A note on isopycnal/diapycnal diffusion for ocean modelling

Eric Deleersnijder, 20 September 2004 (improved 26 September 2004)

It is common knowledge that large-scale diffusion processes in the ocean occur mostly along isopycnal surfaces, i.e. surfaces of equal density. There is also some diapycnal diffusion. The latter is associated with a diffusion flux orthogonal to isopycnal surfaces. The diapycnal and isopycnal diffusion fluxes are commonly parameterised *à la Fourier-Fick*, a formulation involving a diffusion tensor that is not isotropic (Redi 1982). As was seen by Beckers et al. (1998), many discretisations of the isopycnal diffusion term yield discrete operators that are not monotonic — a problem which is particularly annoying.

In this note, the diffusivity tensor to be applied in large-scale ocean models is established and a test case is suggested to assess discretisations of the diffusion term.

The diffusivity tensor

Let t and $\mathbf{x}$ denote time and the position-vector, respectively. The concentration $C(t,\mathbf{x})$ of a constituent of seawater is governed by local production/destruction phenomena and by transport processes. This is modelled by the generic equation

$$\frac{\partial C}{\partial t} = P - \nabla \bullet \mathbf{q} \,, \tag{1}$$

where P is the production/destruction rate of the constituent under study, while $\mathbf{q}$ is the relevant transport flux. The latter is due to processes that are resolved by the model, i.e. advection, and processes that are not resolved. The latter are parameterised herein as diffusion. As is well known, the advective flux is $\mathbf{u}C$, where the vector $\mathbf{u}$ denotes the fluid velocity, i.e. the velocity obtained after filtering out the unresolved fluid motions. So, if $\mathbf{d}$ represents the transport flux due to unresolved processes, (1) may be re-written as

$$\frac{\partial C}{\partial t} = P - \nabla \bullet (\mathbf{u}C + \mathbf{d}) \,. \tag{2}$$

The most general Fourier-Fick parameterisation of flux $\mathbf{d}$ is a linear function of the concentration gradient components:

$$\mathbf{d} = -\mathbf{K} \bullet \nabla C \,, \tag{3}$$

where $\mathbf{K}$ is the relevant diffusivity tensor, which needs to be positive definite — otherwise the associated transport would not necessarily tend to homogenise the concentration and, hence, could not be viewed as being of a diffusive nature.

If the unresolved phenomena are only those occurring at microscopic, i.e. molecular, scales, then the usual parameterisation of $\mathbf{d}$ is

$$\mathbf{d} = -K \nabla c \,, \tag{4}$$

where K is termed the "molecular diffusivity". Flux (4) may be cast into the general form (3) provided the diffusivity tensor $\mathbf{K}$ is

$$\mathbf{K} = \begin{pmatrix} K & 0 & 0 \\ 0 & K & 0 \\ 0 & 0 & K \end{pmatrix} . \tag{5}$$

Clearly, this tensor is invariant under a rotation of the reference frame; this is why it is said to be "isotropic".

If only large scales of motions are actually resolved, the unresolved motions comprise much more that those giving rise to the molecular diffusion. The unresolved phenomena are usually parameterised as non-isotropic diffusion. Such a formulation resorts to two diffusivity coefficients, K^i and K^d, which are the isopycnal diffusivity and the diapycnal diffusivity, respectively. In the principal axes, the associated diffusivity tensor reads

$$\mathbf{K} = \begin{pmatrix} K^i & 0 & 0 \\ 0 & K^i & 0 \\ 0 & 0 & K^d \end{pmatrix} . \tag{6}$$

Then, lengthy calculations are needed in order to express the diffusion term in the commonly used "horizontal-vertical" coordinate system (x,y,z). Fortunately, there exists a much simpler approach to the derivation of the isopycnal-diapycnal diffusion term.

If ρ denotes the density, the diapycnal — i.e. orthogonal to isopycnal surfaces — unit vector is

$$\mathbf{e} = \frac{-\nabla\rho}{|\nabla\rho|} . \tag{7}$$

Then, the "diapycnal gradient" of C is defined as

$$\nabla^d C = \mathbf{e}(\mathbf{e} \bullet \nabla C) , \tag{8}$$

while the "isopycnal gradient" is, quite obviously, the remainder of the gradient, i.e.

$$\nabla^d C = (\nabla - \nabla^i) C . \tag{9}$$

So, the isopycnal-diapycnal diffusion flux must be

$$\mathbf{d} = -K^i \nabla^i C - K^d \nabla^d C , \tag{10}$$

an expression which can be cast into the generic form (3) provided the diffusivity tensor **K** is defined as

$$\mathbf{K} = K^i(\mathbf{I} - \mathbf{ee}) + K^d \mathbf{ee} , \tag{11}$$

with

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} , \tag{12}$$

and

$$\mathbf{e} = \begin{pmatrix} e_x e_x & e_x e_y & e_x e_z \\ e_y e_x & e_y e_y & e_y e_z \\ e_z e_x & e_z e_y & e_z e_z \end{pmatrix} , \tag{13}$$

where $e_s = \mathbf{e} \bullet \mathbf{e}_s$ (s=x,y,z). This yields

$$\mathbf{K} = \frac{1}{\rho_x^2+\rho_y^2+\rho_z^2}\begin{pmatrix} \rho_x^2 K^d + (\rho_y^2+\rho_z^2)K^i & (K^d-K^i)\rho_x\rho_y & (K^d-K^i)\rho_x\rho_z \\ (K^d-K^i)\rho_y\rho_x & \rho_y^2 K^d + (\rho_x^2+\rho_z^2)K^i & (K^d-K^i)\rho_x\rho_y \\ (K^d-K^i)\rho_z\rho_x & (K^d-K^i)\rho_z\rho_y & \rho_z^2 K^d + (\rho_x^2+\rho_y^2)K^i \end{pmatrix}, \quad (14)$$

where $\rho_s = \partial\rho/\partial s$ (s=x,y,z). Simplifications of (14) have been suggested in order to take into account the fact that the slope of the isopycnal surfaces is generally small (Cox 1987).

