Modelling oceanic advection-diffusion by means of random walk algorithms

Eric Deleersnijder, 16 January 2004

Let $C(t,\mathbf{x})$ denote the concentration of a passive — or inert — tracer at time t and location $\mathbf{x}$. The concentration satisfies advection-diffusion equation

$$\frac{\partial C}{\partial t} = -\nabla \bullet (\mathbf{u}C - \mathbf{K} \bullet \nabla C) , \tag{1}$$

where $\mathbf{u}$ is the velocity, which is divergence-free, i.e. $\nabla \bullet \mathbf{u} = 0$; the diffusivity tensor is symmetric and positive definite, and its components are functions of time and position. The boundary Γ of the domain of interest Ω is impermeable, which leads to the following boundary conditions:

$$[\mathbf{u} \bullet \mathbf{n}]_{\mathbf{x}\in\Omega} = 0 , \tag{2}$$

$$[(\mathbf{K} \bullet \nabla C) \bullet \mathbf{n}]_{\mathbf{x}\in\Omega} = 0 . \tag{3}$$

It is possible to solve numerically the partial differential problem (1)-(3) in the Eulerian formalism. However, occasionnally, it may be deemed appropriate to tackle it by means of a Lagrangian algorithm. Then, the tracer is regarded as a set of pointwise particles, which are identified by index i, which ranges from 1 to I; the larger I, the more accurate the Lagrangian solution. The position $\mathbf{r}_i(t)$ of every particle is updated according to the following algorithm:

$$\mathbf{r}_i(t+\Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t)\Delta t , \quad i = 1, 2, \ \ldots \ I . \tag{4}$$

There are at least three issues to be addressed:

1. How to determine the velocity $\mathbf{v}_i(t)$ away from the domain boundaries?
2. How to take into account the boundary conditions (2) and (3)?
3. How to select the time increment Δt for the algorithm (4) to be stable and accurate?

Analytical solutions for assessing Lagrangian models

Eric Deleersnijder, 5 June 2005, 21-28 December 2005

As is well known, Lagrangian transport models must include a term taking into account the space variations of the eddy diffusivity (e.g. Hunter et al. 1993, Visser 1997). These models are generally considered uneasy to validate, because there do not exist many relevant analytical solutions to compare with. Two such solutions, which are inspired by Deleersnijder et al. (2005), are presented herein. Hopefully, they will be of use.

1. Settling and diffusion model

Consider a passive — or inert — constituent settling in a horizontally homogeneous mixed layer adjacent to the surface of the mixed layer. The lower boundary of the surface layer is a pycnocline, in which turbulent diffusion is assumed to be negligible. The sinking velocity, w, and the thickness of the mixed layer, h, are assumed to be constant. Let z denote the vertical coordinate, which is equal to 0 and h at the top of the pycnocline and the water-air interface, respectively, so that the domain of interest is defined by inequalities $0 \le z \le h$ (Figure 1).

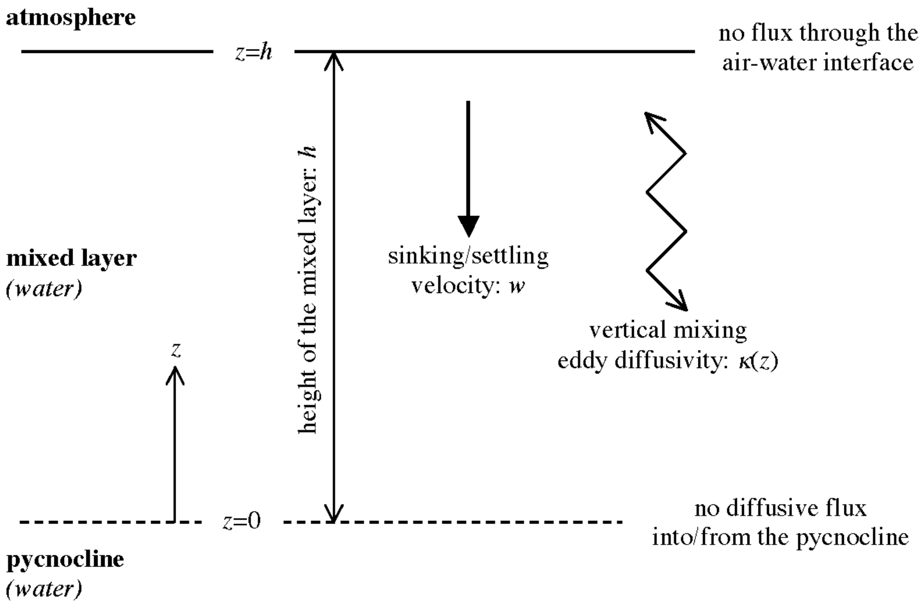

Figure 1. Sinking-diffusion model: illustration of its geometry, parameters and boundary conditions.

