two solutions for a given depth range but even this is not uniformly true.

The Bernoulli method assumes conservation of several variables simultaneously. In the 'snap-shot' data set with which we are working it may be that this is asking too much of the ocean. The β-spiral calculations, however, are very diverse, letting individual quantities be conserved, or collections of them. It performed poorly in the sensitivity tests of Killworth & Bigg (1988) but it was thought that a major reason for this was the strong influence of numerical diffusion in the model. With the GEOSECS inversions, diffusion was found not to improve the solution, with the extra unknowns being unresolved. In figures 5 and 6 we show the 1500 m velocities for the solutions giving the best and worst fits respectively of the trials for the Atlantic and Tongan Trench locations. The Kermadec Trench site gives similar results. As in figure 4 the three different depth-range solutions are shown.

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by which we will check for 'realistic' inversions. One is how well the data fit the equations, i.e. the residuals. The other is to choose a standard water column for the calculations and study the reproducibility of the inverted velocity from case to case, and between considering the whole of the water column and sub-sections of it.

4. The results

(a) *Thermal-wind calculations*

At each of the three sites considered, four different estimates of the thermal-wind shear from 3000 to 400 m were made. Three employed σ_θ as the key variable in the thermal-wind calculation

$$\left.\begin{aligned} u_z &= g(\sigma_\theta)_y/f\rho_0, \\ v_z &= -g(\sigma_\theta)_x/f\rho_0, \end{aligned}\right\} \tag{2}$$

while one used geopotentials (see Gill 1982). The differences between the σ_θ estimates came from the way in which the derivatives at each depth level were evaluated. One method assumed that the density was of the form $a+bx+cy$ at a given level and gave a least-squares fit to the linear coefficients, so giving the derivatives. The others assumed that the stations used to calculate horizontal derivatives by finite differences lay on a longitude–latitude cross. One method let the stations on, say, the longitude arm be unevenly spaced, whereas the other assumed that they were equally spaced. Both of the two calculations gave similar results and will not be separately considered. The geopotential horizontal derivatives were calculated by using the uneven spacing.

The Pacific sites show much greater thermal-wind shear than the Atlantic site and have larger differences between the three methods. This is shown in figure 3 for the Tongan Trench