To see if the diffusivity tensor derived above is positive definite, we consider the product

$$\mathbf{a}\bullet\mathbf{K}\bullet\mathbf{a} = K^i|\mathbf{a}\times\mathbf{e}|^2 + K^d(\mathbf{a}\bullet\mathbf{e})^2 . \quad (15)$$

For any vector $\mathbf{a}\neq\mathbf{0}$, the latter is positive and non-zero provided $K^i, K^d > 0$. QED.

A test case

We assume that the isopycnal surfaces are flat and equally spaced. As a consequence, the vector $\mathbf{e}$ is a constant. Further assuming that the isopycnal diffusivity, the diapycnal diffusivity and the velocity vector components are all constants, we consider the following partial differential problem in an infinite domain:

$$\begin{cases} \dfrac{\partial C}{\partial t} + \mathbf{u}\bullet\nabla C = \nabla\bullet(\mathbf{K}\bullet\nabla C) \\ \left[C(t,\mathbf{x})\right]_{t=0} = \delta(\mathbf{x}-\mathbf{0}) \end{cases}, \quad (16)$$

where δ denotes the Dirac function.

The solution to (16) reads

$$C(t,\mathbf{x}) = \frac{\exp\left[-\dfrac{(\mathbf{x}-\mathbf{u}t)\bullet\mathbf{K}^{-1}\bullet(\mathbf{x}-\mathbf{u}t)}{4t}\right]}{(4\pi t)^{n/2}\sqrt{\det\mathbf{K}}}, \quad (17)$$

where $\det\mathbf{K}$ denotes the determinant of $\mathbf{K}$ while n is the number of space dimensions considered. In other words, n is equal to 1, 2 or 3 according to whether we work in a one-, two- or three-dimensional domain. If thensor $\mathbf{K}$ represents iso- and dia-pycnal diffusion in a three dimensional domain, then

$$\mathbf{K}^{-1} = \left(K^i\right)^{-1}(\mathbf{I}-\mathbf{ee}) + \left(K^d\right)^{-1}\mathbf{ee}, \quad (18)$$

and

$$\det\mathbf{K} = K^d K^d K^i . \quad (19a)$$

Of course, if a two-dimensional "horizontal-vertical" problem is considered, then the determinant of the diffusivity tensor is

$$\det\mathbf{K} = K^d K^i . \quad (19b)$$

Some of the properties of the solution (17) are readily established. First, the concentration is positive at any position $\mathbf{x}$ and any time t>0:

$$C(t,\mathbf{x}) > 0 . \quad (20)$$

Next, the maximum of the concentration is located at

$$\mathbf{r}(t) = \mathbf{u}t . \quad (21)$$

Finally, the total mass of the tracer present in the domain of interest remains constant at time progresses:

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} C(t,\mathbf{x}) \ dxdydz \ = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \delta(\mathbf{x} - \mathbf{0}) \ dxdydz \ = \ 1 \ . \tag{22}$$

It is desirable that a discrete solution of differential problem (16) exhibits the properties (20)-(22).

References

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Checking the solution for a pointwise and instantaneous release of tracer

Eric Deleersnijder, 28 September 2004

We assume that the isopycnal surfaces are flat and equally spaced. As a consequence, the vector $\mathbf{e}$ is a constant. Further assuming that the isopycnal diffusivity, the diapycnal diffusivity and the velocity vector components are all constants, we consider the following partial differential problem in an infinite domain:

$$\begin{cases} \dfrac{\partial C}{\partial t} + \mathbf{u} \bullet \nabla C = \nabla \bullet (\mathbf{K} \bullet \nabla C) \\ \left[C(t,\mathbf{x})\right]_{t=0} = \delta(\mathbf{x} - \mathbf{0}) \end{cases} , \tag{1}$$

where δ denotes the Dirac function.

The solution to (16) reads

$$C(t,\mathbf{x}) = \frac{\exp\left[-\dfrac{(\mathbf{x}-\mathbf{u}t) \bullet \mathbf{K}^{-1} \bullet (\mathbf{x}-\mathbf{u}t)}{4t}\right]}{(4\pi t)^{n/2}\sqrt{\det \mathbf{K}}} , \tag{2}$$

where $\det \mathbf{K}$ denotes the determinant of $\mathbf{K}$ while n is the number of space dimensions considered. In other words, n is equal to 1, 2 or 3 according to whether we work in a one-, two- or three-dimensional domain. If thensor $\mathbf{K}$ represents iso- and dia-pycnal diffusion in a three dimensional domain, then

$$\mathbf{K} = K^i(\mathbf{I} - \mathbf{ee}) + K^d \mathbf{ee} , \tag{3}$$

$$\mathbf{K}^{-1} = \left(K^i\right)^{-1}(\mathbf{I} - \mathbf{ee}) + \left(K^d\right)^{-1} \mathbf{ee} , \tag{4}$$

and

$$\det \mathbf{K} = K^d K^d K^i . \tag{5a}$$

Of course, if a two-dimensional "horizontal-vertical" problem is considered, then the determinant of the diffusivity tensor is

$$\det \mathbf{K} = K^d K^i . \tag{5b}$$

Below, we will verify that expression (2) actually is the solution of (1).

Galilean transformation

Introduce new independent variables:

$$\begin{cases} t' = t \\ \mathbf{x}' = \mathbf{x} - \mathbf{u}t \end{cases} . \tag{6}$$

Then, the differential operators transform as follows:

$$\begin{cases} \dfrac{\partial}{\partial t} = \dfrac{\partial t'}{\partial t}\dfrac{\partial}{\partial t'} + \dfrac{\partial \mathbf{x}'}{\partial t} \bullet \nabla' = \dfrac{\partial}{\partial t'} - \mathbf{u} \bullet \nabla' \\ \nabla = \nabla t' \dfrac{\partial}{\partial t'} + (\nabla \mathbf{x}') \bullet \nabla' = \nabla' \end{cases} , \tag{7}$$

as $\partial t' / \partial t = 1$, $\partial \mathbf{x}' / \partial t = -\mathbf{u}$, $\nabla t' = 0$ and $\nabla \mathbf{x}' = \mathbf{I}$.

