Modeling Vertical and Horizontal Diffusivities with the Sigma Coordinate System

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ABSTRACT

The use of diffusive terms in numerical ocean models is examined relative to different coordinate systems. The conventional model for horizontal diffusion is found to be incorrect when bottom topographical slopes are large. A new formulation is suggested which is simpler than the conventional formulation when transformed to a sigma coordinate system and makes it possible to model realistically both surface Ekman and bottom boundary layers.

1. Introduction

Vertical viscosity and diffusivity related to small turbulence scales characterized by integral macroscales about 0.2–0.5 times the boundary layer thicknesses are now relatively well parameterized using turbulence closure schemes based on hypotheses of Rotta and Kolmogorov (see, for example, Mellor and Yamada, 1982, wherein are references to a number of closure submodels and applications). These hypotheses embody well-defined physical constants, directly measurable in the laboratory. The constants are believed to be sufficiently universal to cover most turbulent flows with accuracy sufficient for most applications.

When the horizontal length scale of mean property variation is large relative to the vertical scale, scale analysis—leading to the turbulent boundary layer approximation—specifically excludes the small-scale horizontal diffusion terms in favor of the vertical terms. The validity of the turbulent boundary layer approximation is indisputable for most laboratory flows documented in the literature. Furthermore, a three-dimensional model study of New York Harbor and Estuary has been completed (but not yet published) wherein the horizontal grid element was 500 m. The vertical coordinate, a sigma system [Phillips, 1957], was divided into 10 levels, such that the vertical grid size was a maximum of 6 m in the deepest water and decreased proportionately as depth decreased. No horizontal viscosity or diffusivity was required. Good vertical resolution was an important factor here. Dispersion was, in effect, explicitly modeled by resolved small-scale horizontal advection followed by vertical mixing, the so-called G. I. Taylor (1954) dispersion process. The correspondence between model simulation and observed current and salinities (an extensive dataset was available) was very good.

It is believed that the New York Harbor experience presages the fact that horizontal diffusion can be eliminated in the future for smaller oceanic domains and as computing costs continue to decrease. In addition, the existing, eddy resolving, two- and three-layer models [Holland, 1978] also suggest this development, although the layer models could further decrease their dependence on horizontal diffusion by using finer vertical resolution and better physics for vertical mixing, important elements for the simulation or forecasting of the oceanic mass fields. However, for most, larger scale, numerical applications, horizontal grid elements are generally much larger than the smallest, two-dimensionally dominant scales dictated by variable bottom topography in shallow water and the baroclinic Rossby radius of deformation in the open ocean. These small, unresolved, mesoscale motions require that modelers use horizontal, subgrid-scale, diffusive terms with diffusivity coefficients, oftentimes much larger than the small scale, vertical diffusivities. Thus, while the situation is improving, many modeling applications will require horizontal mixing for some time into the future. For example, presuming computer storage were available, the current cost of modeling the world ocean with 30 vertical levels on a 1 km $\times$ 1 km grid for one year's simulation is, roughly, ten billion dollars.[1] Since computer costs decrease roughly by a factor of 10

[1] This estimate is based on commercial rates for a Cray-1S computer using a grid of 5×10^9 points and a time step of $\sim$2.5 min (as dictated by numerical stability constraints).

every ten years, it appears, therefore, that for large domain calculations, horizontal mixing coefficients will be needed to fill the gap for the next 40–50 years or more.

The purpose of this paper is to provide the correct formulation of the horizontal mixing terms in a sigma-coordinate system so that both surface Ekman and bottom boundary layers can be realistically modeled, even when the horizontal diffusivities are much larger than the small-scale diffusivity. The discussion presented here, while directed towards ocean modeling, is applicable to atmospheric circulation modeling as well. However, as is appropriate to the ocean environment, and to simplify the discussion, the Boussinesq approximation is used here. The approximation can be removed with no change in the conclusions of the paper.

2. Horizontal and vertical mixing hypotheses and the modeling coordinate system

Consider the three coordinate systems illustrated in Fig. 1: coordinate system A, a conventional x, z coordinate system; coordinate system B, a sigma coordinate system; and coordinate system C, an orthogonal curvilinear system.

