1. INTRODUCTION

There are two main areas where the ocean is important in climate change. Firstly, it is an active lower boundary to much of the atmosphere, for which it is a major source and/or sink of heat, water vapour and carbon dioxide. Secondly, sea-level changes have a direct affect on the coastal environment.

In order to understand the ocean’s role in climate change it is necessary to be able to model the entire depth of the ocean, not just the surface layers. Present day numerical ocean general circulation models (OGCM’s) suffer a number of deficiencies:

1. Climatically important quantities such as poleward heat flux are sensitive to the parameterization of unresolved mixing processes. Present estimates of the vertical diffusivity in the ocean vary by almost two orders of magnitude [2].

2. The present ocean velocity climate is not well-known, which makes validation and tuning of OGCM’s difficult.

Tracer conservation equations provide a relation between velocity, tracer gradients, mixing coefficients and tracer source/sink terms. Several methods exist for inverting these equations to obtain ocean currents, mixing coefficients and source/sink distributions (if the tracer is not conservative). Additional constraints are provided by the assumptions of geostrophy and continuity. The tracer conservation equations are integrated vertically between two neutral surfaces to improve accuracy, and a geostrophic streamfunction is introduced to reduce the number of unknowns. The resulting equations are discretized,
and the matrix equation inverted to find reference level velocities, mixing coefficients and unknown source/sink terms for non-conservative tracers.

The matrix system is typically under-determined; a unique solution is obtained by minimizing a derivative norm of the solution. Positivity constraints are added for mixing coefficients, and for source/sink coefficients where applicable. An example inversion is presented for a section of the eastern North Atlantic influenced by the Mediterranean Water tongue. It is shown that the solution can alter drastically as a function of the relative weighting between solution variables.

Tests conducted with a two-dimensional advective/diffusive problem where the answer is known indicate that the under-determined formulation with a derivative norm has the potential to provide quite accurate answers. Two practical problems remain: firstly, there are many parameters to be estimated, such as smoothing norm differential order and length scales, signal to noise ratio, prior solution mean and relative weighting between different types of unknowns (in this case velocity and mixing coefficients); secondly, an estimate of the validity of the inverse solution is needed. A possible candidate for the parameter estimation problem is a suitable modification of the technique of generalized cross validation (GCV).

2. TRACER CONSERVATION EQUATIONS

The steady-state conservation equation for a tracer $C$ in neutral surface coordinates is [9]

$$
\left[ \mathbf{V}_n - \nabla_n K - K \frac{\partial}{\partial z} (\nabla_n N) \cdot \nabla_n C + eC_z \right]
= K \nabla_n^2 C + (DC_z)_z - \lambda C
$$

where $\mathbf{V}_n$ is the horizontal velocity in a neutral surface, $e$ is the dianeutral velocity (vertical velocity through the surface), $\nabla_n$ is the lateral gradient operator in a neutral surface, $N$ is the height of a neutral surface, $K$ is the epineutral diffusivity, $D$ is the dianeutral diffusivity and $\lambda$ is a consumption coefficient.
The tracer conservation equations are written in the neutral surface framework because mixing is thought to occur preferentially in this plane, which is locally perpendicular to the gradient of buoyancy [8]. The mixing rate is about seven orders of magnitude larger in this plane than perpendicular to it. Using the wrong surface means that some of the much larger quasi-horizontal mixing will be interpreted as vertical mixing. Ocean currents and heat fluxes have been shown to be very sensitive to the magnitude of vertical mixing [2].

The obvious way to proceed is to write the tracer conservation equation on a neutral surface for each tracer, and solve for the 7 unknowns

\[ V_n = (u, v), e, K, D, D_z, \lambda \]

as functions of \((x, y)\).

There are two points to note here:

1. Potential temperature \(\theta\) and salinity \(S\) are related on a neutral surface by \(\alpha \nabla_n \theta = \beta \nabla_n S\), where \(\alpha\) is the thermal expansion coefficient and \(\beta\) is the saline contraction coefficient [8]. Hence only one of these tracers may be used;

2. Vertical second derivatives of the tracer field are needed. These tend to be difficult to estimate accurately in the deep ocean.