Substituting (6)-(7) into (1) and (2) yields

$$\begin{cases} \dfrac{\partial C}{\partial t'} & = & \nabla' \bullet (\mathbf{K} \bullet \nabla' C) \\ \left[C(t', \mathbf{x}')\right]_{t'=0} & = & \delta(\mathbf{x}' - \mathbf{0}) \end{cases} , \tag{8}$$

$$C(t', \mathbf{x}') \;=\; \frac{\exp\left[-\dfrac{\mathbf{x}' \bullet \mathbf{K}^{-1} \bullet \mathbf{x}'}{4t'}\right]}{(4\pi t')^{n/2}\sqrt{\det \mathbf{K}}} . \tag{9}$$

So, in the new coordinates ensuing from the Galilean transformation (6), the problem to be solved involves diffusion only. We now have to see that (9) is indeed the solution of (8).

To simplify the notations, the primes will be omitted from here onward.

The differential equation

After some calculations, we obtain

$$\frac{\partial C}{\partial t} \;=\; \left(\frac{\mathbf{x} \bullet \mathbf{K}^{-1} \bullet \mathbf{x}}{4t^2} - \frac{n}{2t}\right) C \tag{10}$$

and

$$\nabla C \;=\; \frac{\mathbf{K}^{-1} \bullet \mathbf{x}}{2t} C . \tag{11}$$

Hence

$$\mathbf{K} \bullet \nabla C \;=\; -\frac{\mathbf{K} \bullet \mathbf{K}^{-1} \bullet \mathbf{x}}{2t} C \;=\; -\frac{\mathbf{x}}{2t} C , \tag{12}$$

so that

$$\nabla \bullet (\mathbf{K} \bullet \nabla C) \;=\; -\frac{\mathbf{x}}{2t} \bullet \nabla C \;-\; \frac{\nabla \bullet \mathbf{x}}{2t} C \;=\; \left(\frac{\mathbf{x} \bullet \mathbf{K}^{-1} \bullet \mathbf{x}}{4t^2} - \frac{n}{2t}\right) C , \tag{13}$$

since $\nabla \bullet \mathbf{x} = n$. The righ-hand sides of (10) and (13) being equal, the expression (8) satisfies the diffusion equation included in (8). Nonetheless, it remains to be seen that (8) satisfies the initial condition and is associated with a unit mass of tracer.

Initial value and mass conservation

It is readily seen that $\mathbf{K}^{-1}$ is positive definite, which implies that

$$\begin{cases} \lim\limits_{t \to 0} C(t, \mathbf{x}) & = & 0 \quad \text{if} \quad \mathbf{x} \neq \mathbf{0} \\ \lim\limits_{t \to 0} C(t, \mathbf{x}) & = & \infty \quad \text{if} \quad \mathbf{x} = \mathbf{0} \end{cases} . \tag{14}$$

The domain of interest, $\Re^n$, is infinite. Therefore, as the tracer is passive, the total mass of the tracer,

$$M \;=\; \int_{\Re^n} C(t, \mathbf{x}) \; d\mathbf{x} , \tag{15}$$

must remain constant. At the initial instant, the concentration should be equal to $\delta(\mathbf{x} - \mathbf{0})$, so that

$$M = \int_{\Re^n} \delta(\mathbf{x} - \mathbf{0}) \; d\mathbf{x} = 1 \; . \tag{16}$$

It is convenient to rotate the axes to the principal axes of the diffusivity tensor, which is then expressed as

$$\tilde{\mathbf{K}} = \mathrm{diag}(\lambda_1, \; \lambda_2, \; ...) \; , \tag{17}$$

where λ_m (m=1,...n) denote the m-th eigenvalue of **K**. For a two- or a three-dimensional iso-/dia-pycnal diffusion problem, we have $(\lambda_1,\lambda_2) = (K^i,K^d)$ or $(\lambda_1,\lambda_2,\lambda_3) = (K^i,K^i,K^d)$. As the determinant is an invariant of a tensor, we have

$$\det \mathbf{K} = \prod_{m=1}^{n} \lambda_m \; . \tag{18}$$

Thus, if the space coordinates associated with the principal axes are $\tilde{x}_m$ (m=1,...n), using (18), the integral (15) may be transformed to

$$M = \prod_{m=1}^{n} \int_{-\infty}^{+\infty} \frac{\exp\left(-\frac{\tilde{x}_m^2}{4\lambda_m t} \right)}{\sqrt{4\pi\lambda_m t}} \; d\tilde{x}_m \; . \tag{19}$$

If a is a positive constant, it is well known that

$$\int_{-\infty}^{+\infty} e^{-a\xi^2} \; d\xi = \sqrt{\frac{\pi}{a}} \; . \tag{20}$$

Therefore, each of the integral in the product (19) is equal to unity. As a consequence, the total mass of the tracer is conserved, and is equal to unity at any time $t \geq 0$.

Conclusion

Expression (2) is the solution to the partial differential problem (1). QED.

A test case for a Lagrangian model of isopycnal diffusion with non-flat isopycnal surfaces

Eric Deleersnijder, 14 October & 20 December, 2009

Spivakovskaya et al. (2007) considered Lagrangian methods for representing isopycnal/diapycnal diffusion. However, the benchmark they proposed was based on a situation in which the isopycnal surfaces are flat — but obviously not horizontal. Herein, a two-dimensional "horizontal-vertical" test case is suggested in which diapycnal diffusion is zero and the isopycnal surfaces are not flat.

Let x and z denote the horizontal and the vertical coordinate (increasing upwards), respectively. If ρ is the density, the diffusivity tensor reads

$$\mathbf{K} = \begin{pmatrix} \dfrac{\rho_z^2}{\rho_x^2+\rho_z^2} & \dfrac{-\rho_x\rho_z}{\rho_x^2+\rho_z^2} \\ \dfrac{-\rho_x\rho_z}{\rho_x^2+\rho_z^2} & \dfrac{\rho_x^2}{\rho_x^2+\rho_z^2} \end{pmatrix} K^i \ , \tag{1}$$

where K^i is the isopycnal diffusivity.

