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Ocean Models and the Implementation of Vertical Diffusion and Vertical Mixing

Unified Model Version 4.5

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INTRODUCTION

In the current (level) ocean models used at the Met. Office, the mixing of momentum and tracers are treated as though they were distinct processes, with Richardson number dependent diffusion coefficients for momentum and a combination of diffusion coefficients and a bulk mixing scheme at the surface (so called 'Kraus-Turner' schemes) for tracers. While there is indeed evidence that momentum is not as well mixed as tracers near the ocean surface, it is actually the turbulent vertical fluxes which mix the tracer field through the nonlinear advection term. For this reason the turbulent (eddy) diffusivities should be treated in the same way for both momentum and tracer fields. Nevertheless, this formal difference between the mixing of momentum and tracers is part of the ocean code up to and including version 4.4.

Large, McWilliams and Doney (1994), hereafter referred to as LMD, have proposed that mixing of both momentum and tracers should be done in terms of vertical diffusion coefficients alone, thereby abandoning the need for the Kraus-Turner bulk schemes for tracers. The layer at the ocean surface is now viewed as a boundary layer between the 'calmer' ocean in the thermocline and below, and the atmosphere above. This boundary layer is forced by the relevant surface fluxes above, and the mixing results from turbulent fluxes throughout the layer. The application of the relevant turbulent scalings results in the generation of vertical diffusion coefficients for both tracers and momentum. These coefficients are deemed to carry all the information necessary to represent the vertical mixing processes.

As the Met. Office ocean model has grown, so has the number of options and hence possible configurations. The scope of this report is thus aimed at detailing the possible vertical diffusion and mixing options available up to and including version 4.5 – it is up to the user to decide which combination is the best.

1. Implicit Vertical Diffusion Update

1.1 *Numerical Formulation*

In the end, whatever method is used to determine the vertical diffusion coefficients $K(z)$ where z is the vertical coordinate, a diffusion equation for a given parameter $'X'$ of the form,

$$\frac{\partial X}{\partial t} = \frac{\partial}{\partial z}\left(K(z)\frac{\partial X}{\partial z}\right), \tag{1}$$

needs to be solved. Since the vertical scales in the ocean model are much smaller than the horizontal scales, explicit updates of equation (1) would impose impossibly small values for the timestep. To that end equation (1) is solved fully implicitly by writing,

$$X_k^{n+1} - X_k^{n-1} = 2\Delta t \frac{\partial}{\partial z}\left(K(z)^{n-1}\frac{\partial X^{n+1}}{\partial z}\right)_k, \tag{2}$$

thereby guaranteeing a numerically stable solution. Here the time level is given by the superscripts, the vertical levels by the subscripts. The ocean code uses a leap-frog scheme in time (hence the $2\Delta t$ step), with the diffusion coefficients calculated as functions of the ocean state at the time level $(n-1)$.

The grid used in the vertical is shown in Figure 1, with the index 'k' labelling the positions of X increasing away from the ocean surface, whereas the actual depth 'z' increases upwards. The points where K is found lie half-way between each pair of X points, and are labelled by ν. Here the first K point is at the ocean surface given by $\nu = 1$; the first X point $k = 1$ is half-way between the first two K points. Figure 1 also shows relevant distances between grid points, the names being those used in the actual code. The variables dz and dzz are spacings between grid points, whereas zdz and $zdzz$ are the actual depths of each point relative to the ocean surface $z = 0$ at $\nu = 1$.

Resolving equation (2) spatially about grid point k gives,

$$X_k^{n+1} - X_k^{n-1} = \frac{2\Delta t}{dz_k}\left(\left(K^{n-1}\frac{\partial X^{n+1}}{\partial z}\right)_{\nu_k} - \left(K^{n-1}\frac{\partial X^{n+1}}{\partial z}\right)_{\nu_{k+1}}\right), \tag{3}$$

and so the differencing of the remaining spatial terms gives,

$$X_k^{n+1} - X_k^{n-1} = \frac{2\Delta t}{dz_k}\left(\frac{K_{\nu_k}^{n-1}(X_{k-1}^{n+1} - X_k^{n+1})}{dzz_{\nu_k}} - \frac{K_{\nu_{k+1}}^{n-1}(X_k^{n+1} - X_{k+1}^{n+1})}{dzz_{\nu_{k+1}}}\right). \tag{4}$$

Collecting all the forward $(n+1)$ terms on the left hand side of equation (4) yields,

$$-aa_k X_{k-1}^{n+1} + bb_k X_k^{n+1} - cc_k X_{k+1}^{n+1} = X_k^{n-1}, \tag{5}$$

where $bb_k = 1 + aa_k + cc_k$. This is a standard tridiagonal system which can be solved in any number of ways; in the present code the routines VDIFCALC and VDIFCALT do this for momentum and tracers, respectively. These routines set up the coefficients aa_k, bb_k, and cc_k. The matrix is assumed to be eliminated to form a lower-triangular system such that at each level k,

$$-ee_k X_{k-1}^{n+1} + X_k^{n+1} = ff_k. \tag{6}$$

Consider a pair of rows such that row $k+1$ is in equation (6) form, and row k in equation (5) form. Eliminating X_{k+1}^{n+1} between the equations for row $k+1$ and row k results in,

$$-aa_k X_{k-1}^{n+1} + (bb_k - cc_k ee_{k+1}) X_k^{n+1} = X_k^{n-1} + cc_k ff_{k+1}.$$

Tidying up gives the required form for row k as,

$$\left(\frac{-aa_k}{bb_k - ee_{k+1} cc_k} \right) X_{k-1}^{n+1} + X_k^{n+1} = \frac{X_k^{n-1} + cc_k ff_{k+1}}{bb_k - ee_{k+1} cc_k}. \tag{7}$$

This is in the form of row $k+1$ now, so the general forms for ee_k and ff_k are evident; and indeed these are the expressions used in the code. The terms ee_k and ff_k are dependent on ee_{k+1} and ff_{k+1}, respectively, so they are obtained by a sweep up the water column from $k = KM$ to $k = 1$. Once all the coefficients ee_k and ff_k are obtained, then a further single sweep down the water column obtains the required solution X_k^{n+1} from equation (6).