A better strategy is to vertically integrate the tracer conservation equation between two neutral surfaces. Now \(\theta\) and \(S\) give independent information (because \(\alpha\) and \(\beta\) are different functions of depth), and only vertical first derivatives of \(C\) are needed.

One problem is that the number of unknowns has grown enormously; we now need to estimate the unknowns as functions of \((x, y, z)\). It transpires that the number of unknowns can be reduced to 6 on a two-dimensional surface by the use of dynamical constraints, and some simplifying assumptions.

Geostrophy is considered a good assumption in the deep ocean. In addition, it may be shown that a geostrophic streamfunction exists in a neutral surface [11]. Hence the horizontal
velocity on any surface may be written in terms of a streamfunction \( \psi \) on a reference surface:

\[
V_n(z) = f^{-1}k \times \nabla_n \psi + V_{tw}(z)
\]

where

\[
V_{tw}(z) = -\frac{\partial}{\rho f} \int_{z_0}^{z} k \times \nabla_n \rho \, dz
\]

is the thermal wind, \( f \) is the Coriolis parameter, \( \rho \) is water density and \( g \) is the gravitational acceleration.

Geostrophy plus continuity give the linear vorticity balance on a neutral surface [10]

\[
e_z = \frac{\beta u}{f} - \frac{\partial}{\partial z} (V_n \cdot \nabla N)
\]

which can be integrated vertically to give an equation of the form

\[
e(z) = e_0 + \frac{\beta \psi_x}{f^2} (z - z_0) + \frac{\beta}{f} \int_{z_0}^{z} v_{tw} \, dz' - [V_n \cdot \nabla_N]_{z_0}^{z}
\]

where \( \beta \) is the latitudinal derivative of \( f \), \( e_0 \) is the dianeutral velocity on the reference surface, and \( v_{tw} \) is the second component of the thermal wind (4).

It may be shown that if a streamfunction is used, and linear vorticity is enforced exactly, then the resultant velocity field satisfies continuity exactly. Hence it will not be necessary to explicitly include the continuity equation in the inversion.

3. INVERSE MODEL FORMULATION

The tracer equation (1) is now integrated from a point on the reference neutral surface \( z = z_0 \) to a point on another neutral surface \( z = z_a \), which should be sufficiently far from the reference level to ensure that a number of data points are contained between them; otherwise the advantage of vertical integration is lost. The velocity is replaced in terms of the streamfunction at the reference level and the thermal wind according to (3), the vertical
velocity is replaced using (6), and unknown terms are collected on the left-hand side:

\[
(-\psi_y/f, \psi_x/f) \cdot \left( \int_{z_0}^{z_a} \nabla_n C \, dz - \int_{z_0}^{z_a} (\nabla_n N) \, C_z \, dz + \nabla_n N \bigg|_{z_0} (C_a - C_0) \right) + \psi_x \frac{\beta}{f^2} \int_{z_0}^{z_a} (C_a - C) \, dz - \nabla_n K \cdot \int_{z_0}^{z_a} \nabla_n C \, dz
\]

(7) \[+ K \left( -[\nabla_n N \cdot \nabla_n C]_{z_0}^{z_a} + \int_{z_0}^{z_a} \nabla_n N \cdot \frac{\partial}{\partial z} (\nabla_n C) \, dz - \int_{z_0}^{z_a} \nabla_n^2 C \, dz \right) + D_0 C_z|_{z_0} - D_a C_z|_{z_a} + e_0 (C_a - C_0) + \lambda \int_{z_0}^{z_a} C \, dz \]

\[= -\int_{z_0}^{z_a} V_{tw} \cdot \nabla_n C \, dz + \int_{z_0}^{z_a} (V_{tw} \cdot \nabla_n N) \, C_z \, dz - \frac{\beta}{f} \int_{z_0}^{z_a} v_{tw} (C_a - C) \, dz \]

Integration by parts has been used where possible to simplify terms, and to ensure that vertical derivatives of \( \nabla_n N \) are eliminated in favour of vertical derivatives of the tracer. The latter should be less prone to numerical error. It has been assumed that \( K \) and \( \lambda \) are independent of depth.

