Test cases for assessing Lagrangian methods for simulating vertical transport in stratified flows

Eric Deleersnijder, September 10, 2010 and April 6, 2011

For decades Lagrangian simulations in estuaries, coastal regions and seas had recourse to simple, first order schemes (e.g. Dimou and Adams 1993, Hunter et al. 1993, Tartinville et al. 1997, Visser 1997, Spagnol et al. 2002, Bilgili et al. 2005, Proehl et al. 2005). However, the marine modelling community is progressively realising that such schemes are far from optimal (e.g. Stijnen et al. 2006, Spivakovskaya et al. 2007a, Spivakovskaya et al. 2007b, Gräwe 2011, Gräwe and Wolff 2010). Turning to higher-order schemes is one of the improvements that are now believed to be needed. Accordingly, it is necessary to develop Lagrangian test cases focussing on features that cannot be dealt with easily in a Lagrangian mode. For instance, in shallow seas and estuaries, the pycnocline usually is a quasi-impermable barrier to vertical transport: this is easily taken into account by Eulerian models, while obtaining a similar result in Lagrangian simulations is far from trivial. This was illustrated by Stijnen et al. (2006) (Figure 1, Figure 2).

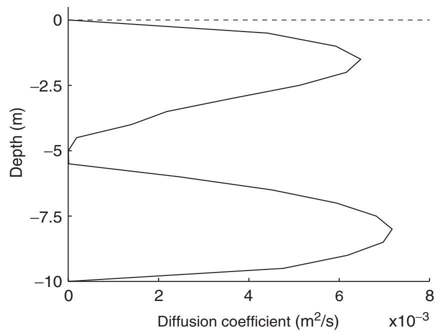

Figure 1. The vertical diffusivity profile in the channel flow simulation of Stijnen et al. (2006).

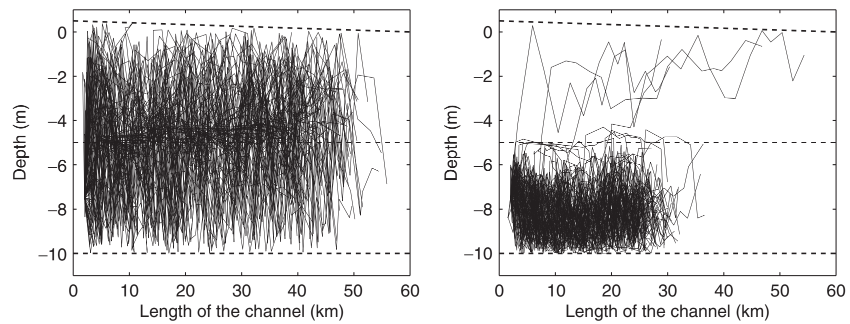

Figure 2. Particule trajectories simulated by Stijnen et al. (2006). With a first-order Euler scheme (left panel), the thermocline does not appear as an impermeable barrier to diffusion, which is quite wrong. Turning to a higher-order scheme leads to a very significant improvement (right panel).

Stijnen et al. (2006) performed Lagrangian simulations in which the pycnocline was seen to be no significant barrier to diffusion when a first-order scheme was used. However, when using a higher-order Lagrangian scheme, the pycnocline remained almost impermeable to diffusive fluxes — as it is supposed to be. Though Stijnen et al. (2006) used a time step that, in my opinion, was much too large, I believe that their results would not change qualitatively if a smaller, more realistic time increment were resorted to. Inspiration may be found in their study for designing a test case for Lagrangian simulation of vertical transport in stratified flows.