The problem is fully specified when the boundary conditions at the top and bottom of the water column are included. Clearly the base of the column will at some level k be bounded by land, and the boundary condition imposed there is to set $K_{\nu_k}^{n-1} = 0$ for each *land point* k. This feeds through into the matrix as $cc_k = 0$ for each *ocean point* k that is bounded below by land.

At the ocean surface $\nu = 1$ there may be a flux Q of X such that,

$$\left(K\frac{\partial X}{\partial z}\right)_{\nu=1} = Q. \tag{8}$$

Substituting this expression in equation (3) at point $k = 1$ the top two rows of the matrix now become,

$$bb_1 X_1^{n+1} - cc_1 X_2^{n+1} = ff_1$$

$$-ee_2 X_1^{n+1} + X_2^{n+1} = ff_2,$$

where $ff_1 = X_1^{n-1} + (2\Delta t Q)/dz_1$. Eliminating between rows 1 and 2 as before, the solution for the top row is then,

$$X_1^{n+1} = \frac{ff_1 + cc_1 ff_2}{bb_1 - ee_2 cc_1}. \tag{9}$$

In the routines VDIFCALC/T the upper boundary condition is determined by setting $aa_1 = 0$ and explicitly putting in the form for ff_1.

1.2 *Truncation Errors in the Vertical*

If the grid spacing in the vertical is a constant Δz, say, then the spatial differencing above results in a leading truncation error term proportional to Δz^2. This is true even if the diffusion coefficient K is not constant with depth.

However, it is not practical to perform climate simulations with a uniformly resolved ocean in the vertical. A non-uniform grid is necessary, and this was anticipated above by labelling the relevant grid spacings with the index k or ν_k. The truncation error in this case reduces to leading order terms of the form $Adz_k(1-r) + Bdz_k^2(1+r) + ...$ for constants A and B, where r is the ratio of successive layer depths, i.e., $r = dz_{k+1}/dz_k$. The effect of the nonuniform grid is to formally lower the trucation error to terms dependent on dz_k and $(1-r)$. Figure 2 shows r as a function of depth for a typical 20 level ocean configuration run at the Met. Office. Not only are there regions where r is not close to 1, but r itself suddenly changes at about $30m$ depth and again at about $1000m$.

Formally, the truncation error relates to how rapidly errors decrease as the resolution is varied. In climate simulation terms this may not be too relevant, given the relatively slow rate at which model resolution changes occur. However, the degree of grid nonuniformity r is known to impact on wave propagation, degrading the numerical dispersion relations further and introducing spurious wave reflections in regions where r is significant. The impact on the fully implicit solve detailed above is not clear; however, most of the ocean code is advanced explicitly, thus raising the (distinct) possibility of noise generation in the code by the nonuniform grid.

2. Richardson Number Dependent Parameterisations

So, given the relevant vertical diffusion coefficients, section 1 shows how the momentum and tracers can be updated. In this section the most widely used parameterisations of the vertical mixing coefficients are discussed. These schemes assume that the mixing depends only on the gradient Richardson number, Ri_g, at each point in the ocean:

$$Ri_g = \left(\frac{-g}{\rho_o}\frac{\partial \rho}{\partial z}\right) / \left((\frac{\partial u}{\partial z})^2 + (\frac{\partial v}{\partial z})^2\right), \tag{10}$$

where g is the gravitational acceleration, ρ_o and ρ are reference and actual densities, and u and v are the zonal and meridional velocities.

Parameterisations of this form are referred to as 'K-theory mixing', and the two in the code are those due to Philander and Pacanowski (1981) ('$P + P$') and Peters et al (1988). The diffusivities from these are set in the routines VERTCOFC/T for momentum/tracers, and at version 4.5 a logical L_OPANDP set to T/F selects $P + P$ or Peters et al, respectively. Although these schemes are strictly formulated to provide appropriate simulations of the equatorial undercurrent (in particular the strong shear zone at the undercurrent edges) the code sets the diffusivities from these schemes everywhere in the ocean, i.e., at all latitudes and longitudes and all depths.

In the deep ocean the above parameterisations result in small background values of the diffusivities relative to those in the upper layers. It turns out, however, that these

background values are *not* consistent with tracer diffusivities observed to occur in the ocean at depth (see Krauss (1990)). Indeed the background values are a few orders of magnitude too small. In order to overcome this weakness, a vertically profiled value of the tracer diffusivity *must* be added to the values arising from the K-theory schemes. This particular diffusivity is carried around by KAPPA_B_SI (set in routine OSETCON), and is a diffusivity that increases with depth. It is simply added to the diffusivities coming from the K-theory schemes for tracers in routine VERTCOFT.

2.1 *STATEC or STATED : That is the Question?*

As equation (10) shows, Ri_g depends on the vertical gradient of the density, or more correctly, the *potential* density. The ocean code has two routines for calculating the potential density ρ, called STATEC and STATED. The former calculates ρ with respect to a reference level either just above or just below the layers of interest. The latter finds the ρ of each layer relative to the surface.

The distinction between the routines arises from the nonlinear nature of the ocean equation of state for ρ, and the differences become exaggerated the deeper the layer of interest is. Indeed, using STATED actually results in negative values of Ri_g in some deep basins in the ocean (notably the Argentine and Brazil basins). The original code in VERTCOFC/T asserted that negative Ri_g should be set to $Ri_g = 0$; in the diffusion parameterisations, $Ri_g = 0$ results in the maximum values of the diffusion coefficients. Thus the incorrect use of STATED at depth results in erroneously high diffusivities in some basins.