At any time t, the concentration of the constituent under consideration, $C(t,z)$, satisfies the following advection-diffusion equation:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(wC + \kappa\frac{\partial C}{\partial z}\right), \tag{1}$$

where κ denotes the eddy diffusivity. For the purposes of the present study, it is convenient to consider that the latter does not depend on time, but further assuming that it is also independent of the vertical coordinate would be too strong an idealisation (Burchard 2002, Umlauf and Burchard 2005). Hence, the eddy diffusivity is assumed to be a non-negative function of the vertical coordinate, i.e. $\kappa(z) \geq 0$. As will be seen, selecting a quadratic diffusivity profile allows for closed-form solutions to be found:

$$\kappa(z) \;=\; 6\bar{\kappa}\,(z/h)(1-z/h)\ , \qquad (2)$$

where $\bar{\kappa}$ is the depth-averaged eddy diffusivity, i.e.

$$\bar{\kappa} \;=\; \frac{1}{h}\int_0^h \kappa(z)\,dz\ . \qquad (3)$$

It is hypothesised that there is no flux of the constituent under study through the air-sea interface, implying that the following boundary condition must be applied:

$$\left[wC + \kappa\frac{\partial C}{\partial z}\right]_{z=h} \;=\; 0\ . \qquad (4)$$

As the pycnocline is a barrier to turbulent diffusion, the associated flux must be prescribed to be zero at the bottom of the mixed layer:

$$\left[\kappa\frac{\partial C}{\partial z}\right]_{z=0} \;=\; 0\ . \qquad (5)$$

At t=0, a unit quantity of the material under study is concentrated at a distance z_0 to the pycnocline: the initial concentration is a Dirac function, i.e.

$$C(0,z) \;=\; \delta(z-z_0)\ . \qquad (6)$$

2. The solution with zero settling velocity

If the settling velocity w is set to zero, the concentration of the constituent under consideration tends to homogenize as time progresses, while its contents in the domain of interest remains constant. This can be expressed mathematically as follows:

$$\lim_{t\to\infty} C(t,z) \;=\; \frac{1}{h}\ , \qquad (7)$$

$$\int_0^1 C(t,z)\,dz \;=\; 1\ . \qquad (8)$$

Demonstrating that (7) and (8)[1] hold valid is trivial, I believe. This remains true for any positive diffusivity. If the diffusivity is given by quadratic expression (2), an analytical solution exists, i.e.

$$\boxed{C(t,z) \;=\; \sum_{n=0}^{\infty} c_n\, e^{-t/\tau_n}\, P_n(2z/h-1)} \qquad (9)$$

[1] It must be stressed that the dimension of the variable that is regarded herein as the concentration is, in fact, the inverse of a length, which is in accordance with the initial condition (6) and the constraint (8). This peculiarity stems from the initial condition being a Dirac function, whose dimension is the inverse of a length.

where P_n denotes the n-order Legendre polynomial and

$$c_n = \frac{2n+1}{h} P_n(2z_0/h-1) , \qquad (10)$$

$$\tau_n = \frac{h^2}{6n(n+1)\overline{\kappa}} . \qquad (11)$$

3. The residence time

If the settling velocity w is not zero, a closed-form solution is hard to obtain. However, as is seen in Deleersnijder et al. (2005), the residence time $\theta(z_0)$ of the particles in the domain of interest may be derived. This timescale is defined as (Bolin and Rodhe, 1973)

$$\theta(z_0) = \int_0^\infty \int_0^h C(t,z)\, dz\, dt , \qquad (12)$$

and, for the present problem, is given by (Deleersnijder et al. 2005)

$$\theta(z_0) = \frac{z_0}{w} + \frac{1}{w} \int_{z_0}^{h} \exp\left[-w \int_{z_0}^{\xi} \frac{d\zeta}{\kappa(\zeta)}\right] d\xi . \qquad (13)$$

The latter satisfies inequalities

$$z_0/w \le \theta(z_0) \le h/w . \qquad (14)$$

If the diffusivity is given by expression (2), the residence time may be seen to be

$$\boxed{\theta(z_0) = \frac{z_0}{w} + \frac{h}{w}\left(\frac{z_0}{h-z_0}\right)^{\mu} B_{1-z_0/h}(1+\mu, 1-\mu)} \qquad (15)$$

where $B_{1-z_0/h}(1+\mu,1-\mu)$ is an incomplete beta function[2] and

$$\mu = \frac{wh}{6\overline{\kappa}} , \qquad (16)$$

References

Bolin, B. and Rodhe, H.: 1973, A note on the concepts of age distribution and transit time in natural reservoirs, *Tellus*, **25**, 58-62.