The density field is such that density decreases as z increases, so that lighter water lies on top of heavier water. The vertical density gradient is assumed to be constant, but the horizontal one is not, so that the isopycnal surfaces are not flat. Accordingly, one may want to consider the following density field

$$\rho(x,z) = \rho_0 \left[1 - \frac{N^2 z}{g} + \alpha \sin(\kappa x) \right] , \tag{2}$$

where ρ_0 is a reference value of the density; N and g are positive constants respresenting the Brunt-Vaisala frequency and the gravitational acceleration, respectively; α and κ are constants.

An isopycnal surface is a surface on which density is constant. Let the latter be denoted ρ^*, then the corresponding isopycnal surface may be represented as follows:

$$z = \frac{g}{N^2}\left(1-\rho^*/\rho_0\right) + \frac{g\alpha}{N^2}\sin(\kappa x) \ . \tag{3}$$

The horizontal and vertical density gradients are

$$\rho_x = \rho_0 \alpha \kappa \cos(\kappa x) \tag{4}$$

and

$$\rho_z = -\frac{\rho_0 N^2}{g} \ . \tag{5}$$

Substituting (4)-(5) into (1) yields

$$\mathbf{K} = \begin{pmatrix} N^4 & \alpha g \kappa N^2 \cos(\kappa x) \\ \alpha g \kappa N^2 \cos(\kappa x) & \alpha^2 g^2 \kappa^2 \cos^2(\kappa x) \end{pmatrix} \frac{K^i}{\alpha^2 g^2 \kappa^2 \cos^2(\kappa x) + N^4} \ . \tag{6}$$

The following values of the parameters seem reasonable

$$K^i \approx 10^3\,\mathrm{m^2\,s^{-1}} \ , \ N^2 \approx 10^{-5}\,\mathrm{s^{-2}} \ , \ g \approx 10\,\mathrm{ms^{-2}} \ , \ \alpha \approx 10^{-3} \ , \ \kappa \approx 10^{-6}\,\mathrm{m} \ . \tag{7}$$

It is noteworthy that they lead to a slope of the isopycnal surfaces with an order of magnitude comparable to that selected by Spivakovskaya et al. (2007):

$$\left|\frac{\rho_x}{\rho_z}\right| = \left|\frac{\alpha\kappa g \cos(\kappa x)}{N^2}\right| \approx \frac{\alpha\kappa g}{N^2} \approx 10^{-3} \ . \tag{8}$$

At the initial instant, J particles[1] are released at $(x,z)=(0,0)$. This point belongs to the isopycnal surface whose equation reads

$$z = \frac{g\alpha}{N^2}\sin(\kappa x) \ . \tag{9}$$

The position vector of every particle is updated by means of an appropriate Lagrangian scheme and is denoted

$$[x_j(t), z_j(t)] \ , \quad j=1,2 \ldots \ J \ . \tag{10}$$

Clearly, the particles should remain on the isopycnal surface represented by (9). However, numerical errors are unavoidable. Their magnitude may be estimated by means of the following error measure

$$\mu(t) = \sqrt{\sum_{j=1}^{J}\left[z_j(t) - \frac{g\alpha}{N^2}\sin[\kappa x_j(t)]\right]^2} \ , \tag{11}$$

which is approximately equal to the standard deviation of the distance[2] of the particles to the isopycnal surface on which they should remain.

It would be interesting to plot $\mu(t)$ as a function of time. I suspect that $\mu(t)$ will increase almost monotonically as time progresses. However, the better the Lagrangian scheme, the slower the increase of $\mu(t)$. This provides a method for assessing various Lagrangian schemes.

Reference

Spivakovskaya D., A.W. Heemink and E. Deleersnijder, 2007, Lagrangian modelling of multi-dimensional advection-diffusion with space-varying diffusivities: theory and idealized test cases, *Ocean Dynamics*, 57, 189-203

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[1] The number of particles, J, should be sufficiently large.

[2] Since the slope of the isopycnal surface defined by (9) is small, the expression $\left|z_j(t) - \frac{g\alpha}{N^2}\sin[\kappa x_j(t)]\right|$ is approximately equal to the distance of the j-th particle to the isopycnal surface under consideration.

A note on the nature of the isopycnal diffusion

Eric Deleersnijder, March 22, 2010

Let x and z denote the horizontal and the vertical coordinate (increasing upwards), respectively. If $\rho(x,z)$ is the density, the 2D "horizontal-vertical" isopycnal diffusivity tensor reads (e.g. Redi 1982)

$$\mathbf{K} = \begin{pmatrix} \dfrac{\rho_z^2}{\rho_x^2+\rho_z^2} & \dfrac{-\rho_x\rho_z}{\rho_x^2+\rho_z^2} \\ \dfrac{-\rho_x\rho_z}{\rho_x^2+\rho_z^2} & \dfrac{\rho_x^2}{\rho_x^2+\rho_z^2} \end{pmatrix} K^i \ , \tag{1}$$

where K^i is the isopycnal diffusivity. Then, the concentration $C(t,x,z)$ of a passive tracer subject to isopycnal diffusion alone obeys the following equations

$$\frac{\partial C}{\partial t} = \nabla \bullet (\mathbf{K} \bullet \nabla C) \tag{2}$$

or, equivalently,

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left[\frac{\rho_z^2 K^i}{\rho_x^2+\rho_z^2}\frac{\partial C}{\partial x} - \frac{\rho_x\rho_z K^i}{\rho_x^2+\rho_z^2}\frac{\partial C}{\partial z}\right] + \frac{\partial}{\partial z}\left[\frac{-\rho_x\rho_z K^i}{\rho_x^2+\rho_z^2}\frac{\partial C}{\partial x} + \frac{\rho_x^2 K^i}{\rho_x^2+\rho_z^2}\frac{\partial C}{\partial z}\right] . \tag{3}$$

This expression is somewhat intricate, which is why it is appropriate to design a coordinate system in which it would become considerably simpler. To do so, it is first necessary to gain insight into the geometry of the isopycnal curves and the nature of the isopycnal diffusion flux.