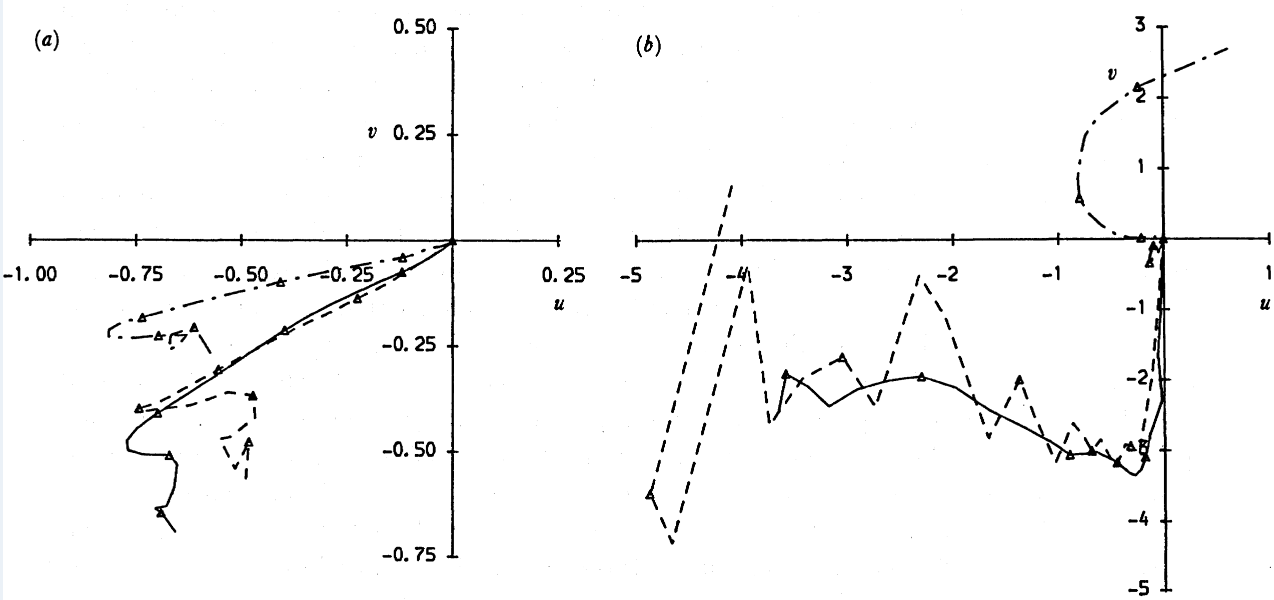

Figure 3. Thermal wind shears (in units of centimetres per second) relative to 3000 m, moving upwards in (*a*) the North Atlantic and (*b*) Tongan Trench locations. Every 500 m above 3000 m is marked by △, finite difference σ_θ estimate, ——; geopotential estimate, ----; σ_θ least-squares estimate, –·–·–.