Burchard, H.: 2002, *Applied Turbulence Modelling in Marine Waters*, Lecture Notes in Earth Sciences Vol. 100, Springer-Verlag, Berlin.

[2] The incomplete beta function is defined to be $B_x(a,b) = \int_0^x \sigma^{a-1}(1-\sigma)^{b-1}\, d\sigma$. There are now many softwares that provide its values on a routine basis. As a consequence, obtaining the value of this function is now almost as easy as getting that of a sine or a cosine. Unfortunately, some numerical packages compute a slightly different incomplete beta function, which actually is the function defined above normalised by a gamma function so that negative arguments are considered unacceptable.

Deleersnijder, E., Beckers, J.-M. and Delhez, E.J.M., 2005, The residence time of settling particles in the surface mixed layer, *Environmental Fluid Mechanics* (in press).

Hunter, J.R., Craig, P.D. and Phillips, H.E.: 1993, On the use of random walk models with spatially variable diffusivity, *Journal of Computational Physics*, **106**, 366-376.

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Visser, A.W.: 1997, Using random walk models to simulate the vertical distribution of particles in a turbulent water column, *Marine Ecology Progress Series*, **158**, 275-281.

Checking an analytical solution using Legendre polynomials

Eric Deleersnijder, 23-28 December 2005

The partial differential problem to solve

Let the domain of interest be defined by inequalities:

$$0 \leq z \leq h \ . \tag{1}$$

The eddy diffusivity is defined to be

$$\kappa(z) = 6\overline{\kappa}\left(\frac{z}{h} - \frac{z^2}{h^2}\right) , \tag{2}$$

where $\overline{\kappa}$ is its depth average, i.e.

$$\overline{\kappa} = \frac{1}{h}\int_0^h \kappa(z)\, dz \ . \tag{3}$$

At any time t (>0), the concentration of the constituent under consideration, $C(t,z)$, satisfies the following diffusion equation:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(\kappa \frac{\partial C}{\partial z}\right) , \tag{4}$$

The domain boundaries are impermeable, implying that no tracer flux is allowed to crossed them. Accordingly, the following boundary conditions must be prescribed:

$$\left[\kappa \frac{\partial C}{\partial z}\right]_{z=0} = 0 = \left[\kappa \frac{\partial C}{\partial z}\right]_{z=h} \ . \tag{5}$$

At t=0, a unit quantity of the tracer under study is concentrated at a distance z_0 to the bottom of the domain of interest; the initial concentration is thus the following Dirac function

$$C(0,z) = \delta(z - z_0) \ , \quad 0 < z_0 < h \ . \tag{6}$$

Theorem

Because of the zero-flux boundary conditions, the tracer content of the domain must remain constant, while diffusion progressively homogeneizes the concentration. This can be expressed mathematically as follows:

$$\int_0^1 C(t,z)\, dz = 1 \ , \tag{7}$$

$$\lim_{t\to\infty} C(t,z) = \frac{1}{h} \ . \tag{8}$$

Demonstration

The solution to partial differential problem (1)-(6) is

$$C(t,z) \;=\; \sum_{n=0}^{\infty} c_n\, e^{-t/\tau_n}\, P_n(2z/h-1) \tag{9}$$

where P_n denotes the n-th order Legendre polynomial and

$$c_n \;=\; \frac{2n+1}{h}\, P_n(2z_0/h-1)\ , \tag{10}$$

$$\tau_n \;=\; \frac{h^2}{6n(n+1)\overline{\kappa}}\ . \tag{11}$$

It is convenient to introduce a new space coordinate:

$$\xi \;=\; \frac{2z-h}{h}\ , \tag{12}$$

with $-1 \le \xi \le 1$. Using the latter, differential equation (4) may be rewritten as

$$\frac{\partial C}{\partial t} \;=\; \frac{6\overline{\kappa}}{h^2}\frac{\partial}{\partial \xi}\left[(1-\xi^2)\frac{\partial C}{\partial \xi}\right]. \tag{13}$$