The sigma coordinate system (Phillips, 1957) is defined[2] as

$$x^* = x, \quad y^* = y, \quad \sigma = \frac{z}{H(x, y)}, \qquad \text{(1a,b,c)}$$

where $\sigma = 0$ at the surface, $z = 0$ and $\sigma = -1$ at the bottom, $z = -H(x, y)$. The three-dimensional ocean circulation model of Blumberg and Mellor (1983, 1985) is a sigma coordinate model that seems to especially benefit from its coordinate system's bottom following capability in dealing with combined baroclinic and topographical effects and in modeling bottom boundary layers.

The curvilinear coordinate system C is comprised of σ surfaces and surfaces orthogonal to these σ surfaces. It is not considered a useful numerical modeling system, but it is useful to this discussion.

Now consider the first (perhaps deceptively) simple step in modeling mixing processes. The momentum flux will be used in the x-component of the vector momentum equation as an example; the results apply to the y-component and to any scalar flux. The net momentum flux for coordinate system A is

$$F_x = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}, \qquad (2)$$

where the stress components are[3]

$$\tau_{xx} = 2A\frac{\partial U}{\partial x}, \quad \tau_{yx} = A\left(\frac{\partial V}{\partial x} + \frac{\partial U}{\partial y}\right), \quad \tau_{zx} = K\left(\frac{\partial U}{\partial z}\right) \qquad \text{(3a, b, c)}$$

Here K is small, $O(10^{-2}\ \mathrm{m^2\ s^{-1}})$ and can be provided by turbulent closure schemes. On the other hand, A can be large, $O(10^2\text{–}10^4\ \mathrm{m^2\ s^{-1}})$; the actual value depends on horizontal resolution—too small and the calculated fields are noisy, too large and resolvable flow structures are removed. Now, at an ocean surface, there is no problem with Eq. (3a, b)—at least in the context of this discussion—since the stress acting on a plane normal to the surface is τ_{zx}. And, although A may be much larger than K, $\partial\tau_{zx}/\partial z$ is, generally, still much larger than the horizontal divergent terms in Eq. (2). However, at the bottom there can be a problem when $A \gg K$ and the bottom slope $\partial H/\partial x$ or $\partial H/\partial y$ is significantly nonzero. Consider the case with $\partial H/\partial x \neq 0$ and $\partial H/\partial y = 0$. The stress near the bottom acting on a surface parallel to the bottom and in the x-direction is $\tau_{nx} = \tau_{zx} - \tau_{xx}\partial H/\partial x = K\partial U/\partial z - 2A\partial H/\partial x\partial U/\partial x$, or approximately $\tau_{nx} \approx (K\Delta U/\delta)[1 - 2(A/K)\cdot(\partial H/\partial x)(\delta/\Delta x)]$ where the change ΔU occurs over a distance δ in the vertical and over a distance Δx in the horizontal direction. Suppose $\delta = 50$ m, $\Delta x = 50$ km, $\partial H/\partial x = -10^{-2}$, $A = 10^4\ \mathrm{m^2\ s^{-1}}$ and $K = 10^{-2}\ \mathrm{m^2\ s^{-1}}$. Then $\tau_{nx} \approx (K\Delta U/\delta)[1 + 20]$; the effective diffusivity for the bottom boundary layer is therefore much larger than K. Furthermore, to realistically model bottom boundary layers this effective diffusivity should approach zero near the bottom where the logarithmic law of the wall prevails and this further exacerbates the problem of using Eqs. (3a, b).

Equations (2) and (3a, b, c) can be transformed into a sigma coordinate system as in the model of Blumberg and Mellor [1983, 1985]. Making the transformation, one obtains

$$F_x = \frac{\partial \tau_{xx}}{\partial x^*} - \frac{\sigma}{H}\frac{\partial H}{\partial x}\frac{\partial \tau_{xx}}{\partial \sigma} + \frac{\partial \tau_{yx}}{\partial y^*} - \frac{\sigma}{H}\frac{\partial H}{\partial y}\frac{\partial \tau_{yx}}{\partial \sigma} + \frac{1}{H}\frac{\partial \tau_{zx}}{\partial \sigma} \qquad (4)$$

[2] Note that a more precise definition is $\sigma = (z - \eta)/(H + \eta)$, where η is the free surface elevation, but we neglect η here to simplify the discussion.