Geometry of isopycnal curves

An isopycnal is a curve in the (x,z) space along which the density is a constant. The unit normal vector to such a curve is (Figure 1)

$$\mathbf{n} = \frac{\nabla\rho}{|\nabla\rho|} = \frac{\rho_x\mathbf{e}_x + \rho_z\mathbf{e}_z}{\sqrt{\rho_x^2+\rho_z^2}} \ , \tag{4}$$

where $\mathbf{e}_x$ and $\mathbf{e}_z$ are unit vectors associated with the x and z coordinate axes, while

$$\rho_x = \left(\frac{\partial\rho}{\partial x}\right)_z \quad \text{and} \quad \rho_z = \left(\frac{\partial\rho}{\partial z}\right)_x . \tag{5}$$

As density increases downwards (lighter water lies on top on heavier water), the derivative ρ_z is negative. On the other hand, ρ_x may be either positive or negative. The unit vector that is tangent to an isopycal is then (Figure 1)

$$\mathbf{t} = (\mathbf{e}_x \times \mathbf{e}_z) \times \mathbf{n} = \frac{-\rho_z\mathbf{e}_x + \rho_x\mathbf{e}_z}{\sqrt{\rho_x^2+\rho_z^2}} . \tag{6}$$

Let σ be the arc length along an isopycnal, implying

$$d\sigma^2 = dx^2 + dz^2 . \tag{7}$$

As

$$\left(\frac{\partial z}{\partial x}\right)_\rho = -\frac{\rho_x}{\rho_z} . \tag{8}$$

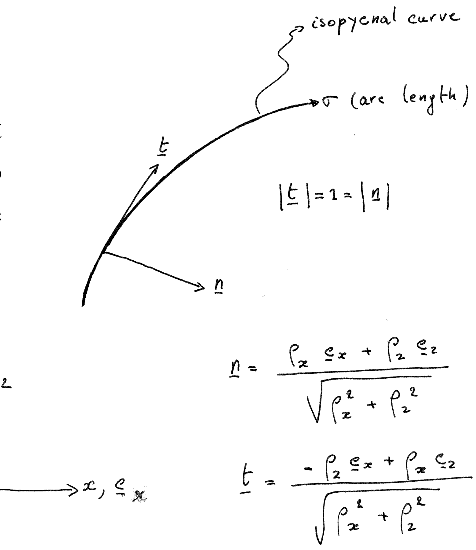
it is readily seen that

$$\left(\frac{\partial x}{\partial \sigma}\right)_\rho = \frac{-\rho_z}{\sqrt{\rho_x^2 + \rho_z^2}} \tag{9}$$

and

$$\left(\frac{\partial z}{\partial \sigma}\right)_\rho = \frac{\rho_x}{\sqrt{\rho_x^2 + \rho_z^2}} . \tag{10}$$

Figure 1. Illustration of the unit normal and tangential vectors to an isopycnal curve



Isopycnal tracer flux

The isopycal tracer flux is

$$\mathbf{q}^i = -\mathbf{K} \bullet \nabla C$$

$$= -\left[\frac{\rho_z^2 K^i}{\rho_x^2 + \rho_z^2}\frac{\partial C}{\partial x} - \frac{\rho_x \rho_z K^i}{\rho_x^2 + \rho_z^2}\frac{\partial C}{\partial z}\right]\mathbf{e}_x - \left[\frac{-\rho_x \rho_z K^i}{\rho_x^2 + \rho_z^2}\frac{\partial C}{\partial x} + \frac{\rho_x^2 K^i}{\rho_x^2 + \rho_z^2}\frac{\partial C}{\partial z}\right]\mathbf{e}_z . \tag{11}$$

Combining (6) and (11) yields

$$\mathbf{q}^i = -K^i (\mathbf{t} \bullet \nabla C)\mathbf{t} , \tag{12}$$

wich is in agreement with elementary physical intuition. This expression may also be transformed to

$$\mathbf{q}^i = -K^i \left(\frac{\partial C}{\partial \sigma}\right)_\rho \mathbf{t} . \tag{13}$$

One has

$$\left(\frac{\partial C}{\partial \sigma}\right)_\rho = \left(\frac{\partial x}{\partial \sigma}\right)_\rho \left(\frac{\partial C}{\partial x}\right)_z + \left(\frac{\partial z}{\partial \sigma}\right)_\rho \left(\frac{\partial C}{\partial z}\right)_x . \tag{14}$$

Then, substituting (6), (9) and (10) into (12), it may be demonstrated that (13) is correct, so that

$$\boxed{\mathbf{q}^i \;=\; -\mathbf{K}\bullet\nabla C \;=\; -K^i(\mathbf{t}\bullet\nabla C)\mathbf{t} \;=\; -K^i\left(\frac{\partial C}{\partial\sigma}\right)_\rho \mathbf{t}} \qquad (15)$$

The tracer equation in isopycnic coordinate

It is now convenient to introduce the following coordinate system

$$\begin{cases}\tau = t\\ \xi = x\\ \rho = \rho(x,z)\end{cases} \qquad (16)$$

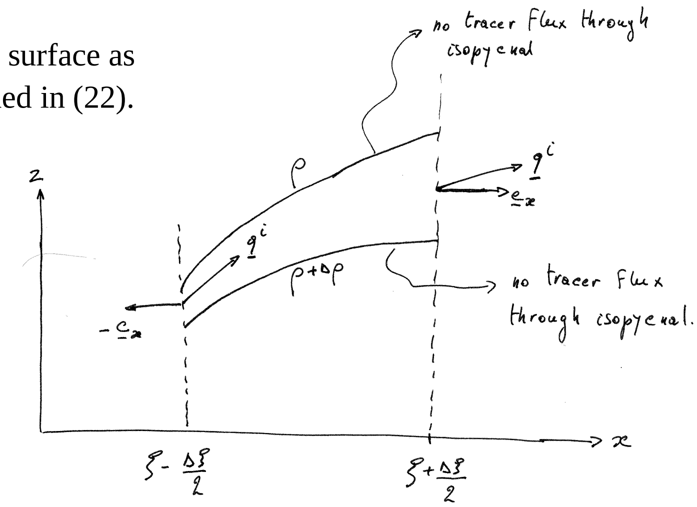
Then, on has

$$\left(\frac{\partial}{\partial\sigma}\right)_\rho \;=\; \left(\frac{\partial\xi}{\partial\sigma}\right)_\rho\left(\frac{\partial}{\partial\xi}\right)_\rho \;=\; \left(\frac{\partial x}{\partial\sigma}\right)_\rho\left(\frac{\partial}{\partial\xi}\right)_\rho . \qquad (17)$$

Then, substituting (9) into (17) yields

$$\left(\frac{\partial}{\partial\sigma}\right)_\rho \;=\; \frac{-\rho_z}{\sqrt{\rho_x^2+\rho_z^2}}\left(\frac{\partial}{\partial\xi}\right)_\rho . \qquad (18)$$

Figure 2. Control surface as defined in (22).