Substituting (9)-(11) into (13) and setting $\xi_0 = 2z_0/h-1$ lead to

$$\frac{\partial C}{\partial t} \;=\; -\frac{6\overline{\kappa}}{h^3}\sum_{n=0}^{\infty} n(n+1)(2n+1)P_n(\xi_0)\exp\!\left(-\frac{6n(n+1)\overline{\kappa}t}{h^2}\right)P_n(\xi) \tag{14}$$

and

$$\frac{6\overline{\kappa}}{h^2}\frac{\partial}{\partial \xi}\left[(1-\xi^2)\frac{\partial C}{\partial \xi}\right] \;=\; \frac{6\overline{\kappa}}{h^3}\sum_{n=0}^{\infty}(2n+1)P_n(\xi_0)\exp\!\left(-\frac{6n(n+1)\overline{\kappa}t}{h^2}\right)\frac{d}{d\xi}\left[(1-\xi^2)\frac{dP_n(\xi)}{d\xi}\right]. \tag{15}$$

As is well known, Legendre polynomials satisfy the following differential equation

$$\frac{d}{d\xi}\left[(1-\xi^2)\frac{dP_n(\xi)}{d\xi}\right] \;=\; -n(n+1)P_n(\xi)\ . \tag{16}$$

Therefore, (14) and (15) are equal to each other, so that the series (9) satisfies the partial differential equation (13) or, equivalently, (4).

At $\xi = \pm 1$, the first derivative of Legendre polynomials is finite and the eddy diffusivity is zero. As a result, the boundary conditions (5) are satisfied.

The initial condition (6) is met if the following relation

$$\frac{1}{h}\sum_{n=0}^{\infty}(2n+1)P_n(\xi_0)P_n(\xi) \;=\; \delta(z-z_0) \tag{17}$$

holds true — only in a “weak sense”, I suppose. Given that

$$\int_{-1}^{1} P_m(\xi)P_n(\xi)\,d\xi \;=\; \begin{cases} 0 & \text{if} \quad m \ne n \\ 2/(2n+1) & \text{if} \quad m = n \end{cases}, \tag{18}$$

demonstrating that the initial condition is satisfied is tantamount to showing that

$$\frac{1}{h}(2n+1)P_n(\xi_0)\int_0^h \left[P_n(\xi)\right]^2 dz \;=\; \int_0^h \delta(z-z_0)P_n(\xi)\,dz\ . \tag{19}$$

Then, it is readily seen that

$$\frac{1}{h}(2n+1)P_n(\xi_0)\int_0^h\left[P_n(\xi)\right]^2 dz \;=\; \frac{1}{h}(2n+1)P_n(\xi_0)\,\frac{h}{2}\underbrace{\int_0^h\left[P_n(\xi)\right]^2 d\xi}_{2/(2n+1)} \;=\; P_n(\xi_0)\ , \tag{20}$$

and

$$\int_0^h \delta(z-z_0)P_n(\xi)\,dz \;=\; P_n(\xi_0)\ . \tag{21}$$

As a consequence, (19) holds valid, which we consider to be a satisfactory proof of the exactness of (17).

To summarise, we have seen that the series (9) satisfies the differential equation (4), the boundary condition (5) and the initial condition (6), implying that (9) must be regarded as the solution to the problem under study.

By virtue of (9), the tracer content of the domain of interest may be expressed as

$$\int_0^1 C(t,z)\,dz \;=\; \frac{h}{2}\int_{-1}^1\sum_{n=0}^{\infty} c_n\,e^{-t/\tau_n}\,P_n(\xi)\ . \tag{22}$$

As is well known, $P_0(\xi)=1$, implying that (18) yields

$$\int_{-1}^1 P_0(\xi)P_n(\xi)\,d\xi \;=\; \int_{-1}^1 P_n(\xi)\,d\xi \;=\; \begin{cases}0 & \text{if}\quad n=1,2,\ldots\\ 2 & \text{if}\quad n=0\end{cases}\ . \tag{23}$$

Then, (22) transforms to

$$\int_0^1 C(t,z)\,dz \;=\; h\,c_0\,e^{-t/\tau_0}\ . \tag{24}$$

Since $c_0=1/h$ and $1/\tau_0=0$, if follows that *integral (7) holds valid*.