[3] The full stress tensor which is axisymmetric about the z coordinate and subject to $\partial U_k/\partial x_k = 0$ is $\tau_{ij} = C_1(\partial U_i/\partial x_j + \partial U_j/\partial x_i) + C_2(\lambda_i\partial W/\partial x_j + \lambda_j\partial W/\partial x_i) + C_3(\lambda_i\partial U_j/\partial z + \lambda_j\partial U_i/\partial z) + C_4\delta_{ij}\partial W/\partial z$ where $\lambda_i = (\lambda_x, \lambda_y, \lambda_z) = (0, 0, 1)$ is a vector normal to the $x - y$ plane. $\partial W/\partial x$ terms have been neglected in Eq. (3a, b, c) according to boundary layer scale analysis. Also the vertical divergence, $\partial W/\partial z$, has been neglected as is appropriate to oceans and perhaps to the earth's atmosphere (Williams, 1972). Alternately, in the absence of more physics, one simply posits a constitutive relation where $C_4 = 0$.

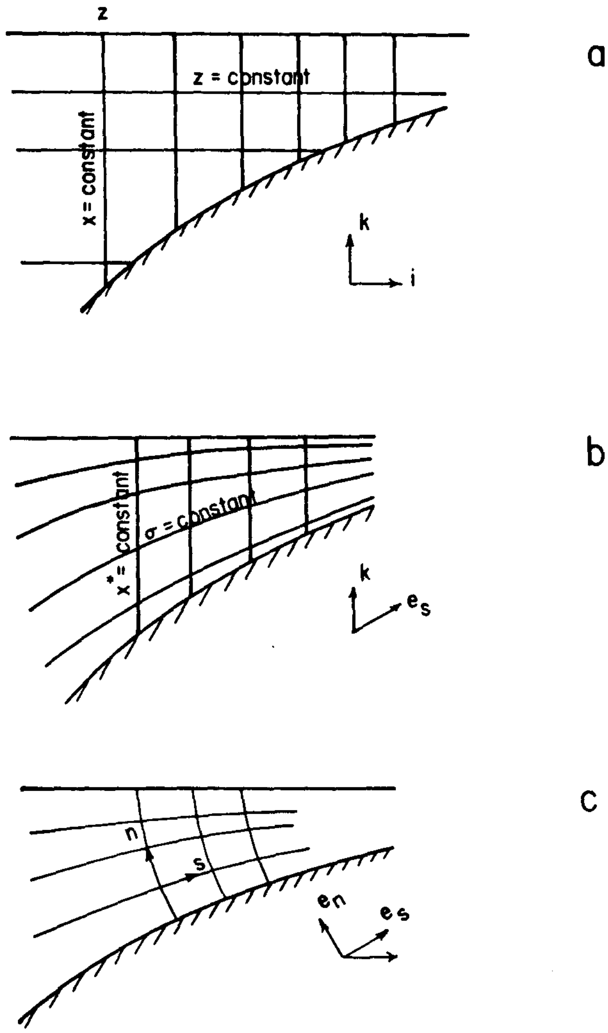

FIG. 1. Schematic of three coordinate systems: (a) a conventional x, z system; (b) a sigma system; and (c) an orthogonal curvilinear system.

and

$$\tau_{xx} = 2A\left[\frac{\partial U}{\partial x^*} - \frac{\sigma}{H}\frac{\partial H}{\partial x}\frac{\partial U}{\partial \sigma}\right] \quad (5a)$$

$$\tau_{yx} = A\left[\frac{\partial V}{\partial x^*} + \frac{\partial U}{\partial y^*} - \frac{\sigma}{H}\frac{\partial H}{\partial x}\frac{\partial V}{\partial \sigma} - \frac{\sigma}{H}\frac{\partial H}{\partial y}\frac{\partial U}{\partial \sigma}\right] \quad (5b)$$

$$\tau_{zx} = \frac{K}{H}\frac{\partial U}{\partial \sigma}. \quad (5c)$$

On continental slopes it was found that the Blumberg–Mellor model could not simulate physically reasonable bottom boundary layers; for example, the logarithmic velocity behavior is not obtained. The point is, of course, that a coordinate transformation does not change the physics of the governing equations. The previous discussion in terms of Eqs. (2) and (3a, b) applies equally to Eqs. (4) and (5a, b, c).