There are six unknowns in (7):

(i) \( \psi \), streamfunction on the reference surface \( z = z_0; \)

(ii) \( K \), average epineural diffusivity between the two depths;

(iii) \( D_0 \), dianeutral diffusivity on the reference surface;

(iv) \( D_a \), dianeutral diffusivity on the surface \( z = z_a; \)

(v) \( e_0 \), vertical velocity through the reference surface;

(vi) \( \lambda \), average biological consumption coefficient between the two depths (oxygen only).

Equation (7) is written in finite-difference form on a uniform grid for each available tracer, giving the matrix system

(8) \[ A x = b \]

where each line of \( A \) represents one discrete equation for one grid cell, and each element is the coefficient of a variable, \( x \) is the model vector containing all the variables on a two-
dimensional grid:

\[ x = \begin{bmatrix} \cdots \psi_{ij} \cdots K_{ij} \cdots D_{ij}^0 \cdots D_{ij}^u \cdots e_{0}^j \cdots \lambda_{ij} \cdots \end{bmatrix}^T \]

\[ = \begin{bmatrix} \Psi^T & K^T & D_{0}^T & D_{u}^T & e_{0}^T & \Lambda^T \end{bmatrix}^T \]

and \( b \) is the data vector containing the known forcing terms in the tracer equation.

Once (8) has been inverted to find all the variables comprising \( x \), one can diagnose for the three-dimensional horizontal flow field \( V_n(z) \) using (4), the dianeutral velocity \( e(z) \) using (6), and \( D(z) \) using the original tracer equation (1).

4. INVERSION METHOD

The system of equations (8) is underdetermined; a unique solution is obtained by minimizing a weighted measure of solution size:

\[ x^T W_x x = \begin{bmatrix} a^2 W_{\psi} & 0 & \cdots \\ 0 & b^2 W_K & \cdots \\ \vdots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} a^2 W_{\psi} & 0 & \cdots \\ 0 & b^2 W_K & \cdots \\ \vdots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} \Psi \\ K \end{bmatrix} \]

where \( a, b, \text{etc.} \) are constants determining the relative weighting between the constituent variables of \( x \).

The least-squares criterion, where \( W_x \) is just the unit matrix, often gives poor solutions. For example, it is not at all clear that the size of \( \psi \) should be made small. It would be better to minimize a physically interpretable quantity such as kinetic energy (although, again, it is not at all clear that this is appropriate.)

There are a number of mathematically desirable properties that any solution should possess:

1. \( \psi \) must be differentiable to obtain velocity;
2. The solution should be sufficiently differentiable so that the finite-difference scheme used to obtain \( Ax = b \) converges.
In order to ensure that the solution is suitably differentiable, it is necessary to define the weight matrices in terms of a Sobolev norm [1]. These norms contain the integral of the sum of the squares of all possible derivatives up to some order. An example (in two dimensions) is

\[
\|f\|^2 = \iint \left\{ f^2 + 2I^2 (f_x^2 + f_y^2) + t^4 (f_{xx}^2 + 2f_{xy}^2 + f_{yy}^2) + \cdots \right\} \, dx \, dy
\]

In two dimensions, if the highest weak derivative in the norm is of order \(d\), then \(f\) is continuously differentiable of order \(d - 2\) [1].

In discrete form, each weight matrix \(W_\Phi, W_K\) etc. in (10) represents a Sobolev norm (also referred to as a smoothing norm) of the form

\[
W = \sum_{i=0}^{d} t^2 D_i^T D_i
\]

where (in the case of a one-dimensional grid for clarity)

\[
D_i = \frac{1}{\Delta x} \begin{bmatrix}
-1 & 1 \\
-1 & 1 \\
\vdots & \ddots & \ddots \\
\vdots & & \ddots & \ddots \\
-1 & 1
\end{bmatrix}
\]

In two dimensions, this matrix will look slightly different because of the need to represent derivatives in each dimension.

It may be shown that there is a one-to-one correspondence between the deterministic approach to inverse problems and the statistical approach, where the prior solution covariance function (or matrix) is specified, and a minimum variance solution sought [13]. \(W_x\) may be interpreted as the inverse of the solution covariance matrix \(C_x^{-1}\).