Vertical eddy diffusivity

It is desirable that the CPU cost of each run be modest so that many runs can be performed within a reasonably small amount of time, allowing numerous schemes with a wide spectrum of parameter values to be assessed. This is why it is suggested that one turns to a 1D, vertical problem in which transport is due to vertical, turbulent diffusion, with the possible addition of settling processes (e.g. Deleersnijder et al. 2006a, Deleersnijder et al. 2006b, Spivakovskaya et al. 2007a, Gräwe and Wolff 2010, de Brauwere and Deleersnijder 2010); horizontal transport processes are not taken into account. A pycnocline associated with a strong density gradient must be present, so that the eddy diffusivity at the location of the pycnocline is negligible, thereby representing an impermeable barrier to vertical diffusive transport. Without any loss of generality, the thermocline can be assumed to be located in the middle of the water column. Accordingly, it is suggested that the vertical eddy diffusivity be equal to

(1) $$\kappa(z) = \begin{cases} \dfrac{2(1+a)(1+2a)}{a^2 h^{1+1/a}} z(h-2z)^{1/a}\bar{\kappa} \ , & 0 < z < h/2 \\ \dfrac{2(1+a)(1+2a)}{a^2 h^{1+1/a}} (h-z)(2z-h)^{1/a}\bar{\kappa} \ , & h/2 < z < h \end{cases}$$

where h denotes the height of the water column and the constant a is larger than or equal to unity; z is the distance to the seabed, which is located at z=0, while the sea surface is at z=h. It is readily seen that the constant $\bar{\kappa}$ is the depth-averaged value of the eddy diffusivity $\kappa(z)$.

The diffusivity profile (1), which illustrated in Figure 3, admits the following asymptotic behaviours:

(2) $$\kappa(z) \sim \frac{2(1+a)(1+2a)\bar{\kappa}}{a^2}\frac{z}{h} \ , \quad \frac{z}{h} \to 0 \ ,$$

(3) $$\kappa(z) \sim \frac{2^{1/a}(1+a)(1+2a)\bar{\kappa}}{a^2}\left|1/2 - z/h\right|^{1/a} \ , \quad \frac{z}{h} \to \frac{1}{2} \ ,$$

(4) $$\kappa(z) \sim \frac{2(1+a)(1+2a)\bar{\kappa}}{a^2}(1-z/h) \ , \quad \frac{z}{h} \to 1 \ .$$

Thus, the eddy diffusivity is a linear function of the distance to the upper and lower boundaries of the domain: such a behaviour is generally believed to be acceptable for idealised test cases. In addition, the eddy diffusivity is zero at the pycnocline and, in the vicinity of the latter, the parameter *a* controls the steepness of the diffusivity profile; the larger the value of *a*, the larger the vertical diffusivity gradient (Figure 3).

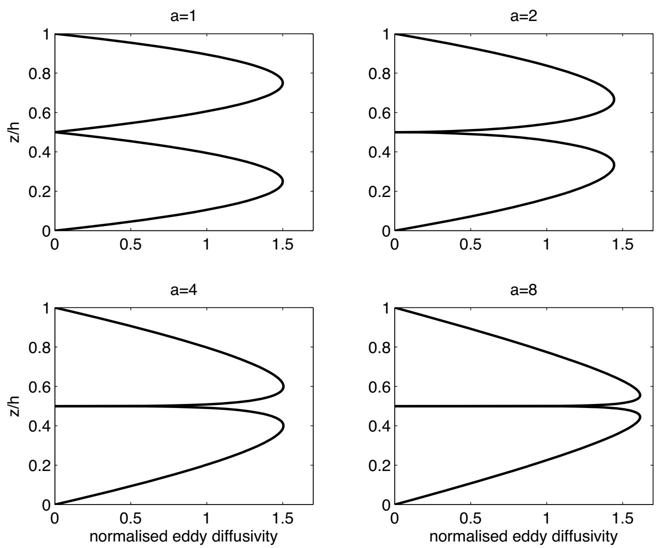

Figure 3. Eddy diffusivity profiles obtained from expression (1) for various values of the parameter *a*.

First test case

To asses to what extent the pycnocline actually is a barrier to vertical diffusion, N particles may be released somewhere in the upper half of the water column. The upper and lower boundaries are assumed to be impermeable to diffusion. Therefore, as time t progresses, the number of particles present in the water column must remain constant. One should display the number $n(t)$ of particles present in the lower half of the domain. Clearly, the better the scheme under consideration, the smaller the ratio $n(t)/N$.