To proceed towards a correct model for horizontal diffusion, another form of Eq. (2) or Eq. (4) is convenient. It may be verified that

$$F_x = \frac{1}{H}\frac{\partial}{\partial x}(H\tau_{xx}) + \frac{1}{H}\frac{\partial}{\partial y}(H\tau_{xy}) + \frac{1}{H}\frac{\partial \tau_{\sigma x}}{\partial \sigma} \quad (6)$$

is equivalent to Eq. (4) and therefore to Eq. (2) by letting $\tau_{\sigma x} \equiv \tau_{zx} - \sigma(\partial H/\partial x)\tau_{xx} - \sigma(\partial H/\partial y)\tau$. Note that $\tau_{\sigma x}$ consists of terms containing A and is largest near the bottom ($\sigma = -1$). Also note that τ_{xx}, τ_{xy} and $\tau_{\sigma x}$ are stresses in the x-direction acting on surfaces of constant x^*, y^* and σ, respectively. ($\tau_{\sigma x}$ is actually the shear force per unit area projected on a z = constant plane.) If one refers to Fig. 1b, one sees that they are natural stress definitions for use on a small volume element, $\Delta\sigma H \Delta x^* \Delta y^*$ in sigma coordinates.

To develop a proper formulation valid near the ocean surface and bottom, a replacement constitutive relation for Eq. (3a, b, c) or, equivalently Equation (5a, b, c) is needed; a relation that does not include a component containing A, acting on surfaces parallel to the bottom.

By considering coordinates s and m parallel to the bottom and n normal to the bottom, as in Fig. 1c, a new constitutive relation in this curvilinear orthogonal system can be written as

$$\tau_{ss} = 2A\frac{\partial U_s}{\partial s}, \quad \tau_{ms} = A\left(\frac{\partial U_m}{\partial s} + \frac{\partial U_s}{\partial m}\right), \quad \tau_{ns} = K\frac{\partial U_s}{\partial n} \quad (7a, b, c)$$

where now the stress components acting on the plane parallel to both the surface and bottom contains K and not the much larger value A. To see why this is correct, define $K \equiv v_K l_K$ and $A \equiv v_A l_A$ where v_K, v_A are velocity scales and l_K, l_A corresponding length scales. The velocity scales of both unresolved subgrid scale, parallel motion v_A and small scale turbulent, normal motion v_K are roughly of the same order, $O(10^{-2}$ m s$^{-1})$. It is, however, known that scales of motion normal to solid surfaces, $l_K = O(1$ m$)$ whereas, one supposes, $l_A = O(\Delta x) = O(10^3\text{–}10^5$ m$)$. Equation (7a, b, c) where $A \gg K$ is in accord with this scaling, whereas the stress defined by Eq. (3a, b, c), where also $A \gg K$, are not.

A difficulty with Eq. (7a, b, c) is that, when τ_{ss}, τ_{ms}, τ_{ns} are transformed without any approximations to τ_{xx}, τ_{yx}, $\tau_{\sigma x}$ and the velocities to U and V, the result is very complicated except at the surface, $z = 0$, where they reduce to Eqs. (2) and (3a, b, c). The situation can be improved by taking advantage of the fact that bottom slopes are small numbers; for example, $\partial H/\partial x = 0.1$ is an upper limit of values encountered in the ocean. If $\phi_x \approx \sin \phi_x \equiv -\sigma\partial H/\partial x$ where ϕ_x is the angle between the sigma surface and the horizontal (see Fig. 1c), it can be shown that $\tau_{xx} = \cos^2 \phi_x \tau_{ss} + \cos \phi_x \sin \phi_x \tau_{ns} \approx (1 - \phi_x^2)\tau_{ss} + \phi_x \tau_{ns} \approx \tau_{ss}$ and similarly that $\tau_{ss} \approx 2A\partial U/\partial x^*$.