The equivalent covariance function for the norm given by (11) may be shown to be [12]

\[
C(r) = (r/l)^{d-1} K_{d-1} (r/l)
\]
where $K_{d-1}$ is the modified Bessel function of order $d - 1$. In discrete form, the equivalent covariance function can always be determined numerically by inverting $W_x$. The parameter $l$ may be interpreted as a length scale for fixed $d$ (see Fig. 1). The highest derivative appearing in the norm affects the shape of the equivalent covariance function. Two choices are compared to a Gaussian covariance function in Fig. 2. It should be noted that $l$ is not a good measure of the width of the peak. A better measure is the integral length scale

$$I_l = \int_0^\infty |C(r)/C(0)| \, dr$$

and it is this value which remains constant for all covariance functions in Fig. 2.

Figure 1. Dependence of covariance function associated with the $d = 2$ norm on length parameter $l$.

Figure 2. Smoothing norm equivalent covariance functions for $d = 2$ ($l = 1.3$) and $d = 5$ ($l = 0.6$) compared to a Gaussian profile. The integral length scale (area under the curve) has the value 2 for all functions.
One reason for dwelling at some length on the covariance function interpretation of the smoothing norm method is that the solution will shortly be interpreted as being composed of a sum of covariance functions. This in turn gives some idea of the consequences of choosing large or small values for $l$.

In the underdetermined case, it is always possible to satisfy the equations exactly. However, one can allow for equation error by minimizing an augmented version of (10):

\begin{equation}
    e^T W_e e + \mu^2 x^T W_x x
\end{equation}

where $e = Ax - b$ is the equation error and $\mu$ is a parameter which trades-off smoothing against satisfaction of the equations. Two forms of the solution which minimizes (16) are:

\begin{equation}
    x = \left( A^T W_e A + \mu^2 W_x \right)^{-1} A^T W_e b
\end{equation}

and

\begin{equation}
    x = W_x^{-1} A^T \left( AW_x^{-1} A^T + \mu^2 W_e^{-1} \right)^{-1} b
\end{equation}

It is clear from this last form that the solution is represented in terms of a linear combination of the columns of $W_x^{-1}$, that is, as a linear combination of covariance functions. The same interpretation is made in the case of data interpolation based on the Gauss-Markov theorem (statistical interpolation or objective mapping) [12].

It is believed that mixing coefficients should be positive. However, most of the early solutions obtained had negative mixing coefficients in some places. It is possible to enforce positivity on the mixing coefficients (and on the consumption coefficient $\lambda$ where applicable, as is the case when the tracer is oxygen), using programs provided by Menke [13]. One of the disadvantages of this procedure is that it is no longer possible to explicitly write down the solution in a form like (17) or (18), and so it is harder to see the structure of the solution. In particular, it is entirely possible that the solution will no longer be representable as a linear combination of the data, because one could envision a case where the data is all zero,
but the solution is restricted to be non-trivial. However, an advantage of using positivity
constraints is that they will show whether the information at hand is consistent with positive
mixing coefficients.

5. NORTH ATLANTIC MODEL

The data set and region studied here are the same as used by Hogg [5]. That is, a subset
of the 1° Levitus [7] data set in the eastern North Atlantic is used, over which an 8×8 grid is
defined with a spacing of 3°, from 43.5°W to 22.5°W, and from 22.5°N to 43.5°N. Neutral
surfaces are chosen to match the depth of Hoggs’ potential density surfaces at the centre of
the region. The tracer equation (7) is written in finite-difference form at each point of the grid
for which a centred-difference estimate of $\psi$ and $K$ horizontal derivatives is available. Hence
all edges and corners of the grid are excluded, as well as points surrounding a seamount in the
northeast corner of the region. The Levitus data set has already been smoothed horizontally
with a length-scale of 700–1000 km. No further smoothing was done here.

The discretized tracer equation is written for the three tracers: potential temperature,$\theta$; salinity, $S$; and dissolved oxygen, $O_2$. This leads to a system of 96 equations in 238
variables. The variables comprise 55 each of $\psi$ and $K$ on the full grid, but excluding corners
and a region around the seamount, and 32 each of $D_0$, $D_u$, $e_0$ and $\lambda$ at each point for which
an equation is written.