Combining (2) and (15) yields

$$\frac{\partial C}{\partial t} \;=\; \nabla\bullet\left[K^i\left(\frac{\partial C}{\partial\sigma}\right)_\rho \mathbf{t}\right]. \qquad (19)$$

Integrating the latter on a control surface Ω and using the divergence theorem leads to

$$\frac{d}{dt}\int_\Omega C\,d\Omega \;=\; \int_\Gamma K^i\left(\frac{\partial C}{\partial\sigma}\right)_\rho \mathbf{t}\bullet\mathbf{m}\,d\Gamma\ , \qquad (20)$$

where Γ is the boundary of Ω and $\mathbf{m}$ is the outward unit vector. Now assume that the control surface is (Figure 2)

$$\Omega = [\xi - \Delta\xi/2, \xi + \Delta\xi/2] \times [\rho - \Delta\rho/2, \rho + \Delta\rho/2] . \quad (21)$$

If $\Delta\xi, \Delta\rho \to 0$, the mass budget (20) is asymptotically equal to

$$\Delta\xi\,\Delta z \frac{\partial C}{\partial \tau} \sim \left[K^i \left(\frac{\partial C}{\partial \sigma} \right)_\rho (\mathbf{t} \bullet \mathbf{e}_x) \Delta z \right]_{\xi - \Delta\xi/2}^{\xi + \Delta\xi/2} . \quad (22)$$

Given that

$$\Delta z = \frac{\Delta\rho}{-\rho_z} \quad (23)$$

and

$$\mathbf{t} \bullet \mathbf{e}_x = \frac{-\rho_z}{\sqrt{\rho_x^2 + \rho_z^2}} , \quad (24)$$

(22) transforms to

$$\frac{\partial C}{\partial \tau} \sim -\rho_z \frac{\left[\frac{K^i}{\sqrt{\rho_x^2 + \rho_z^2}} \frac{\partial C}{\partial \sigma} \right]_{\xi - \Delta\xi/2}^{\xi + \Delta\xi/2}}{\Delta\xi} , \quad \Delta\xi \to 0 . \quad (25)$$

Taking the limit of this expression for $\Delta\xi \to 0$ yields

$$\frac{\partial C}{\partial \tau} = -\rho_z \frac{\partial}{\partial \xi} \left[\frac{K^i}{\sqrt{\rho_x^2 + \rho_z^2}} \frac{\partial C}{\partial \sigma} \right] . \quad (26)$$

By having recourse to (18), the equation above may be rewritten as

$$\boxed{\frac{\partial C}{\partial \tau} = \rho_z \frac{\partial}{\partial \xi} \left[\frac{K^i \rho_z}{\rho_x^2 + \rho_z^2} \frac{\partial C}{\partial \xi} \right] = \sqrt{\rho_x^2 + \rho_z^2} \frac{\partial}{\partial \sigma} \left[\frac{K^i}{\sqrt{\rho_x^2 + \rho_z^2}} \frac{\partial C}{\partial \sigma} \right]} \quad (27)$$

Spivakovskaya (2007) considered a case in which isopycnal surface are flat, but not horizontal, implying that ρ_x and ρ_z are constants. As a result, (27) simplifies to

$$\frac{\partial C}{\partial \tau} = \cos^2\theta \frac{\partial}{\partial \xi} \left(K^i \frac{\partial C}{\partial \xi} \right) = \frac{\partial}{\partial \sigma} \left(K^i \frac{\partial C}{\partial \sigma} \right) , \quad (29)$$

where θ is an angle whose tangent is the slope of the isopycnals. In other words, this angle is zero or $\pi/2$ according to whether the isopycnals are horizontal or vertical, respectively.

That equation (27) reduces to a well-known formula in the particular case considered in Spivakovskaya (2007) is reassuring as to its relevance.

Reference

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On the impact of isopycnal diffusion on the density field

Eric Deleersnijder, April 1, 2011

It is common knowledge that large-scale diffusion processes in the ocean occur mostly along isopycnal surfaces, i.e. surfaces of equal density. There is also some diapycnal diffusion. The latter is associated with a diffusion flux orthogonal to isopycnal surfaces. The diapycnal and isopycnal diffusion fluxes are commonly parameterised *à la Fourier-Fick*, a formulation involving a non-isotropic diffusion tensor (Redi 1982).

In most ocean models, density is not obtained from the solution of a transport equation. Instead, it is evaluated by means of the relevant equation of state. For a simple version of the latter, density may be seen to obey a remarkable property, which is established herein.

The diffusicity tensor

Let t and $\mathbf{x}$ denote time and the position-vector, respectively. The evolution of a scalar variable $\psi(t,\mathbf{x})$ is governed the generic equation

$$\frac{\partial\psi}{\partial t} = P - \nabla \bullet \mathbf{q} , \tag{1}$$

where P is the production/destruction rate, while $\mathbf{q}$ is the relevant transport flux. The latter is due to processes that are resolved by the model, i.e. advection, and processes that are not resolved. The latter are parameterised herein as diffusion. As is well known, the advective flux is $\mathbf{u}\psi$, where the vector $\mathbf{u}$ denotes the fluid velocity, i.e. the velocity obtained after filtering out the unresolved fluid motions. So, if $\mathbf{d}$ represents the transport flux due to unresolved processes, (1) may be re-written as

$$\frac{\partial\psi}{\partial t} = P - \nabla \bullet (\mathbf{u}\psi + \mathbf{d}) . \tag{2}$$

The most general Fourier-Fick parameterisation of flux $\mathbf{d}$ is a linear function of the concentration gradient components:

$$\mathbf{d} = -\mathbf{K} \bullet \nabla\psi , \tag{3}$$

where $\mathbf{K}$ is the relevant diffusivity tensor, which needs to be positive definite — otherwise the associated transport would not necessarily tend to homogenise the concentration and, hence, could not be viewed as being of a diffusive nature.