Thus, to very good approximation

$$\tau_{xx} = 2A\frac{\partial U}{\partial x^*} \tag{8a}$$

and similarly

$$\tau_{xy} = A\left(\frac{\partial U}{\partial y^*} + \frac{\partial V}{\partial x^*}\right) \tag{8b}$$

$$\tau_{\sigma x} = \frac{K}{H}\frac{\partial U}{\partial \sigma}. \tag{8c}$$

Specifically, Eq. (8c) does not contain A. Furthermore, Eq. (6) together with Eq. (8a, b, c) which as shown here is physically correct, is much simpler than Eqs. (4) and (5a, b, c).

A complete list of equations for momentum and heat diffusion is contained in the Appendix. The modeling of heat flux near the bottom also benefits by recasting the heat flux constitutive relations.

3. Discussion

The best modeling of horizontal diffusion terms are null terms, but if they need be included which, presently, is almost always the case, then Eqs. (6) and (8) are the correct representation instead of either Eqs. (2) and (3) or, equivalently, Eqs. (4) and (5). A problem with Eqs. (6) and (8) has been encountered, however. Namely, if there is no initial motion and temperature, salinity and density are functions of z with the horizontal thermal diffusivity (A_H) equal to a constant, Eq. (A2) will result in cross-slope heat transfer followed by a baroclinically driven flow. In spite of this, Eq. (A2) is correct physically. What is not correct is that A_H be nonzero when there is no motion. Another parameterization for A_H is needed such as the grid and velocity gradient dependent horizontal diffusivity formulation of Smagorinsky [1963] or some other velocity dependent (and buoyancy gradient dependent) relation. If A_H = constant is to be maintained, which does make the level of diffusiveness in a model easy to report, then a "fix" would be to subtract out an area averaged $\bar{T}(z)$ from $T(x, y, z)$ before evaluating the heat flux and similarly, the salinity flux terms. This removes most of the cross-slope diffusion, particularly in deep water where the problem is most acute.

The new horizontal diffusion terms have been inserted into the Blumberg–Mellor ocean model. Figure 2 is a sample, two-dimensional (x, σ) calculation mapped into (x, z) space after 60 days of model integration. The physical setting is upwelling induced by an applied, southward (negative y-direction) surface wind stress of 0.6 dyn cm^{-2}. Initially the velocity field is null, $T = T(z)$ and $S = S(z)$; T is temperature and S is salinity. Realistic bottom boundary layers are obtained which, if detailed, show an Ekman velocity spiral over a logarithmic near bottom layer. Temperature and salinity in the boundary layers are well mixed vertically.