The limit for $t\to\infty$ of the tracer concentration is readily estimated:

$$\begin{aligned}\lim_{t\to\infty}C(t,z) \;&=\; \lim_{t\to\infty}\sum_{n=0}^{\infty} c_n\,e^{-t/\tau_n}\,P_n(2z/h-1)\\ &\qquad\qquad \lim_{t\to\infty}c_0\underbrace{e^{-t/\tau_0}}_{=1}\underbrace{P_0(2z/h-1)}_{=1} \;=\; c_0 \;=\; \frac{1}{h}\end{aligned}\ . \tag{25}$$

As a consequence, the *limit (8) is correct*. QED.

A general solution to a diffusion problem — involving a variable eddy coefficient — for assessing Lagrangian algorithms

Eric Deleersnijder, 12 January 2006

In previous working notes, I have suggested a one-dimensional diffusion problem of which the analytical solution may be used to assess Lagrangian algorithms involving random walks. The key feature of this problem was that the eddy diffusivity was a function of the space coordinate, which requires the introduction of a corrective velocity in the Lagrangian algorithm. A generalised version of this problem is suggested herein, along with a general solution and three closed-form solutions for special diffusivity profiles.

The problem to solve

Let t and z denote time and a space coordinate. The domain of interest is defined by the inequalities

(1) $$0 \le t \ , \ \ 0 \le z \le h \ ,$$

where h is a positive constant. The concentration of the tracer under study, $C(t,z)$, is the solution of the following partial differential problem:

(2) $$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(\kappa \frac{\partial C}{\partial z}\right) , \quad \left[\kappa \frac{\partial C}{\partial z}\right]_{z=0,h} = 0 \ , \quad C(0,z) = C_0(z) \ \ge \ 0 \ ,$$

where $\kappa(z)$ is the eddy diffusivity. The latter is positive and non-zero in the interval $0 < z < h$.

Dimensionless formulation

For the sake of generality, it is convenient to reformulate the problem above using dimensionless variables. The latter are defined to be

(3) $$t' = \frac{t}{h^2/\overline{\kappa}} \ , \quad z' = \frac{z}{h} \ , \quad \left(C',C_0'\right) = \frac{\left(C,C_0\right)}{\overline{C}_0} \ , \quad \kappa' = \frac{\kappa}{\overline{\kappa}} \ ,$$

where $\overline{\kappa}$ and $\overline{C}_0$ denote the averages over the domain of interest of the eddy diffusivity and the initial concentration, respectively, i.e.

(4) $$\overline{\kappa} = h^{-1}\int_0^h \kappa(z)\,dz \ , \quad \overline{C}_0 = h^{-1}\int_0^h C_0(z)\,dz \ .$$

From here on, only dimensionless quantities will be used. This is why we will drop the primes. So, using dimensionless variables, the domain of interest and the problem to be solved may be rewritten as follows:

(5) $$0 \le t \ , \quad 0 \le z \le 1$$

(6) $$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(\kappa \frac{\partial C}{\partial z}\right) , \quad \left[\kappa \frac{\partial C}{\partial z}\right]_{z=0,1} = 0 \ , \quad C(0,z) = C_0(z) \ \ge \ 0$$

where the — dimensionless — domain-averaged values of the eddy diffusivity and initial concentration must be equal to unity, i.e.

(7) $$\overline{\kappa} = \int_0^1 \kappa(z)\,dz = 1 \ , \quad \overline{C}_0 = \int_0^1 C_0(z)\,dz = 1 \ .$$

It is readily seen that the solution of the problem above must satisfy the constraints:

(8) $$\boxed{\overline{C}(t) = \int_0^1 C(t,z)\,dz = 1 \ , \quad \lim_{t\to\infty} C(t,z) = 1}$$

General solution

Let $\psi_n(z)$ and λ_n (n=0,1,2,3...) denote the eigenfunctions and the eigenvalues — with $\lambda_n < \lambda_{n+1}$ — ensuing from the Sturm-Liouville problem

(9) $$\frac{d}{dz}\left(\kappa \frac{d\psi_n}{dz}\right) + \lambda_n \psi_n = 0 \ , \quad \left[\kappa \frac{d\psi_n}{dz}\right]_{z=0,1} = 0 \ .$$

As is well known, the eigenfunctions are orthogonal. They may be normalised so that