If the unresolved phenomena are only those occurring at microscopic (i.e. molecular) scales, then the usual parameterisation of $\mathbf{d}$ is

$$\mathbf{d} = -K\nabla\psi , \tag{4}$$

where K is termed the "molecular diffusivity". Flux (4) may be cast into the general form (3) provided the diffusivity tensor $\mathbf{K}$ is

$$\mathbf{K} = \begin{pmatrix} K & 0 & 0 \\ 0 & K & 0 \\ 0 & 0 & K \end{pmatrix} . \tag{5}$$

Clearly, this tensor is invariant under a rotation of the reference frame; this is why it is said to be "isotropic".

If only large scales of motions are actually resolved, the unresolved motions comprise much more that those giving rise to the molecular diffusion. The unresolved phenomena are usually parameterised as non-isotropic diffusion. Such a formulation resorts to two diffusivity coefficients, K^i and K^d, which are the isopycnal diffusivity and the diapycnal diffusivity, respectively. In the principal axes, the associated diffusivity tensor reads

$$\mathbf{K} = \begin{pmatrix} K^i & 0 & 0 \\ 0 & K^i & 0 \\ 0 & 0 & K^d \end{pmatrix} . \tag{6}$$

Then, lengthy calculations are needed in order to express the diffusion term in the commonly used "horizontal-vertical" coordinate system (*x,y,z*). Fortunately, there exists a much simpler approach to the derivation of the isopycnal-diapycnal diffusion term.

If ρ denotes the density, the diapycnal — i.e. orthogonal to isopycnal surfaces — unit vector is

$$\mathbf{e} = \frac{-\nabla\rho}{|\nabla\rho|} . \tag{7}$$

Then, the "diapycnal gradient" of ψ is defined as

$$\nabla^d\psi = \mathbf{e}(\mathbf{e}\bullet\nabla\psi) , \tag{8}$$

while the "isopycnal gradient" is, quite obviously, the remainder of the gradient, i.e.

$$\nabla^d\psi = (\nabla - \nabla^i)\psi . \tag{9}$$

So, the isopycnal-diapycnal diffusion flux must be

$$\mathbf{d} = - K^i\nabla^i\psi - K^d\nabla^d\psi , \tag{10}$$

an expression which can be cast into the generic form (3) provided the diffusivity tensor **K** is defined as

$$\mathbf{K} = K^i(\mathbf{I} - \mathbf{ee}) + K^d\mathbf{ee} , \tag{11}$$

with

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} , \tag{12}$$

and

$$\mathbf{e} = \begin{pmatrix} e_x e_x & e_x e_y & e_x e_z \\ e_y e_x & e_y e_y & e_y e_z \\ e_z e_x & e_z e_y & e_z e_z \end{pmatrix} , \tag{13}$$

where $e_s = \mathbf{e}\bullet\mathbf{e}_s$ (s=x,y,z). This yields

$$\mathbf{K} = \frac{1}{\rho_x^2+\rho_y^2+\rho_z^2}\begin{pmatrix} \rho_x^2 K^d + (\rho_y^2+\rho_z^2)K^i & (K^d - K^i)\rho_x\rho_y & (K^d - K^i)\rho_x\rho_z \\ (K^d - K^i)\rho_y\rho_x & \rho_y^2 K^d + (\rho_x^2+\rho_z^2)K^i & (K^d - K^i)\rho_x\rho_y \\ (K^d - K^i)\rho_z\rho_x & (K^d - K^i)\rho_z\rho_y & \rho_z^2 K^d + (\rho_x^2+\rho_y^2)K^i \end{pmatrix} , \tag{14}$$

where $\rho_s = \partial\rho/\partial s$ (s=x,y,z). Simplifications to (14) have been suggested in order to take into account the fact that the slope of the isopycnal surfaces is generally small (Cox 1987).

To see if the diffusivity tensor derived above is positive definite, we consider the product

$$\mathbf{a} \bullet \mathbf{K} \bullet \mathbf{a} \;=\; K^i|\mathbf{a} \times \mathbf{e}|^2 \;+\; K^d(\mathbf{a} \bullet \mathbf{e})^2 \;. \tag{15}$$

For any vector $\mathbf{a} \neq \mathbf{0}$, the latter is positive and non-zero provided $K^i, K^d > 0$. QED.

A special case

Assume that temperature $\theta(t,\mathbf{x})$ and salinity $S(t,\mathbf{x})$ behave as passive tracers, implying that they obey the following evolution equations:

$$\frac{\partial\theta}{\partial t} \;=\; -\nabla \bullet (\mathbf{u}\theta - \mathbf{K} \bullet \nabla\theta) \;, \tag{16}$$

$$\frac{\partial S}{\partial t} \;=\; -\nabla \bullet (\mathbf{u}S - \mathbf{K} \bullet \nabla S) \;. \tag{17}$$

Further assume that density is linear function of temperature and salinity, i.e.

$$\rho(\theta,S) \;=\; \rho_0 \;+\; a(\theta - \theta_0) \;+\; b(S - S_0) \;, \tag{18}$$

where a, b, ρ_0, θ_0 and S_0 are constants. Then, combining (16)-(18) yields

$$\frac{\partial\rho}{\partial t} \;=\; -\nabla \bullet (\mathbf{u}\rho - \mathbf{K} \bullet \nabla\rho) \;. \tag{19}$$