The norm length scale $l$ is chosen to be comparable to the spatial averaging of the Levitus
data set (about 700km), and to be the same for each variable. The relative weightings between
variables ($a$, $b$ etc.) are chosen to be inversely proportional to an estimate of the size of the
variable. This is an unsatisfactory procedure. The values chosen are very rough estimates,
particularly in the case of $\psi$, and the solution tends to have a magnitude of about these
estimates.

Results were accordingly disappointing. Although it was possible to obtain a solution
when positivity constraints were enforced, the solution could look quite different depending on the relative weighting between different variables. Two solutions for the streamfunction only are shown in Fig. 3 and Fig. 4. There is a considerable difference between them, and neither resemble Hoggs' solution (not shown here).

Figure 3. Streamfunction on reference surface. Typical velocity is 0.1 mm/s.

Figure 4. Streamfunction on reference surface. Typical velocity is 1.0 mm/s.
It would appear that there is much to be learnt about choosing parameters in underdetermined inverse problems. To gain some experience in a simple problem where the answer is known, a two-dimensional advective/diffusive problem is studied.

6. SIMPLIFIED TEST PROBLEM

Fiadeiro and Veronis [4] and Lee and Veronis [6] have studied a simplified advective/diffusive inverse problem in a two-dimensional channel. Their steady-state tracer conservation equation is

\[
\nabla \cdot (\mathbf{v}c) - \nabla \cdot (K \nabla c) = \lambda c
\]

where \( c \) is the tracer concentration, \( \mathbf{v} \) is velocity, \( K \) is the mixing coefficient and \( \lambda \) is a consumption or decay coefficient. Conservation of mass is ensured by the introduction of a streamfunction \( \psi = k \times \nabla \psi \) where \( k \) is normal to the plane of the channel. The tracer conservation equation becomes

\[
k \cdot \nabla \psi \times \nabla c - \nabla \cdot (K \nabla c) = -\lambda c
\]

The forward problem is: knowing \( \psi \) and \( K \) and values of \( c \) or its derivatives on the boundary, find \( c(x, y) \) in the interior.

The inverse problem is: knowing \( c(x, y) \) (maybe more than one tracer) in an interior region of the channel, estimate \( \psi \) and \( K \) in that region.

It should be noted that if two linearly independent tracers are available, then the only factor preventing the estimation of \( \psi \) and \( K \) by solving (20) as a forward problem is the absence of suitable boundary conditions.

The imposed streamfunction together with the solution of the forward problem for two tracers are shown in Fig. 5, Fig. 6 and Fig. 7 respectively.
Two inversion regions are considered: one in the uniform flow region at the eastern end of the channel, and the other containing the smaller of the two eddies. Data is taken at every second numerical grid point used in the forward calculation to introduce truncation error. The reader is referred to the work by Lee and Veronis [6] for further details.
Many experiments were carried out, of which only a few are shown here. The stream-function and diffusivity in the uniform flow region are shown in Fig. 8 and Fig. 9 respectively. The goal of the inversions is to reproduce these figures as accurately as possible.

![Figure 8. True streamfunction in uniform flow region.](image)

![Figure 9. True diffusivity in uniform flow region.](image)
The first experiment is to calculate the standard least-squares solution. This is shown in Fig. 10 and Fig. 11. Clearly it is a bad estimate of the true solution.

A much better solution is obtained by using a smoothing norm with \( d = 2 \) and the length scale \( l \) chosen to be 10 grid units. The relative weighting between \( \psi \) and \( K \) was chosen to be approximately the true value, but a factor of 3 either way made little difference to the solution. The solution is shown in Fig. 12 and Fig. 13. This may be seen to be an unfair test because the underlying solution is quite smooth, but it does indicate the utility of the
smoothing norm approach in obtaining a smooth solution. Note that the diffusivity is positive everywhere, and that no positivity constraints were used.

![Figure 12. \( d = 2, l = 10 \) norm streamfunction in uniform flow region.](image)

Figure 12. \( d = 2, l = 10 \) norm streamfunction in uniform flow region.