Second test case

Now consider particles having a negative buoyancy, causing them to migrate downward with the settling velocity w, which is assumed to be a constant. As in the previous test case, the upper and lower boundaries of the water column are assumed to be impermeable to diffusion, implying that particles leave the domain — once and for all — at the instant they hit the seabed. Therefore, the number of particles present in the water column decreases monotonically as time progresses.

The Eulerian counterpart of this Lagrangian problem admits no closed form solution. However, it is possible to calculate the residence time $\theta(z)$. The latter is the average time that particles released at a distance z to the sea bottom spend in the water column — assuming that the number of particles released is arbitrarily large. According to Deleersnijder et al. (2006a), one has

$$\theta(z) = \frac{z}{w} + \frac{1}{w}\int_z^h \exp\left[-w\int_z^\xi \frac{d\zeta}{\kappa(\zeta)}\right] d\xi \ . \tag{5}$$

Therefore, numerical, Lagrangian estimates of the residence time can be compared with expression (5), which can be computed with a high accuracy. The residence time at the top of the water column (z=h) is equal to h/w for any diffusivity profile. It is probably worth assessing to what extent Lagrangian residence time estimates satisfy this property.

For the lower half of the water column ($0 \le z < h/2$), formula (5) may be transformed to

$$\theta(z) = \frac{z}{w} + \frac{1}{w}\int_z^{h/2} \exp\left[-w\int_z^\xi \frac{d\zeta}{\kappa(\zeta)}\right] d\xi \quad (0 < z < h/2) \ . \tag{6}$$

This is because the pycnocline is an impermeable barrier to diffusion. If $a = 1$, then one has

$$\theta(z) = \begin{cases} \dfrac{h/2}{w} + \dfrac{\eta}{w} + \dfrac{1}{w}\displaystyle\int_\eta^{h/2} \exp\left[-w\int_\eta^\xi \frac{d\zeta}{\kappa(\zeta)}\right] d\xi \ , & h/2 < z < h \\ \dfrac{\eta}{w} + \dfrac{1}{w}\displaystyle\int_\eta^{h/2} \exp\left[-w\int_\eta^\xi \frac{d\zeta}{\kappa(\zeta)}\right] d\xi \ , & 0 < z < h/2 \end{cases} \tag{7}$$

with

(8) $$\eta = \begin{cases} z - h/2 \ , & h/2 < z < h \\ z \ , & 0 < z < h/2 \end{cases}$$

implying that the residence time satisfies the remarkable property

(9) $$\boxed{\theta(h/2+\eta) = \frac{h/2}{w} + \theta(\eta) \quad (a=1)}$$

It is worth assessing to what extent Lagrangian residence time estimates satisfy this remarkable property.

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On the spurious particle flux crossing the pycnocline in a Lagrangian model

Eric Deleersnijder, May 26, 2011

In shallow seas, the pycnocline usually is a very thin layer that is an almost impermeable barrier to turbulent diffusion. In idealised test cases, it is acceptable to assume that the diffusivity in the pycnocline is zero, implying that the tracer flux crossing it must be zero. This is easily represented in Eulerian numerical models. In Lagrangian simulations, however, it is almost impossible to prevent some particles from crossing the pycnocline, thereby causing simulation errors the magnitude of which has to be assessed. A simple method for doing so is suggested herein.

Consider a 1D, vertical model. The pycnocline is assumed to be located in the middle of the water column, whose depth is h. The seabed and the sea surface are impermeable. The diffusivity profile is symmetric with respect to the pycnocline. Let $\overline{\kappa}$ denote the depth-averaged vertical tracer diffusivity. The vertical mixing timescale is of the order of

$$\tau = \frac{(h/2)^2}{\overline{\kappa}} = \frac{h^2}{4\overline{\kappa}} . \tag{1}$$

Now consider a Lagrangian representation of the vertical diffusion of a passive tracer. No particle should cross the pycnocline. However, because the model is not perfect, some particles will do. These events are independent of each other. Assuming that there is only one mechanism (a deficiency in the Lagrangian model) causing such numerical artefacts, the number of particles originating from the lower half of the water column that will cross the pycnocline during the time interval Δt tends to $\mu \Delta t C$ as $\Delta t \to 0$, where μ and C are the mean speed at which particles are crossing the pycnocline and the particle density (number of particles per unit height) just under the pycnocline. Clearly, a formula of the same type may be used to estimate the number of particle crossing the pycnocline in the opposite direction, i.e. from the upper half of the water column to the lower one.