Then, by using (7) and (11), the "density flux" $-\mathbf{K} \bullet \nabla\rho$ is seen to be be independent of the isopycnal diffusivity:

$$\begin{aligned} -\mathbf{K} \bullet \nabla\rho \;&=\; -[K^i(\mathbf{I} - \mathbf{ee}) + K^d\mathbf{ee}] \bullet \big[-|\nabla\rho|\mathbf{e}\big] \\ &=\; |\nabla\rho|K^i\underbrace{(\underbrace{\mathbf{I} \bullet \mathbf{e}}_{=\mathbf{e}} - \mathbf{e}\underbrace{\mathbf{e} \bullet \mathbf{e}}_{=1})}_{=0} + |\nabla\rho|K^d\mathbf{e}\underbrace{\mathbf{e} \bullet \mathbf{e}}_{=1} \\ &=\; |\nabla\rho|K^d\mathbf{e} \;=\; -K^d\nabla\rho \end{aligned} \tag{20}$$

Finally, substituting (20) into (19) leads to

$$\boxed{\frac{\partial\rho}{\partial t} \;=\; -\nabla \bullet (\mathbf{u}\rho - K^d\nabla\rho)} \tag{21}$$

For the simplified density equation considered herein, isopycnal diffusion has no impact on the evolution of density. Thus, if advection and isopycnal diffusion are negligible, the density must remain constant, i.e. $\rho(t,\mathbf{x}) = \rho(0,\mathbf{x})$.

References

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A three-dimensional test case for Lagrangian models of isopycnal diffusion with non-flat isopycnal surfaces

Eric Deleersnijder, April 30, 2013

Spivakovskaya et al. (2007) considered Lagrangian methods for representing isopycnal/diapycnal diffusion. However, the benchmark they proposed was based on a situation in which the isopycnal surfaces are flat — and obviously not horizontal. Deleersnijder (2009) suggested a two-dimensional "horizontal-vertical" test case in which diapycnal diffusion is zero and the isopycnal surfaces are not flat. This test case was dealt with by Shah et al. (2011) and Shah et al. (2013). In the present working note, a three-dimensional benchmark is designed, which is largely inspired by the aforementioned two-dimensional test case.

Let x and y denote the horizontal coordinates, while z denotes the vertical coordinate (increasing upwards). If ρ is the density, the isopycnal diffusivity tensor reads

$$\mathbf{K} = \frac{K^i}{\rho_x^2+\rho_y^2+\rho_z^2}\begin{pmatrix} \rho_y^2+\rho_z^2 & -\rho_x\rho_y & -\rho_x\rho_z \\ -\rho_y\rho_x & \rho_x^2+\rho_z^2 & -\rho_y\rho_z \\ -\rho_z\rho_x & -\rho_z\rho_y & \rho_x^2+\rho_y^2 \end{pmatrix} \tag{1}$$

where K^i is the isopycnal diffusivity.

Density decreases as z increases, so that lighter water lies on top of heavier water. The vertical density gradient is assumed to be constant, but the horizontal one is not, so that the isopycnal surfaces are not flat. Accordingly, one may want to consider the following density field

$$\rho(x,z) = \rho_0\left[1+\alpha_x\sin(\kappa_x x)+\alpha_y\sin(\kappa_y y)-\frac{N^2 z}{g}\right] , \tag{2}$$

where ρ_0 is a reference value of the density; N and g are positive constants representing the Brunt-Vaisala frequency and the gravitational acceleration, respectively; α_x, α_y, κ_x and κ_y are constants.

An isopycnal surface is a surface on which density is constant. Let the latter be denoted ρ^*, then the corresponding isopycnal surface may be represented as follows:

$$z = \frac{g}{N^2}\left(1-\rho^*/\rho_0\right) + \frac{g\alpha_x}{N^2}\sin(\kappa_x x) + \frac{g\alpha_y}{N^2}\sin(\kappa_y y) . \tag{3}$$

The horizontal and vertical density gradients are

$$\rho_x = \rho_0\alpha_x\kappa_x\cos(\kappa_x x) , \quad \rho_y = \rho_0\alpha_y\kappa_y\cos(\kappa_y y) , \tag{4}$$

and

$$\rho_z = -\frac{\rho_0 N^2}{g} . \tag{5}$$

These formulas are to be substituted into (1) to obtain the actual expressions of the components of the diffusivity tensor.

The following values of the parameters seem reasonable

$$K^i \approx 10^3\,\mathrm{m^2\,s^{-1}}\ ,\ N^2 \approx 10^{-5}\,\mathrm{s^{-2}}\ ,\ g \approx 10\,\mathrm{m\,s^{-2}}\ ,\ \alpha_\xi \approx 10^{-3}\ ,\ \kappa_\xi \approx 10^{-6}\,\mathrm{m}\ , \tag{6}$$

with $\xi = x, y$.

At the initial instant, J particles are released at $(x,y,z) = (0,0,0)$. This point belongs to the isopycnal surface whose equation reads

$$z = \frac{g\alpha_x}{N^2}\sin(\kappa_x x) + \frac{g\alpha_y}{N^2}\sin(\kappa_y y)\ . \tag{7}$$

The position vector of every particle is updated by means of an appropriate Lagrangian scheme and is denoted

$$[x_j(t), y_j(t), z_j(t)],\quad j = 1,2 \ldots J\ . \tag{8}$$

Clearly, the particles should remain on the isopycnal surface represented by (7). However, numerical errors are unavoidable. Their magnitude may be estimated by means of the following error measure

$$\mu(t) = \sqrt{\sum_{j=1}^{J}\left[z_j(t) - \frac{g\alpha_x}{N^2}\sin(\kappa_x x) - \frac{g\alpha_y}{N^2}\sin(\kappa_y y)\right]^2}\ , \tag{9}$$

which is approximately equal to the standard deviation of the distance of the particles to the isopycnal surface on which they should remain.

It would be interesting to plot $\mu(t)$ as a function of time. I suspect that $\mu(t)$ will increase almost monotonically as time progresses. However, the better the Lagrangian scheme, the slower the increase of $\mu(t)$. This provides a method for assessing various Lagrangian schemes.

Reference

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