While some may argue that high diffusivities at depth arising from the turbulent bottom boundary layer are realistic, it was never the intention of the $P+P$ and Peters et al schemes to produce them. And indeed, the proper application of a local measure of ρ through STATEC removes the problem altogether. This has been included in the version 4.5 code. The choice of which scheme to use is flagged by the logical variable L_OSTATEC, being T/F for STATEC/D, respectively.

3. Bulk Mixed Layer Schemes

The Richardson number schemes, while formally applied everywhere, are known to significantly underestimate the mixing that takes place in the relatively shallow zone between the atmosphere above and the calmer thermocline below. The effect on the momentum is to produce Ekman currents that are too strong relative to the local geostrophic currents, and that are too far to the right of the wind (in the northern hemisphere) (see Gordon and Roberts, 1997). The impact on tracers is to give surface layers that are too stratified relative to the well-mixed layers anticipated for tracers.

A solution to these problems is to implement a separate mixing scheme specifically for the surface region. And indeed such schemes for tracers are well documented, coming under the generic name of 'bulk mixed layer schemes'. The particular flavour used in the Met. Office ocean code is the 'Kraus-Turner' (K-T) bulk scheme, and is detailed in UMDP No. 41 by Foreman (1990). The scheme uses energetic arguements to mix the upper layer, guaranteeing neutrally stable vertical profiles for the tracers down to depths dependent on the balance between the energy available to drive the mixing, and the local structure of the layer being mixed.

The K-T scheme is fundamentally different from the diffusion equation approach in its application; the differential nature of the latter is to be contrasted with the 'physical' application of the former. However, when the K-T scheme is applied to tracers, the simulated upper layers are more than adequate representations of those observed. Applying K-T schemes to momentum is another matter; the vertical structures produced for tracers are not what are found for momentum, so the bulk schemes are clearly not at all appropriate in this case.

Early versions of the ocean model lived with this mixture; momentum was updated via a single diffusion equation solve (VERTCOFC/VDIFCALC), while the tracers had both a diffusion equation solve (VERTCOFT/VDIFCALT) followed by a K-T sweep (MIXLAY) to tidy up the upper layers. The surface current errors therefore remained.

4. Oceanic Boundary Layers : 'Large et al' Schemes

It would be satisfying if the vertical mixing of momentum and tracers came from a single formulation. The pick and mix nature described previously could then be abandoned. Such a formulation is described in LMD, in which mixing at *all* depths in the ocean can be cast in the form of equation (1). The major result of LMD is to find a prescription for the diffusion coefficient $K(z)$ that can represent the processes in the upper layers, in the thermocline region (particularly the equatorial undercurrent) and in the deep ocean.

LMD build on the experience of atmospheric modellers who treat the transition zone between the ground and the 'free air' above as a turbulent boundary layer. Within the oceanic boundary layer (OBL) the diffusion coefficients are found as parameterised functions of the vertical turbulent fluxes, and further depend on whether the surface forcing is stable/unstable, i.e., the tendency of the forcing to result in a more/less stable layer, respectively. Once the coefficients are obtained it is then a simple matter to solve equation (1) as described. The key for the ocean is to find the right parameterisation for $K(z)$ for the variety of conditions possible in the OBL for both tracers and momentum. LMD argue that their formulation is the key.

4.1 *The LMD Scheme*

The two steps leading to the diffusion equation for the boundary layer are,

$$\frac{\partial X}{\partial t} = -\frac{\partial < wx > (z)}{\partial z},$$

linking the time evolution of X by layer eddies to the vertical turbulent flux $< wx >$, and

$$< wx > (z) = -K(z)\frac{\partial X}{\partial z},$$

the assumption that the turbulent fluxes are dependent on the vertical gradient of X with the constant of proportionality being K. The result of these is to give equation (1).

The main steps in the LMD scheme are;

(1) Use the Richardson number parameterisations (or other equivalents) to set $K_0(z)$ at *all* depths in the ocean;

(2) Determine the forcing terms at the ocean surface;

(3) Find the boundary layer depth $h(x, y)$ consistent with the state of the water column at each point (x, y);

(4) Find $K(z)$ within the OBL between the ocean surface and $h(x, y)$ such that $K(z)$ suitably matches the values for $K_0(z)$ found in (1) at $h(x, y)$;

(5) Finally solve equation (1).

In the LMD scheme, the parameterisation for the diffusivity takes the form,

$$K(\sigma) = hw(\sigma)G(\sigma), \tag{11}$$

where $w(\sigma)$ is the turbulent velocity scale, $G(\sigma)$ is a dimensionless vertical shape function, and σ is the dimensionless coordinate varying between 0 at the ocean surface to 1 at a depth $d = h$ (i.e., $\sigma = d/h$ with d being the depth). This form shows that K is proportional not only to the turbulence within the layer through $w(\sigma)$, but also depends on the layer depth h, thereby reflecting the ability of deeper boundary layers to contain larger (and presumably) more efficient eddies. This choice of K also ensures that the surface layer turbulence is confined to the boundary layer.

The turbulent velocity scale is of the form,

$$w(\sigma) \approx \frac{\kappa_v u_\star}{\Phi(d/L)}, \tag{12}$$

where κ_v is von Karman's constant (usually 0.4), $u_\star$ is the friction velocity given by,

$${u_\star}^2 = \tau_o/\rho_o, \tag{13}$$

where τ_o and ρ_o are the surface stress and density, respectively. The Monin-Obukov length scale L is given by,

$$L = {u_\star}^3/(\kappa_v B_f), \tag{14}$$

where B_f is the surface buoyancy forcing.

The functions $\Phi(d/L)$ are empirically determined from measurements, but "there is no concensus about their precise functional form". The effect of $\Phi(d/L)$ is to scale

$w(\sigma)$ with respect to $\kappa_v u_\star$, such that $\Phi(d/L) = 1$ for neutral forcing, i.e., $(d/L) = 0$, and $\Phi(d/L)$ is less/greater than 1 for unstable $((d/L) < 0)$/stable $((d/L) > 0)$ conditions. These functions have different scalings for momentum and tracers; thus, along with the respective surface boundary conditions, the LMD formulation is able to accommodate all the vertical mixing processes in a single scheme.