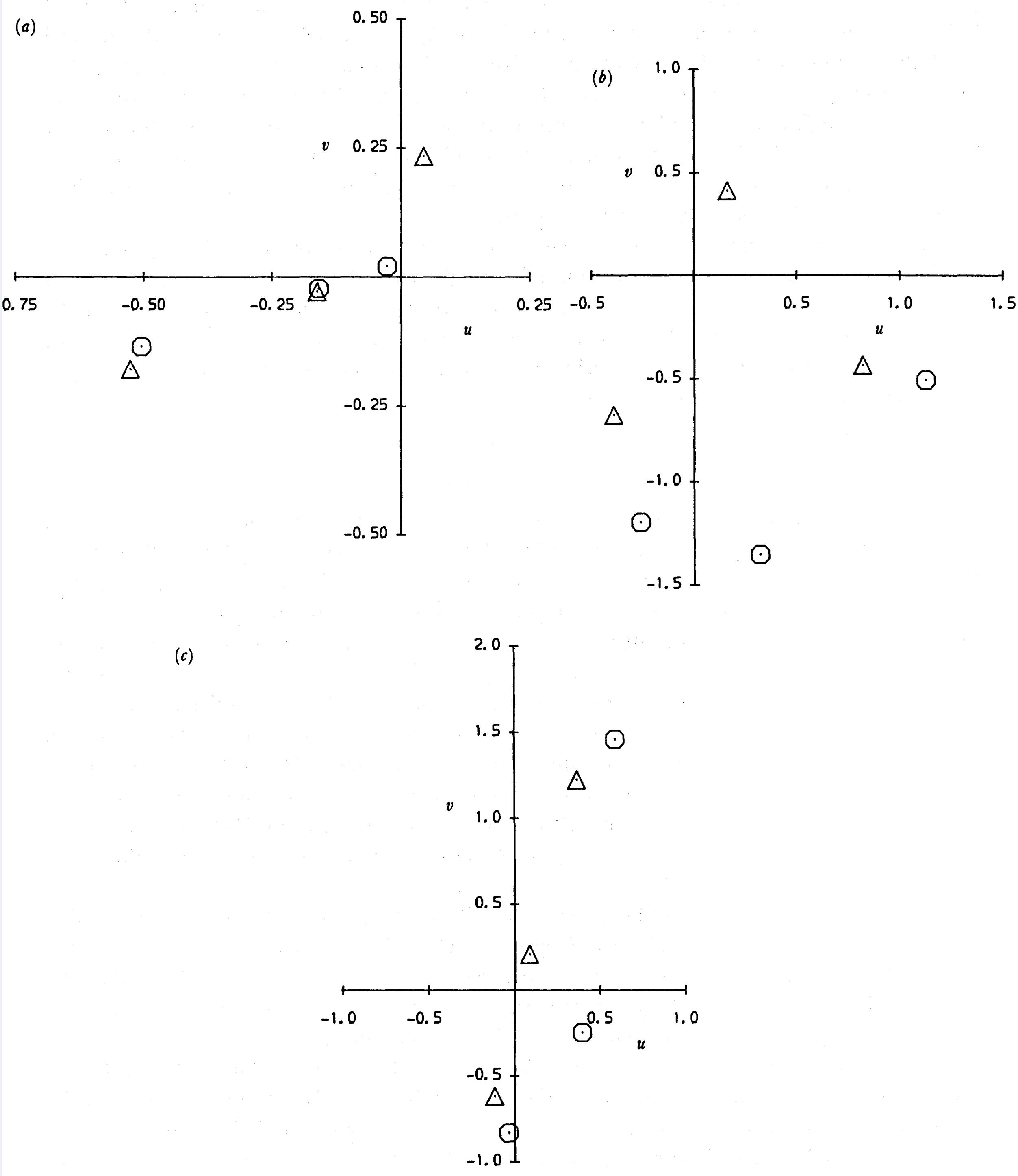

FIGURE 4. Bernoulli inversion velocities (in units of centimetres per second) at 1500 m. Three depth-range cases (ρ, q) inversions, ○; (ρ, NO) inversions, △. (*a*) Atlantic site, (*b*) Tongan Trench (B), (*c*) Kermadec Trench (C).

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The inconsistency between the various solutions and depth ranges is manifest. The inversions combining conservation of ρ, q and NO tend to give the largest residuals (and hence the worst fits) whereas the ρ-only results tend to give the smallest residuals. There are significant exceptions to these statements. In particular, the good fits of PO in the Atlantic illustrate the compatibility of the PO construction with more conventional conserved quantities.

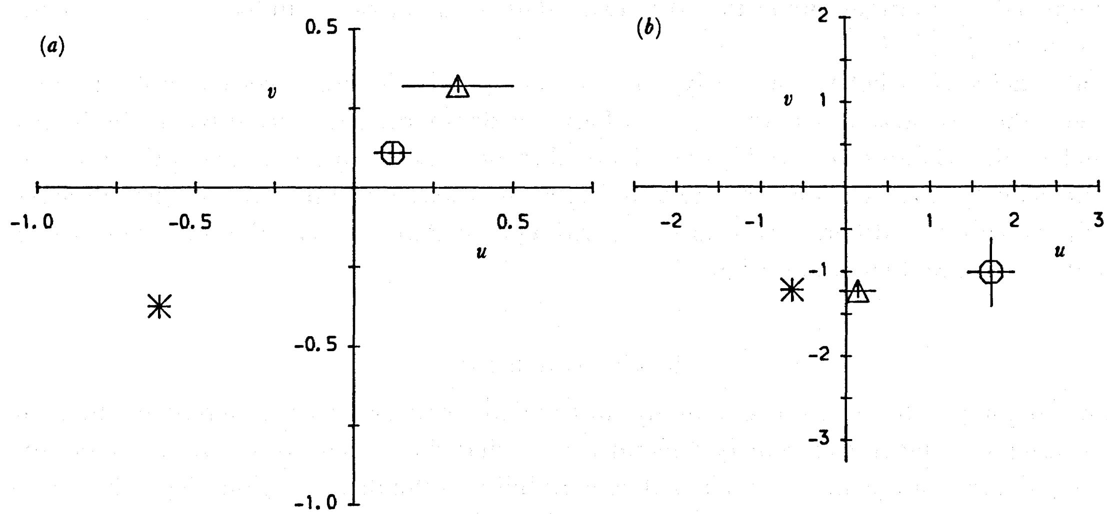

FIGURE 5. The best fit β-spiral velocities (centimetres per second) at 1500 m. Three depth ranges: full depth, △; upper range, ○; lower range, ×. (*a*) Atlantic site (variable runs providing best fit: △, PO; ○, PO; ×, ρ). (*b*) Tongan Trench (B) (variable runs providing best fit: △, ρ; ○, ρ; ×, ρ).