(10) $$\int_0^1 \psi_m(z)\psi_n(z)\,dz = \begin{cases} 1 & \text{if } m=n \\ 0 & \text{if } m \neq n \end{cases}.$$

For n=0, the eigenfunction and eigenvalue are

(11) $$\psi_0(z) = 1 \ , \quad \lambda_0 = 0 \ ,$$

no matter the eddy diffusivity profile. This implies that, for n≥1, the eigenfunctions have zero mean:

(12) $$\int_0^1 \psi_n(z)\,dz = 0 \ , \quad n = 1,2,3,\ldots \ .$$

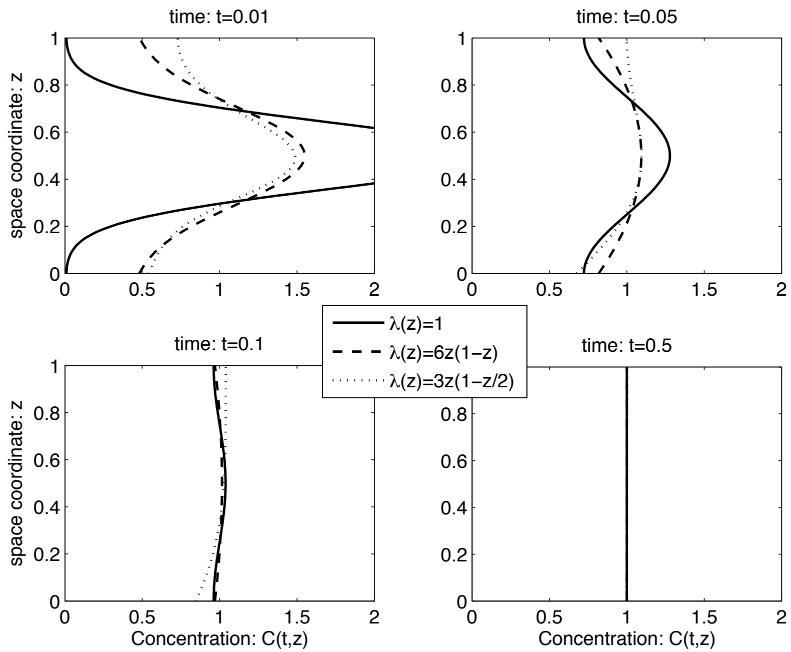
The solution of the partial differential problem (6) may be written as a series of the abovementioned eigenfunctions:

(13) $$\boxed{C(t,z) = 1 + \sum_{n=1}^{\infty} \gamma_n e^{-\lambda_n t} \psi_n(z) \ , \quad \text{with } \gamma_n = \int_0^1 C_0(z)\psi_n(z)\,dz}$$

It is straightforward to demonstrate that solution (13) satisfies the constraints (8).

Assuming that the initial concentration is the Dirac impulse located at $z = z_0$, i.e. $C_0(z) = \delta(z - z_0)$, there exist a few diffusivity profiles for which the eigenfunctions and eigenvalues may be obtained analytically. This is illustrated in the table below, where P_n denotes the n-th order Legendre polynomial. See also the figure, which was obtained for $z_0 = 1/2$.

$\kappa(z) = 1$	$\kappa(z) = 6z(1-z)$	$\kappa(z) = 3z(1-z/2)$
$C_0 = \delta(z-z_0)$	$C_0 = \delta(z-z_0)$	$C_0 = \delta(z-z_0)$
$\gamma_n = \sqrt{2}\cos(n\pi z_0)$	$\gamma_n = \sqrt{2n+1}\,P_n(2z_0-1)$	$\gamma_n = \sqrt{4n+1}\,P_{2n}(1-z_0)$
$\lambda_n = n^2\pi^2$	$\lambda_n = 6n(n+1)$	$\lambda_n = 3n(2n+1)$
$\psi_n(z) = \sqrt{2}\cos(n\pi z)$	$\psi_n(z) = \sqrt{2n+1}\,P_n(2z-1)$	$\psi_n(z) = \sqrt{4n+1}\,P_{2n}(1-z)$



It is useful to keep in mind that Legendre Polynomials satisfy the differential equation and integral

(14) $$\frac{d}{d\xi}\left[(1-\xi^2)\frac{dP_n(\xi)}{d\xi}\right] + n(n+1)P_n(\xi) = 0 \ , \quad \int_{-1}^{+1} P_n^2(\xi)\,d\xi = \frac{2}{2n+1} \ , \quad n = 1,2,3,\ldots \ .$$

In addition, Legendre polynomials exhibit the following properties:

(15) $$P_{2n}(\xi) = P_{2n}(-\xi) \ , \quad \left[\frac{dP_{2n}(\xi)}{d\xi}\right]_{\xi=0} = 0 \ , \quad P_{2n-1}(\xi) = -P_{2n-1}(-\xi) \ , \quad n = 1,2,3,\ldots \ .$$

Acknowledgements. Many thanks to Laurent White, who carefully checked the mathematical developments above.