4.2 *Ocean Model Flavours of the LMD Scheme*

At version 4.5, there are two possible implementations of the LMD scheme, referred to as 'Quadratic Large' (QL) and 'Full Large' (FL).

4.2.1 *QL*

This is a scaled-down version of the LMD scheme, and has been designed to deal with the surface current errors noted in section 3. The function $G(\sigma)$ is chosen to be a quadratic function, viz,

$$G(\sigma) = a_0 + a_1\sigma + a_2\sigma^2. \tag{15}$$

There is no turbulent transport across the ocean surface, implying that $K = 0$ there; this can only be satisfied by setting $a_0 = 0$. Equation (12) for $w(\sigma)$ is obtained on the basis that near to the surface $a_1 + a_2\sigma =< wx > (d)/ < wx > (0)$. Clearly, $a_1 = 1$ for this relationship to hold at the ocean surface. The remaining coefficient is set by requiring that K from equation (11) is equal to K_0 at the layer depth $d = h$, giving $a_2 = ((K_0(h)/(h\kappa_v u_\star)) - 1)$.

The QL scheme also takes the basic profile to be neutral, so that the function $\Phi(d/L)$ is always equal to 1. This approximation removes the need to find L and so the QL scheme is relatively insensitive to the surface forcing. A final concern is guaranteeing that K within the boundary layer be positive definite. For the coefficients in the QL scheme this is so since turning points will occur only when $\sigma = 1/(1 - (K_0(h)/(h\kappa_v u_\star)))$; clearly the turning points are outside the layer range $0 < \sigma < 1$.

The QL scheme improves the surface current errors, but as it is a reduced version of FL, it is not considered sufficient to provide a realistic mixed layer for tracers. It is therefore still necessary to use the K-T scheme through MIXLAY to generate the surface mixed layer for tracers. When the QL scheme is chosen through the logical variable L_OQLARGE, it is applied to both momentum and tracers by the setting of the diffusion coefficients in VERTCOFC/T and the solution of equation (1) in VDIFCALC/T, exactly as before.

4.2.2 *FL*

In FL advocated by LMD, the shape function $G(\sigma)$ is chosen to be a cubic, thereby introducing an extra constant a_3. The extra boundary condition is now not only continuity of K at h, but also continuity of the first derivative of K at h. Applying all these conditions at $d = h$ results in,

$$a_2 = -2 + 3G(1) - \frac{\partial G(1)}{\partial \sigma}, \qquad a_3 = +1 - 2G(1) + \frac{\partial G(1)}{\partial \sigma}, \tag{16}$$

with,

$$G(1) = \frac{K_0(h)}{hw(1)}, \qquad \frac{\partial G(1)}{\partial \sigma} = -\frac{\partial K_0(h)/\partial z}{w(1)} - \frac{K_0(h)\partial w(1)/\partial \sigma}{hw^2(1)}. \tag{17}$$

Note that the sign of $\partial K_0(h)/\partial z$ in equation (17) is correct; the derivatives are with respect to σ which increases (downwards) in the opposite sense to z. Using equation (17) to get $G(1)$ and $\partial G(1)/\partial \sigma$ leads to a_2 and a_3, and hence $G(\sigma)$. Unlike QL, FL evaluates the turbulent velocity scale $w(\sigma)$ in equation (12) using $\Phi(d/L)$.

Does the FL scheme guarantee a positive definite K in the upper layer? Since $a_0 = 0$ equation (11) can be written,

$$K(\sigma) = hw(\sigma)\sigma\Psi(\sigma), \qquad \Psi(\sigma) = 1 + a_2\sigma + a_3\sigma^2. \tag{18}$$

$\Psi(\sigma)$ at $\sigma = 0$ and $\sigma = 1$ is 1 and $G(1)$, respectively, thus at each end of the range of interest $\Psi(\sigma)$ is positive. To prevent a zero of $\Psi(\sigma)$ occurring between $\sigma = 0$ and $\sigma = 1$ it is sufficient to require that $\partial\Psi/\partial\sigma < 0$ at $\sigma = 1$. Using equations (16) and

(17) it can be shown that,

$$\frac{\partial \Psi}{\partial \sigma}(1) = \frac{\partial G(1)}{\partial \sigma} - G(1) = -\frac{\partial K_0(h)/\partial z}{w(1)} - G(1)(1 + \frac{1}{w(1)}\frac{\partial w(1)}{\partial \sigma}). \qquad (19)$$

Both $G(1)$ and $w(\sigma)$ are positive. If the forcing is unstable ($L < 0$) then LMD limit $w(\sigma)$ such that $\partial w(1)/\partial \sigma = 0$. In this case setting $\partial K_0(h)/\partial z \geq 0$ satisfies the constraint $\partial \Psi(1)/\partial \sigma < 0$. For stable forcing, it can be shown that the term multiplying $G(1)$ in equation (19) is positive, so that $\partial K_0(h)/\partial z \geq 0$ is again sufficient to guarantee positive $K(\sigma)$ for all conditions.

So, in order to prevent unphysical negative $K(\sigma)$ values in the boundary layer, the routines VERTCOFC/T check the sign of $\partial K_0(h)/\partial z$; if it is less than zero, then the code resets the value to be zero.