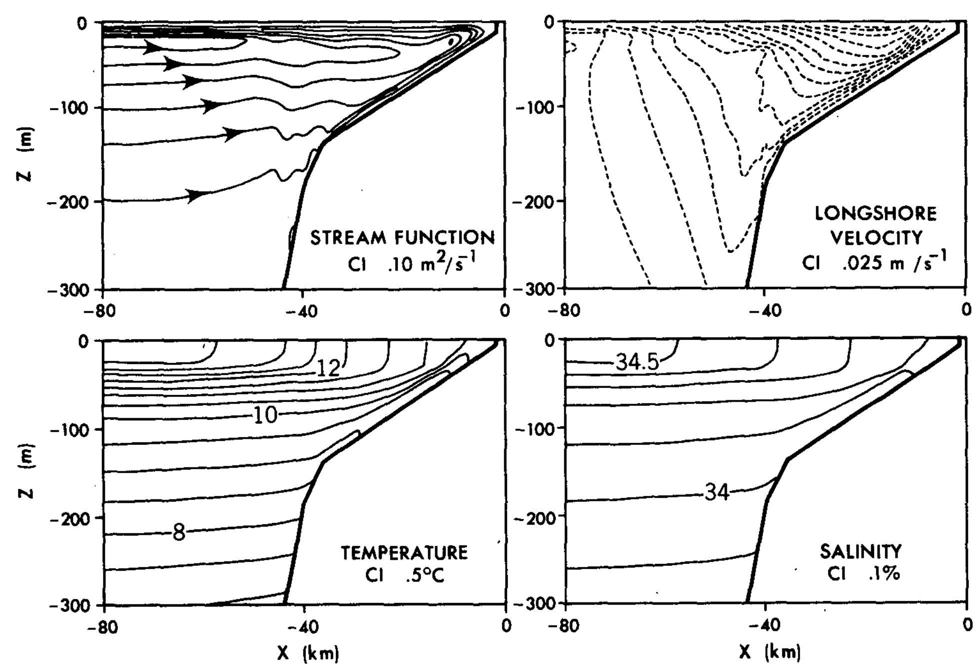

FIG. 2. The flow and mass fields after 60 days of integration. Initially the velocity field is null, $T = T(z)$ and $S = S(z)$. The upwelling flow is induced by a southward (negative y) surface wind stress of 0.6 dyn cm^{-2}. Note the formation of a well-defined bottom boundary layer. Note also the entrainment of upwelled water into the boundary layer.

4. Conclusions

The conventional definition of horizontal diffusion has been found to be physically incorrect near sloping bottoms when the horizontal diffusivity is larger than the vertical diffusivity. The conventional definition leads to a net flux component normal to the bottom which can be large, whereas fluctuating velocities and length scales normal to the bottom cannot be large and, in fact, must approach zero at the bottom. When converted to a sigma coordinate system, the conventional formulation behaved poorly in the Blumberg–Mellor model on sloping bottoms; the bottom boundary layer was unrecognizable relative to known bottom layer properties.

A new formulation of the diffusive terms used in numerical ocean models has been presented and tested. This formulation not only provides for an accurate computation of bottom boundary layers on steep continental slopes but, it turns out, is also much simpler mathematically and requires less computer resources than the conventional formulation when transformed to a sigma coordinate system.

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APPENDIX

Complete List of Diffusion Terms for the Sigma Coordinate System

The complete equations for net heat diffusion are

$$Q = \frac{1}{H}\frac{\partial}{\partial x^*}(Hq_x) + \frac{1}{H}\frac{\partial}{\partial y^*}(Hq_y) + \frac{1}{H}\frac{\partial q_\sigma}{\partial \sigma} \quad \text{(A1)}$$

where

$$(q_x, q_y, q_\sigma) = A_H\left(\frac{\partial T}{\partial x^*}, \frac{\partial \mathrm{T}}{\partial y^*}, 0\right) + \frac{K_H}{H}\left(0, 0, \frac{\partial T}{\partial \sigma}\right) \quad \text{(A2)}$$

which also applies to salinity or any other scalar. The eddy diffusivity coefficients for heat are denoted by A_H and K_H.

The corresponding equations for the momentum component equations are

$$F_\alpha = \frac{1}{H}\frac{\partial}{\partial x^*}(H\tau_{x\alpha}) + \frac{1}{H}\frac{\partial}{\partial y^*}(H\tau_{y\alpha}) + \frac{1}{H}\frac{\partial}{\partial \sigma}(\tau_{\sigma\alpha}) \quad \text{(A3)}$$

where

$$(\tau_{x\alpha}, \tau_{y\alpha}, \tau_{\sigma\alpha}) = A_M\left(\frac{\partial U}{\partial x_\alpha} + \frac{\partial U_\alpha}{\partial x^*}, \frac{\partial V}{\partial x_\alpha} + \frac{\partial U_\alpha}{\partial y^*}, 0\right) = \frac{K_M}{H}\left(0, 0, \frac{\partial U_\alpha}{\partial \sigma}\right). \quad \text{(A4)}$$

Here the subscript α is either x or y and U_α is either $U_x = U$ or $U_y = V$; A_M and K_M are the eddy viscosity coefficients.

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