The timescale

$$\gamma^{-1} = \frac{h}{2\mu} \tag{2}$$

is associated with the rate at which particles are crossing the pycnocline. Now assume that this timescale is much larger that the mixing timescale defined above, τ, i.e.

$$\gamma\tau = \frac{\mu h}{2\overline{\kappa}} << 1 . \tag{3}$$

Under this hypothesis, the particle density will tend to be homogeneous in every half of the water column. Therefore, denoting t, $n_1(t)$ and $n_2(t)$ the time, the number of particles in the lower half of the water column and that in the upper half of the domain, respectively, the governing equations of the phenomena under study are

$$\frac{dn_1}{dt} = -\gamma(n_1 - n_2) , \tag{4}$$

$$\frac{dn_2}{dt} = -\gamma(n_2 - n_1) . \tag{5}$$

Clearly, these equations are valid if the number of particles is sufficiently large.

Upon denoting $n_{1,0} = n_1(0)$ and $n_{2,0} = n_2(0)$, the solution to (4)-(5) reads

$$n_1(t) = \frac{n_{1,0} + n_{2,0}}{2} + \frac{n_{1,0} - n_{2,0}}{2} e^{-\gamma t} , \tag{6}$$

$$n_2(t) = \frac{n_{1,0} + n_{2,0}}{2} - \frac{n_{1,0} - n_{2,0}}{2} e^{-\gamma t} . \tag{7}$$

The number of particles present in the whole water column remains constant,

$$n_1(t) + n_2(t) = n_{1,0} + n_{2,0} . \tag{8}$$

This is because the upper and lower boundaries of the domain are impermeable, implying that particles are not allowed to leave the domain. Another important property of the solutions above is related to their large-time limit:

$$\lim_{\gamma t \to \infty} n_1(t) = \frac{n_{1,0} + n_{2,0}}{2} = \lim_{\gamma t \to \infty} n_2(t) . \tag{9}$$

For a given set of parameters, one could evaluate the value of γ from numerical simulations. Then, the smaller the dimensionless parameter $\gamma\tau$, the better the Lagrangian method under consideration.

Response to a remark by Arnold Heemink on Ulf Gräwe's draft manuscript

Eric Deleersnijder, September 9, 2011

On September 6, 2011, Arnold Heemink wrote the following remark on Ulf Gräwe's draft manuscript (Gräwe et al., 2011):

> *In your paper you write at a number of locations that particles crossing the pycnocline is a problem of particle models only and not of Eulerian models. I don't think that this is the case. Of course if you know exactly where the pycnocline is (as in the test case) it is easy to model this as an impermeable boundary in Eulerian models. But in that case it would also have been very easy to model this as an impermeable boundary in a particle model (e.g. by reflexion or by time step reduction unless the particle does not cross the boundary). It seems to me that the real problem is if the pycnocline is not known in advance. This was e.g. the case described in Stijnen (2006) where the diffusivity had been computed by the flow model (including k-eps turbulence model) showing a (variable) pycnocline. In these kind of cases it is not possible to include an impermeable boundary at the pycnocline (which may not be complete impermeable at all), not in Eulerian and not in particle models. This makes the value of the test case much higher (not only discussing a problem of a particle model). I wonder how an Eulerian model would would perform whithout including a impermeable boundary at the pycnocline from the start ....*

Nowadays the vertical eddy (or viscosity) field commonly is predicted by means of sophisticated turbulence closure schemes (e.g. GOTM, www.gotm.net) implemented in Eulerian models. These schemes are able to reproduce huge vertical gradients of the eddy diffusivity. In other words, over the distance of one space increment, the eddy diffusivity may vary by several orders of magnitude. Clearly, very small values of the eddy coefficient may be obtained, which, for all practical purposes, may be regarded as zero. Therefore, if a suitable discretisation of the vertical turbulent fluxes is implemented, a small value of the eddy coefficient will give rise to an almost impermeable barrier to diffusion — without artificially prescribing impermeable boundary conditions inside the water column. This is seen below.