4.2.3 *UM Atmosphere Approach*

The LMD scheme is based on parameterisations used by the atmospheric modelling community. Following their lead, a variant used by the UM atmosphere modellers is now available within the ocean model. Equation (11) remains the basis for determining $K(\sigma)$; however $G(\sigma)$ is now taken to be,

$$G(\sigma) = \sigma(1 - a_4\sigma)^2, \qquad (20)$$

where, as before, $a_0 = 0$ and $a_1 = 1$ have been used to match the surface conditions. Unlike FL, equation (20) has only one free parameter, a_4. This is set by matching to $K_0(h)$. In this case, $K_0(h)$ is *not* the diffusivity from the background, but is a diffusivity K_{ent} parameterised in terms of an explicit entrainment velocity, w_{ent} say, calculated at the boundary layer depth h. The matching condition requires,

$$a_4 = 1 \pm \sqrt{G(1)}, \qquad (21)$$

where $G(1) = K_{ent}/(hw(1))$. The positive root for a_4 leads to a zero for $K(\sigma)$ in the boundary layer and so the negative root must be chosen. This choice in equation (20) guarantees a positive $K(\sigma)$.

The UM modellers impose a further constraint on a_4 by arguing that the $K(\sigma)$ profile should not peak at the boundary layer depth h. The reason for this is that it is felt that the contribution there should generally be smaller than that at the heart of the layer. This can be achieved by not letting a_4 get too small; i.e. effectively limiting the parameterised amplitude of K_{ent}. Thus, a_4 is chosen as

$$a_4 = max(1 - \sqrt{G(1)}, 2/3). \tag{22}$$

Note that the resultant K profile from this scheme will now be discontinuous at the layer base. The amplitude of this jump will presumably reflect the amount of entrainment occurring there. The details of this vertical entrainment scheme parameterisation ("VESPAR") to determine w_{ent} and hence K_{ent} are given in section 4.6.

4.3 *Numerical Aspects of the LMD Scheme*

The point of FL is the unification of vertical diffusion and mixing into a single formulation. The implementation of FL must therefore dispense with the K-T scheme. It is now important to consider where within the computational cycle to actually solve equation (1) using FL.

In the UM Ocean code, equation (1) is cast numerically in the form of equation (2), so that the required solution X_k^{n+1} is obtained by stepping forward from the previous solution X_k^{n-1}. This is the strict interpretation of equation (2) as written. However, the interpretation of X_k^{n-1} depends on when exactly equation (1) is solved within a single cycle of the ocean code.

There is no K-T scheme for momentum. Thus in routine CLINIC the time at which K is found via VERTCOFC and equation (1) is solved in VDIFCALC are not compromised by the use or otherwise of a LMD scheme. However, for the tracers using the K-T scheme, the actual step to obtain the mixed water column via K-T does not take place until other processes have been accounted for in the column of water. Such processes include the contributions due to penetrating radiation (in routine

SOLADD), surface changes due to fluxes between ice and the ocean (ICEFLUX), and adjustments preventing water temperatures falling below a minimum temperature TFREEZE (FREEZEUP). The surface fluxes of heat and salinity are also accounted for by assuming that they are initially absorbed in the top ocean layer (SFCADD). Once all these updates have been performed the K-T scheme proceeds to impose the full mixing.

As a consequence, the K-T scheme operates not on X_k^{n-1} but rather a next best update, $X_k^{\dagger(n-1)}$ say, incorporating all the processes just described. Separating out all the factors leading to $X_k^{\dagger(n-1)}$ enables a range of 'complex' physical processes to be applied that are not easily expressible in the simple differential form of equation (1). In VDIFCALC, conversely, the surface boundary fluxes *are* included. There is no 'splitting' of processes in the momentum update.

With K-T present VERTCOFT and VDIFCALT are performed *before* all the above-mentioned processes are added in. Clearly, if FL is to replace K-T, then equation (1) must be solved where K-T presently sits; in this way the diffusion process can update from $X_k^{\dagger(n-1)}$ which has incorporated the surface boundary conditions through SFCADD. Thus, when FL is used VDIFCALT must now be called from where MIXLAY presently is. This movement of VDIFCALT is important since equation (1) is solved in VDIFCALT subject to the upper boundary condition of zero flux through the ocean surface. The actual transfer of the boundary fluxes is of course via SFCADD which produces an update for $X_1^{(n-1)}$ in $X_1^{\dagger(n-1)}$ consistent with those fluxes.

Note that if SFCADD is called after VDIFCALT then the value of $X_1^{\dagger(n-1)}$ is simply the value placed in it by SFCADD. On the other hand, if SFCADD is called first, then the implicit solve in VDIFCALT implies propagation of the bottom boundary conditions up the water column in the first sweep, followed by the final update sweeping down the water column. The sweeps interact with $X_1^{\dagger(n-1)}$, modifying it on the way up, and then using that new value to influence the solution on the way down.

4.4 *The Boundary Layer Depth in LMD Schemes*

The final crucial element in the LMD schemes is the determination of the boundary layer depth h. At h, K in the OBL is to some degree 'forced' by $K_0(h)$ and its vertical derivative through equations (16) and (17). Furthermore, the amplitude of K is directly proportional to h (see equation (11)). LMD propose that h is determined by use of a bulk Richardson number of the form,

$$Ri_b(d) = \frac{(B_o - B(d))d}{|\mathbf{V}_o - \mathbf{V}(d)|^2 + V_t^2(d)}, \tag{23}$$

where B_o and $\mathbf{V}_o$ are the buoyancy and currents averaged over a near surface layer defined by $0 < \sigma < \epsilon$ (where typically $\epsilon = 0.1$), and $B(d)$ and $\mathbf{V}(d)$ are the respective values at depth d. The term V_t^2 is meant to account for turbulent velocity shear within the layer, which is "most important in pure convection and other situations of little or no mean shear". This is given as,

$$V_t^2(d) = A(N(d)dw(d)), \tag{24}$$

where A is a constant, and $N(d)$ is the stratification. Equation (24) has been derived by taking the case of pure convection, and then going over to the general case with the purely convective result as a necessary limit.