A settling-diffusion problem: analytical solutions for assessing Lagrangian algorithms

Eric Deleersnijder, 16 January 2006

Settling and diffusion model

Consider a passive — or inert — constituent settling in a horizontally homogeneous mixed layer adjacent to the surface of the mixed layer. The lower boundary of the surface layer is a pycnocline, in which turbulent diffusion is assumed to be negligible. The sinking velocity, w (>0), and the thickness of the mixed layer, h, are assumed to be constant. Let z denote the vertical coordinate, which is equal to 0 and h at the top of the pycnocline and the water-air interface, respectively, so that the domain of interest is defined by inequalities $0 \leq z \leq h$ (Figure 1).

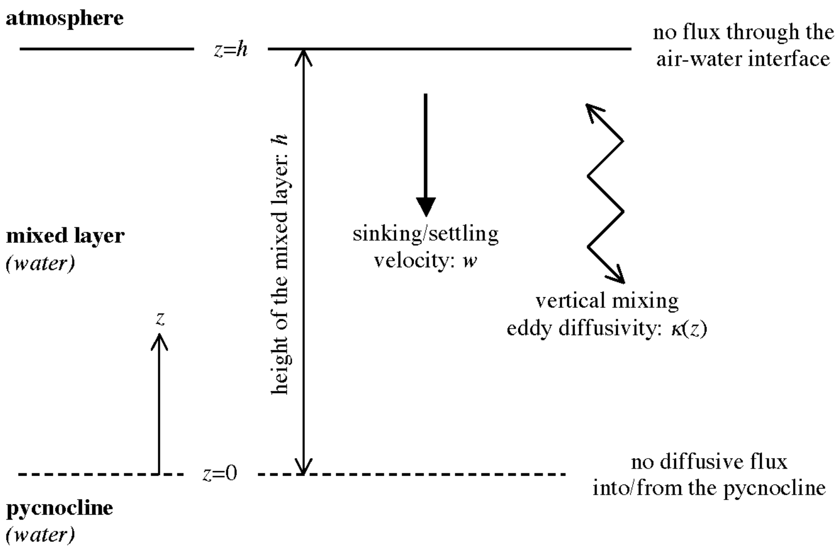


Figure 1. Sinking-diffusion model: illustration of its geometry, parameters and boundary conditions.

At any time t, the concentration of the constituent under consideration, $C(t,z)$, satisfies the following advection-diffusion equation:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(wC + \kappa \frac{\partial C}{\partial z} \right) , \tag{1}$$

where κ denotes the eddy diffusivity. For the purposes of the present study, it is convenient to consider that the latter does not depend on time, but further assuming that it is also independent of the vertical coordinate would be too strong an idealisation (Burchard 2002, Umlauf and Burchard 2005). Hence, the eddy diffusivity is assumed to be a non-negative function of the vertical coordinate.

It is hypothesised that there is no flux of the constituent under study through the air-sea interface, implying that the following boundary condition must be applied:

$$\left[wC + \kappa \frac{\partial C}{\partial z} \right]_{z=h} = 0 \ . \tag{2}$$

As the pycnocline is a barrier to turbulent diffusion, the turbulent diffusion flux must be prescribed to be zero at the bottom of the mixed layer:

$$\left[\kappa \frac{\partial C}{\partial z} \right]_{z=0} = 0 \ . \tag{3}$$

Upon specifying the initial profile of the concentration, $C(0,z)$, the concentration $C(t,z)$ may, in principle, be obtained at any point and any time t>0.

To obtain the residence time $\theta(z_0)$, a unit amount of tracer is released at the initial time at a distance z_0 to the pycnocline. In other words, the initial condition reads

$$C(0,z) = \delta(z - z_0) \ . \tag{4}$$

As is well known (Bolin and Rodhe 1973, Delhez et al. 2004), the residence time may be evaluated as follows:

$$\theta(z_0) = \int_0^{\infty} \int_0^{h} C(t,z) \, dz \, dt \ . \tag{5}$$

Then, the latter may be re-written as a function of z, i.e. $\theta(z)$, which is the form that will be used in most instances below.