Consider the following standard vertical diffusion equation:

$$\frac{\partial C}{\partial t} = -\frac{\partial \phi}{\partial z} , \tag{1}$$

where t and z are the time and the vertical coordinate, respectively; $C(t,z)$ is the concentration under study; the associated turbulent flux is denoted ϕ. The latter is parameterised *à la* Fourier-Fick, i.e.

$$\phi = -K \frac{\partial C}{\partial z} . \tag{2}$$

Therefore, combining (1) and (2), yields

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(K\frac{\partial C}{\partial z}\right) . \tag{3}$$

Now consider the space discretisation of (1)-(3). It is convenient to adopt the following notation

$$C_k(t) = C(t, k\Delta z) , \tag{4}$$

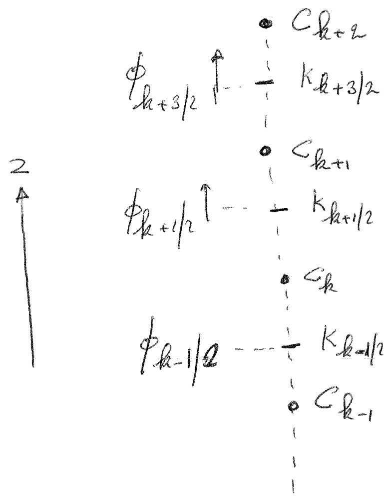
where k is an integer and Δz is the vertical grid size. The standard space arrangement of variables is such that the eddy coefficient is not calculated at the same point as the concentration. In fact, it is appropriate to do so between the concentration levels, leading to

$$K_{k+1/2}(t) = K[t,(k+1/2)\Delta z] . \tag{5}$$

Therefore, it is also convenient — and quite natural — to compute the fluxes between the concentrations points:

$$\phi_{k+1/2}(t) = K_{k+1/2}(t)\,\frac{C_{k+1}(t)-C_k(t)}{\Delta z} . \tag{6}$$

The space location of these discrete variables is illustrated in the figure below.



It is readily seen that at $x = k\Delta z$ and $x = (k+1)\Delta z$ the discretisation in space of the aforementioned continuous equation is

$$\frac{dC_{k+1}}{dt} = -\frac{\phi_{k+3/2}-\phi_{k+1/2}}{\Delta z} = \frac{K_{k+3/2}\dfrac{C_{k+2}-C_{k+1}}{\Delta z} - K_{k+1/2}\dfrac{C_{k+1}-C_k}{\Delta z}}{\Delta z} , \tag{7a}$$

$$\frac{dC_k}{dt} = -\frac{\phi_{k+1/2}-\phi_{k-1/2}}{\Delta z} = \frac{K_{k+1/2}\dfrac{C_{k+1}-C_{k1}}{\Delta z} - K_{k-1/2}\dfrac{C_k-C_{k-1}}{\Delta z}}{\Delta z} . \tag{7b}$$

Now assume that the numerical turbulence closure scheme being used predicts that the diffusivity $K_{k+1/2}$ is so small that it presumably is acceptabe to consider its value to be zero. Then, the corresponding flux $\phi_{k+1/2}$ is zero. As a result, $C_k(t)$ and $C_{k+1}(t)$ do not influence each other, as can be seen by setting $K_{k+1/2} = 0$ or $\phi_{k+1/2} = 0$ in (7a) and (7b):

$$\frac{dC_{k+1}}{dt} = -\frac{\phi_{k+3/2}}{\Delta z} = K_{k+3/2}\frac{C_{k+2}-C_{k+1}}{\Delta z^2}\ , \tag{8a}$$

$$\frac{dC_k}{dt} = -\frac{-\phi_{k-1/2}}{\Delta z} = -K_{k-1/2}\frac{C_k-C_{k-1}}{\Delta z^2}\ . \tag{8b}$$

Therefore, there is no doubt that the level k+1/2 is a barrier to vertical diffusion.

Reference

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