The term V_t^2 is intended to represent the impact of entrainment processes occurring at the base of the mixed layer. Thus h is not the depth of the mixed layer, h_m say, but will actually lie at some deeper point depending upon the relative amplitude of V_t^2 and the strength of the surface forcing through B_o. The 'typical mixed layer' on which LMD base their analysis to derive the V_t^2 is shown in Figure 3. The so-called 'penetrative convection' invoked by LMD generates eddies whose extent reaches beyond h_m, thereby enabling the entrainment of fluid from below. Between h_m and h there is a buoyancy jump of the order $B_o - B(d)$ (assuming, of course, that this layer is so well mixed that the buoyancy is constant from the surface down to h_m), and it is this jump that external processes have to work against in order to entrain the heavier material below. In generalising V_t^2 it is intended that Ri_b given by equation (23) will cover *all* processes leading to entrainment; the proof of this will be in the eating.

The depth h is defined to be where Ri_b is equal to a critical bulk number Ri_{bc}, say. The constants A and Ri_{bc} are determined by running a variety of experiments for different oceanic conditions, and obtaining the best fits to observations; LMD find that $A \approx 4.4$ and $Ri_{bc} \approx 0.3$ are appropriate.

4.5 *The LMD Boundary Layer Depth in the UM Ocean Models*

The QL version of the LMD scheme represents a (useful) simplification since it provides a fair representation of the turbulent Ekman layer. The depth h is set by using a *gradient* Richardson number and finding where a critical number CRIT_RI (usually 0.3) occurs. There is also a limit imposed on the maximum depth that h can be, set by the parameter MAX_QLARGE_DEPTH (usually 80 m); h is seen as a measure of the boundary layer depth and so it would seem sensible to limit its extent to the 'surface'. Clearly, in regions where strong convection from the surface downwards is occurring (for example the northern Atlantic in winter) then h on the basis of CRIT_RI alone could be many hundreds of metres.

CRIT_RI_FL and MAX_LARGE_DEPTH are the equivalent parameters for FL. The model can also set h via a gradient or bulk Richardson number using the routines CALC_MLD_LARGEG/B, respectively. The choices reflect the fact that the form recommended by LMD does not (at time of writing) produce an adequate seasonal variation in the modelled mixed-layer depths relative to the climatology. The experience is that using Ri_b with a CRIT_RI_FL of 0.3 and a MAX_LARGE_DEPTH of $80m$ produces mixed layers that are generally much too shallow, particularly in the southern ocean in the southern hemisphere summer months. The reasons for these results are not obvious, but appear to be related to the inability of the Ri_b to handle entrainment (and hence layer deepening) when stable layers are wind driven.

The best combination found to date is to use a gradient Richardson number with a CRIT_RI_FL of 1 and again set MAX_LARGE_DEPTH to $80m$, giving a depth h_g, say. If the layer is stably forced ($L > 0$) then a second depth h_L, say, is calculated which is proportional to L itself, since theory suggests that in such conditions L is a

natural scalelength for the boundary layer. If $L > 0$ then h is set to be the larger of h_g or h_L. Seasonal variations of mixed layer depths are now vastly improved relative to the Ri_b formulation.

4.6 *VESPAR Details*

Figure 3 shows that in the 'idealised' mixed layer, the buoyancy is close to a constant B_o down to h_m. There is then a jump ΔB at the layer base over a distance Δz before there is a more gradual decline in buoyancy into the thermocline and beyond. In terms of a turbulent flux of buoyancy $< wb >$ associated with the jump ΔB it is plausible to suggest that,

$$< wb > (h_m) \approx w_{ent} \Delta B \approx K_{ent} \Delta B / \Delta z, \tag{25}$$

so that the parameterisation we seek is simply $K_{ent} = w_{ent} \Delta z$.

In common with all these schemes, the critical issue is determining the boundary layer depth at which to find K_{ent}. At present this is done by finding where the gradient Richardson number exceeds CRIT_RI_FL (typically set to 1). The relationship between this point and the grid used in the model is shown in Figure 4. The Richardson number is found at the ν points. So, suppose the critical number is exceeded at $\nu = 3$; the boundary layer depth is then simply taken to be zdz_2 (see Figure 1). There is no attempt to interpolate between grid points. Since the density is found at the k points, the buoyancy jump calculated is that straddling the bottom of the layer, with an associated $\Delta z = dzz_3$ in this case.

If the surface forcing tendency is unstable, i.e., the Monin-Obukov length L is negative, then the "empirical rule of convection" is invoked, viz

$$< wb > (h_m) / < wb > (0) \approx constant \approx -0.2,$$

so that the upward flux at the surface $< wb > (0)$ is associated with a downward convective flux $< wb > (h_m)$ at the layer base. It is this "penetrative convection" that supplies the excess turbulent kinetic energy to enable entrainment of fluid below the

layer to be mixed up into the layer, thereby leading to layer deepening. Identifying $< wb > (h_m) = -w_{ent}\Delta B$ (as before) the parameterisation is then

$$w_{ent} = \frac{0.2 < wb > (0)}{\Delta B}. \tag{26}$$

In the stable case it seems pertinent to appeal to the bulk layer ideas used to derive the Kraus-Turner scheme. If the wind mixing energy through ${u_\star}^3$ is the dominant term then (approximately),

$$w_{ent} h_m \Delta B \approx 2\lambda {u_\star}^3 f(z), \tag{27}$$

where λ is a constant (typically 0.7), and $f(z)$ is a term that modulates ${u_\star}^3$ so that its effect dimishes with depth. Typically $f(z) = exp(-z/\delta)$, where δ is a constant of the order of $100m$.

4.7 *Vertical Components from Isopycnal Diffusion*

Routine TRACER is the driver for the tracer processes. In particular, the isopycnal diffusion is implemented here. As the Ocean UMDP 51 by Roberts (1999) details, all the components of the isopycnal diffusion that contain horizontal derivatives are updated explicitly via routine ISOFLUX. The purely vertical component (labelled 'zz' in the matrix) has to be updated implicitly to avoid severe timestep constraints. This isopycnal component is added to that set in VERTCOFT (through variable GNU) in routine AI_CALC, eventually emerging in variable K33. Before VDIFCALT is finally called to do the total vertical diffusion update, K33 is passed into variable FK3_GNU.