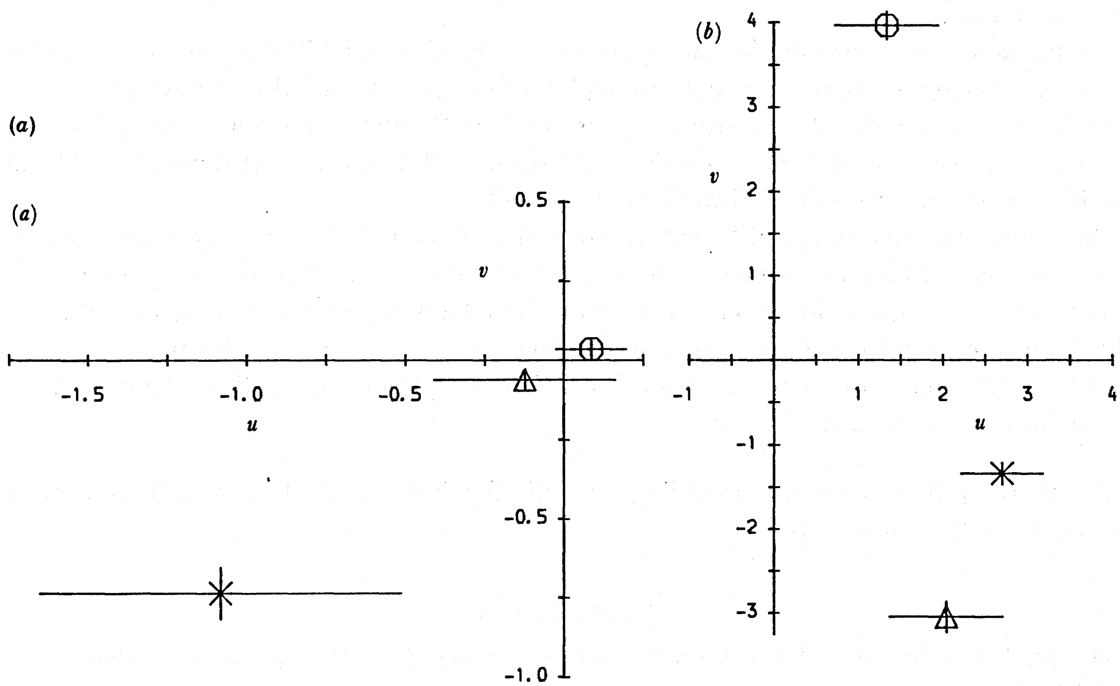

FIGURE 6. As for figure 5, but for worst fits. (*a*) Atlantic site (variable runs providing worst fit: △, $\rho+q+$NO; ○, q; ×, NO). (*b*) Tongan Trench (B) (variable runs providing worst fit: △, $\rho+q+$NO; ○, $\rho+q+$NO; ×, $\rho+q+$NO).

The upper-Atlantic depth range is the only set where both best and worst solutions fall within the respective error bars (interestingly the density inversion is not the best fit here). Note the smallness of the velocity predicted. The information from the deeper regions at this location seems to be completely at variance with the consistency of the upper region. Examining the thermal wind (figure 3*a*) shows a significant *u* reversal around 1500 m. Presumably the dynamics of this transition region violate the model equations, perhaps through nonlinearities. The upper-level Bernoulli inversions (the two results near the origin in figure 4*a*) give similar results to the β-spiral.

Both Pacific sites behave similarly, that is, very poorly. There is considerable difference between the best and worst fits and also between depth ranges. Curiously, in the Tongan Trench section (figures 5*b* and 6*b*) both fits tend to agree between the three depth-range cases for one velocity, but it is *u* for the best fits and *v* for the worst! The different runs (not all shown) clearly indicate that different tracers are providing orthogonal information to each other, but they do not share a common origin.

5. Conclusions

The major conclusion from our many and varied inversions with different methods and depth ranges is that it is extremely difficult to say what the velocity field was in the ocean at the time the measurements were taken. The variability in the thermal wind, depending on the method of calculation, was to some degree lost in inversion. However, the inconsistency between different inversions leads one to conclude that there are some important discrepancies between the GEOSECS ocean and the dynamical models used. Only at the North Atlantic site, over a limited depth range where velocities were less than 0.5 cm s^{-1}, can consistency be claimed for the inversions.

What, then, are we missing in our equations? Temporal variability seems the most likely candidate. Trying to use conservation principles over a sparsely sampled data set, even if it is near synoptic as in the Pacific sites, appears to fail. Possibly using more data, in a grid arrangement over a smaller area, would be more successful. Looking at time-averaged data should also be more fruitful (Killworth & Bigg 1988).

Our conclusion then is that although the constructs NO and PO possess the right properties to be considered as useful adjuncts to more conventional conservative tracers, present cruise strategies are inadequate for inverse methods to be reliably applied to our sparse data base. These tracers clearly have potential in different circumstances, some of which have been alluded to above. However, a different approach is required to extract the useful material contained in present-day tracer measurements.

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