![Figure 13. \( d = 2, l = 10 \) norm diffusivity in uniform flow region.](image)

Figure 13. \( d = 2, l = 10 \) norm diffusivity in uniform flow region.

The second experiment involved the small eddy region; the true solution is shown in Fig. 14 and Fig. 15, while one of the best solutions obtained by trial-and-error is shown in Fig. 16 and Fig. 17. This solution used different length scales for \( \psi \) \((l = 2)\) and \( K \) \((l = 14)\). If a uniform length scale of \( l = 10 \) was used, the \( \psi \) solution hardly resolved the eddy (it looked very like the uniform flow region solution), and the diffusivity was smooth but
negative in some places. Clearly it is necessary to have a good idea about the length scales expected in the solution. In this case, there is much more detail in the flow field than in the diffusivity, and choosing norm length scales to reflect this gives good results.

Many more experiments were conducted, and all indicated the same thing: it is important to estimate the various parameters such as length-scales, norm differential order, relative weighting between different variables, and equation error in a consistent and accurate manner in order to get an acceptable solution to an underdetermined inverse problem.
7. PARAMETER ESTIMATION

Generalized cross-validation (GCV) provides a measure of the error in predicting the “data” (right-hand side of the equations) when they are excluded one at a time from the inversion [3] [14]. The average prediction error may be approximated without repeatedly
inverting the matrix A with one row missing. The expression is:

\[ V = \frac{N^{-1}e^TW_e e}{\|N^{-1}\text{tr}(I - AA^{-g})\|^2} \]

\[ = \left( \frac{\text{Mean weighted equation error}}{\text{Mean diagonal non-resolution}} \right)^2 \]

The second expression comes from noting that \( AA^{-g} \) is the “data” resolution matrix \([13]\) relating the observed and predicted “data” values according to

\[ b_{\text{pred}} = AA^{-g}b_{\text{obs}} \equiv R_{\phi}b_{\text{obs}} \]

Ideally, the resolution matrix should equal the unit matrix, so that the observed data are reproduced by the model. The extent to which the diagonal elements of \( AA^{-g} \) are different from unity is one measure of the inability of the system to perfectly resolve the “data”. Hence GCV can be interpreted as optimizing the “data” fit (that is, the equation error) relative to the systems ability to resolve the “data”.

GCV can be used to estimate unknown parameters such as length scales, highest derivative in the smoothing norm and the amount of smoothing.. Each parameter choice will generally require one inversion of the original system of equations, except that only one inversion is required to optimize \( \mu \).

Experimentation with GCV has just started, but the results so far are quite encouraging. Fixing the norm differential order at \( d = 2 \) leaves four parameters to estimate: the streamfunction and diffusivity length scales, the relative weighting between streamfunction and diffusivity fields, and the smoothing parameter \( \mu \). Fig. 18 and Fig. 19 show the best possible inverse solution for the streamfunction and diffusivity respectively, obtained by choosing the parameters to minimize the rms error between it and the true solution. Fig. 20 and Fig. 21 show the solution obtained using GCV. The streamfunction field is quite acceptable, while the diffusivity field is positive everywhere and of about the right magnitude.
8. CONCLUSION

The time-averaged ocean circulation and mixing coefficients may in principle be determined by inverting tracer conservation equations together with the dynamical constraints continuity and geostrophy. Vertical integration of the tracer equation between two quasi-horizontal surfaces is desirable because:

1. Vertical second derivatives of the tracer field need not be calculated;
2. \( \theta \) and \( S \) may be used as independent tracers;
3. The number of unknowns is reduced;
4. Tracer data within the layer is utilized.

Continuity is enforced implicitly by the use of a streamfunction together with the linear vorticity balance.

The problem is underdetermined, and so a minimum norm solution is sought. The solution depends on parameters such as norm length scale, differential order, relative weighting between different variable types, and signal-to-noise ratio.
A simple two-dimensional advection/diffusion model was used to test if good solutions were possible, and also whether generalized cross-validation (GCV) was a useful parameter estimation tool. Preliminary experiments indicate that GCV is capable of estimating parameters sufficiently accurately to obtain a useful solution.

REFERENCES


CSIRO Division of Oceanography, GPO Box 1538, Hobart 7001, Australia.