4.8 *UMUI Vertical Diffusion at Version 4.5*

To take account of the unification implied by FL, the UMUI windows at version 4.5 now reflect the extra choices available. They are clearly set up to reflect the fact that FL and K-T are mutually exclusive; you can only have one or the other. And as previously noted the logical variable L_OPANDP is available to select between $P+P$ or Peters et al.

One extra choice of interest relates to the method used to calculate the surface friction velocity $u_\star$, defined in equation (13). There $u_\star$ is given in terms of the magnitude of the stress τ_o. However, the stress is a function of the atmospheric winds, and so the value passed to the ocean within the model depends on how often the atmospheric fields are coupled to the ocean. This coupling period is usually taken to be one day, i.e., over each atmospheric timestep (typically half an hour) τ_o is recorded, summed and then meaned before being finally used to force the ocean.

The stress, however, is a vector, so that it is plausible that over a day the components could reverse, leading to a mean value close to zero, whereas in fact there had been significant forcing applied throughout the day. To overcome this possible shortfall, $u_\star$ can be calculated using not a vector but a scalar, the so-called wind mixing energy (wme), such that,

$$u_\star{}^3 = wme_o/\rho_o. \tag{28}$$

A logical variable L_OUSTARWME reflects this choice, being T/F for $u_\star$ being found through equation (28)/(13), respectively.

5. Testing the Vertical Mixing Schemes

It has to be said that LMD present a fairly exhaustive set of tests of their scheme, for both a range of surface forcing conditions, and (just as importantly) for different vertical grid spacings and staggerings. In particular there are a lot of "single column model" experiments that permitted tuning of the various parameters advocated by LMD. And indeed it is this flexibility that is perhaps most appealing about the LMD scheme; it is arguably more appropriate than the bulk models for the general range of conditions and scales that are found both in the ocean and in the ocean models, and the mixing formulation for tracers and momentum is unified.

However, it also has to be said that our experience with the FL version of the LMD scheme is that it does not do a good job of modelling the wind-driven stable layers, particularly those in the southern ocean around March; the tendency is for

the layers to be too shallow, thus warming (even more) the southern ocean relative to climatology. This weakness motivated the inclusion of VESPAR which, despite the simplicity (and crudeness) appears to work very well in all seasons. Unlike LMD, however, VESPAR has only been tested in the global ocean model. No specific test tuning has been done (although experience from the Kraus-Turner modelling has of course been used).

Caution then in the long run. There is a very strong grid dependence built into these schemes, first through the determination of the boundary layer depth, and then through the parameterisation of the processes at that depth. LMD appeal to continuity in their matching, and interpolate so that the scheme appears to operate on (piecewise) continuous information. This would seem to reduce the grid dependence to some degree, and is suggested by the results from their tests. However, the weak link in LMD appears to revolve around determining the layer depth; the use of R_{ib} in equation (23) does not seem to capture the entrainment processes satisfactorily, despite the presence of V_t^2.

By directly attacking the entrainment flux, VESPAR mitigates the LMD problems (at least for the global model). However, there is a very strong grid scale built in, since there is no attempt to interpolate, and the buoyancy jump is entirely that found between the grid points spanning the critical depth. Furthermore there is an inbuilt arbitrariness in that the coefficient a_4 is limited in amplitude in order to maintain a "realistic" diffusion profile through the boundary layer; this may be appropriate when there are many grid points resolving the layer, but may be suspect when the layers are shallow and hence (relatively) poorly resolved.

For present coarse vertical scales, the VESPAR approach may be entirely appropriate. However, as the grid scale decreases further there are legitimate concerns over both the determination of the layer depth, and exactly where the buoyancy jump is that contributes to the entrainment flux. It may be that VESPAR in its present form will scale poorly to finer grids, whereas LMD will perform well. Time alone will tell.

ACKNOWLEDGEMENTS

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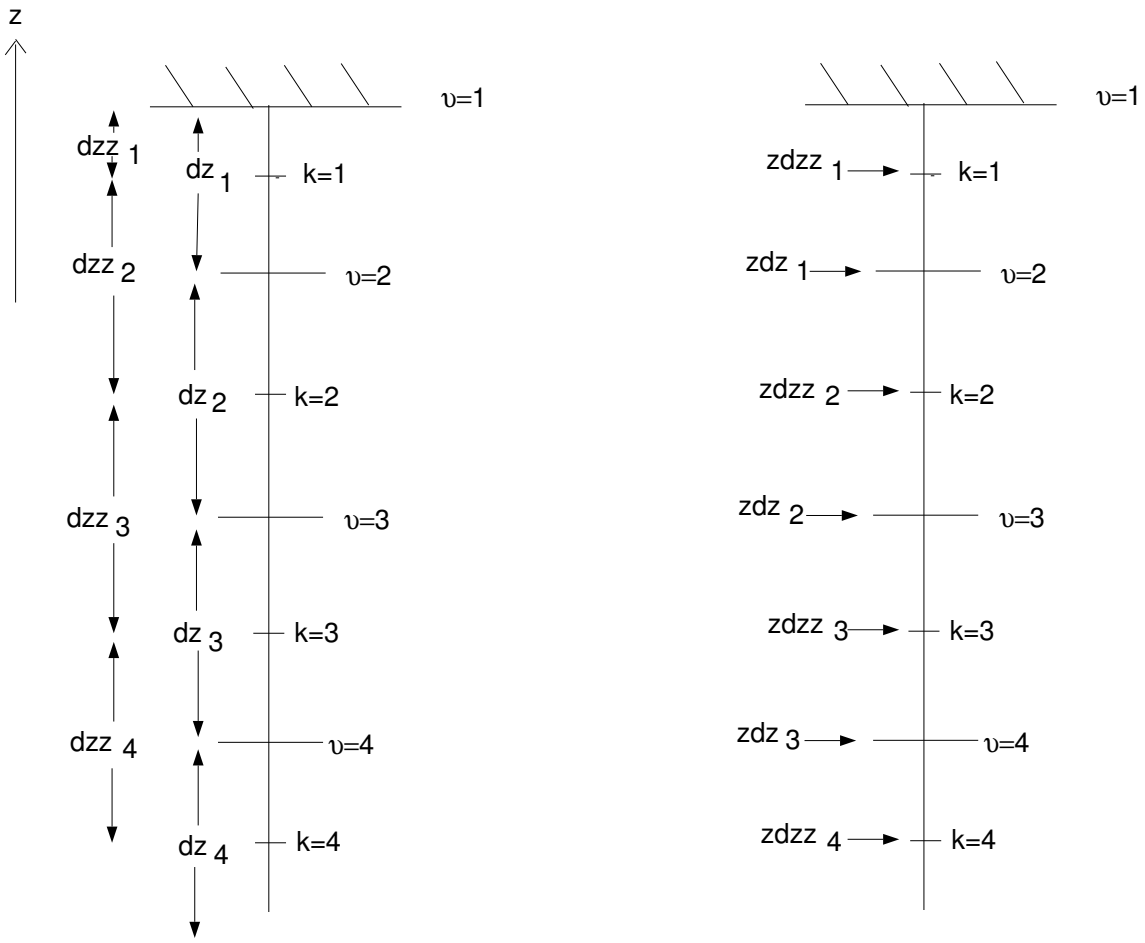

Figure 1

Figure 1: Vertical grid labelling in the ocean model.

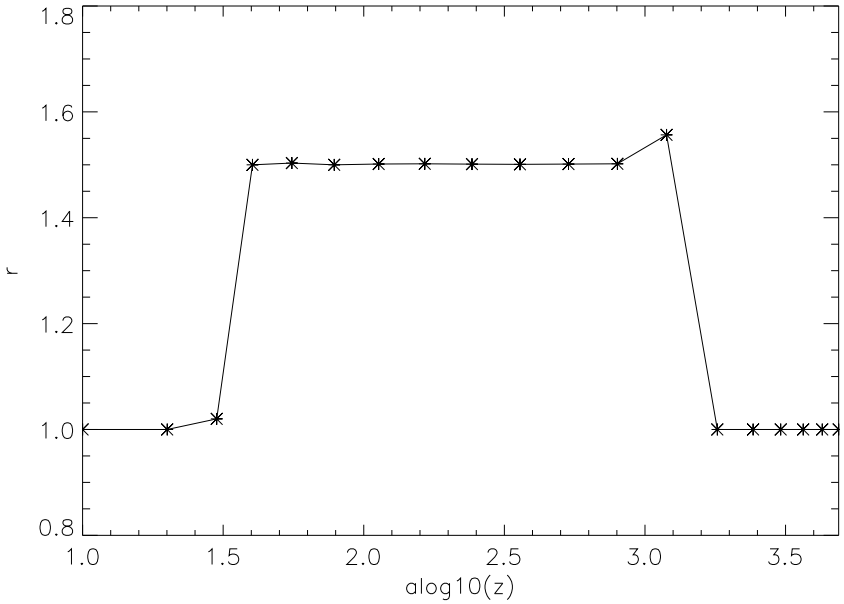

Figure 2

Figure 2: Rate of change of grid spacing 'r' with depth for typical model set-up.

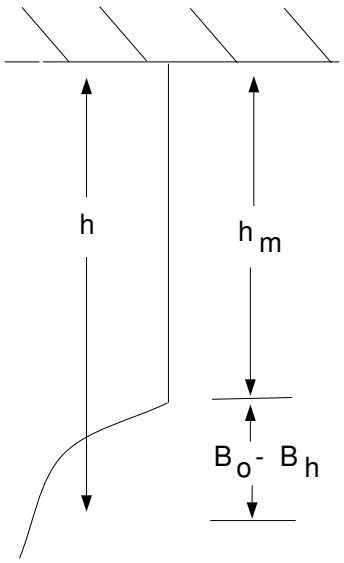

Figure 3

Figure 3: Boundary layer depth definitions for a typical well-mixed zone.

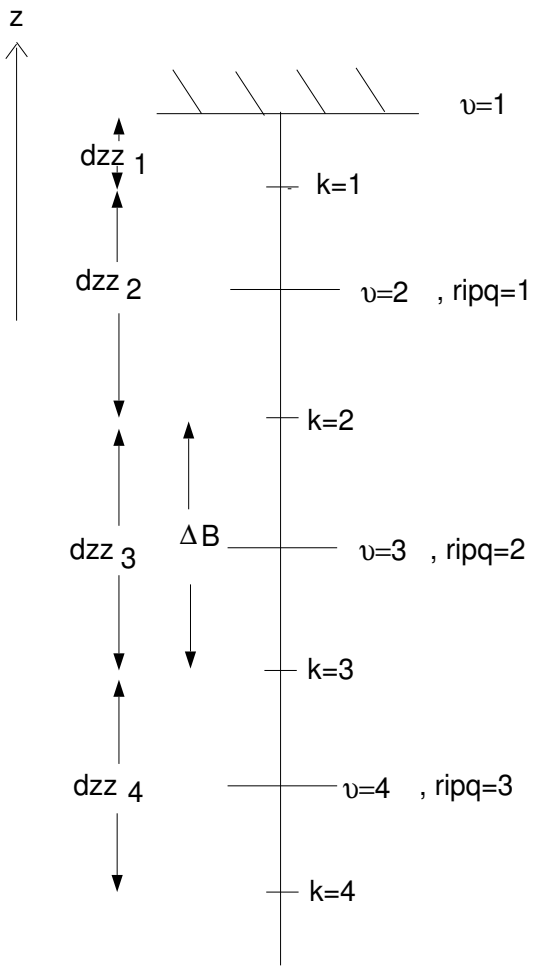

Figure 4

Figure 4: Grid labelling for VESPAR scheme.