Closed-form expressions of the concentration are hard to derive, especially when the eddy diffusivity is not constant in space. Therefore, for the problem under study, the residence time can hardly ever be obtained from the direct application of (5). It is however possible to establish an analytical expression of the residence time by having recourse to an adjoint model approach.

An adjoint model approach

In accordance with the adjoint model approach of Delhez et al. (2004), the residence time $\theta(z)$ satisfies the following differential problem:

$$\frac{d}{dz}\left(w\theta - \kappa \frac{d\theta}{dz} \right) = 1 \ , \tag{6}$$

$$\left[\kappa \frac{d\theta}{dz} \right]_{z=h} = 0 \ , \tag{7}$$

$$\left[w\theta - \kappa \frac{d\theta}{dz} \right]_{z=0} = 0 \ . \tag{8}$$

Then, it is readily seen that the residence time is

$$\theta(z) = \frac{z}{w} + \frac{1}{w} \int_z^h \exp\left[-w \int_z^{\xi} \frac{d\zeta}{\kappa(\zeta)} \right] d\xi \tag{9}$$

Notice that at the top of the mixed layer, $z = h$, the residence time is equal to h/w, no matter the eddy diffusivity profile and magnitude!

Dimensionless formulation

It is convenient to introduce dimensionless variables:

$$t' = \frac{t}{h/w} \ , \ (z', z_0') = \frac{(z, z_0)}{h} \ , \ \kappa' = \frac{\kappa}{\overline{\kappa}} \ , \ C' = \frac{C}{\overline{C}(0)} \ , \ \theta' = \frac{\theta}{h/w} \ , \tag{10}$$

where $\overline{\kappa}$ and $\overline{C}(0)$ denote the average over the mixed layer height of the eddy diffusivity and the initial value of the concentration, i.e.

$$\overline{\kappa} \ = \ \frac{1}{h}\int_0^h \kappa(z)\, dz \ , \tag{11}$$

and

$$\overline{C}(0) \ = \ \frac{1}{h}\int_0^h C(0,z)\, dz \ . \tag{12}$$

Finally, the Peclet number is defined to be

$$Pe \ = \ \frac{wh}{\overline{\kappa}} \ . \tag{13}$$

From now on, only dimensionless variables will be used, so that it is appropriate to drop the primes. Accordingly, the domain of interest is now defined as $0 \le t$ and $0 \le z \le 1$, while the differential problem obeyed by the concentration is

$$\frac{\partial C}{\partial t} \ = \ \frac{\partial}{\partial z}\left(wC + \frac{\kappa}{Pe}\frac{\partial C}{\partial z} \right) , \tag{14}$$

$$\left[C + \frac{\kappa}{Pe}\frac{\partial C}{\partial z} \right]_{z=h} \ = \ 0 \ . \tag{15}$$

$$\left[\frac{\kappa}{Pe}\frac{\partial C}{\partial z} \right]_{z=0} \ = \ 0 \ . \tag{16}$$

$$C(0,z) \ = \ \delta(z - z_0) \ . \tag{17}$$

The residence time,

$$\theta(z_0) \ = \ \int_0^\infty \int_0^h C(t,z)\, dz\, dt \ , \tag{18}$$

may be obtained by solving the adjoint problem

$$\frac{d}{dz}\left(\theta - \frac{\kappa}{Pe}\frac{d\theta}{dz} \right) \ = \ 1 \ , \tag{19}$$

$$\left[\frac{\kappa}{Pe}\frac{d\theta}{dz} \right]_{z=h} \ = \ 0 \ , \tag{20}$$

$$\left[\theta - \frac{\kappa}{Pe}\frac{d\theta}{dz} \right]_{z=0} \ = \ 0 \ , \tag{21}$$

yielding

$$\boxed{\theta(z) \ = \ z \ + \ \int_z^1 \exp\left[-Pe\int_z^\xi \frac{d\zeta}{\kappa(\zeta)} \right] d\xi} \tag{22}$$

Illustration

If the eddy diffusivity is constant, $\kappa = 1$, the residence time is (Figure 2)

$$\theta(z) \;=\; z \;+\; \frac{1 - e^{-Pe(1-z)}}{Pe} \;. \tag{23}$$

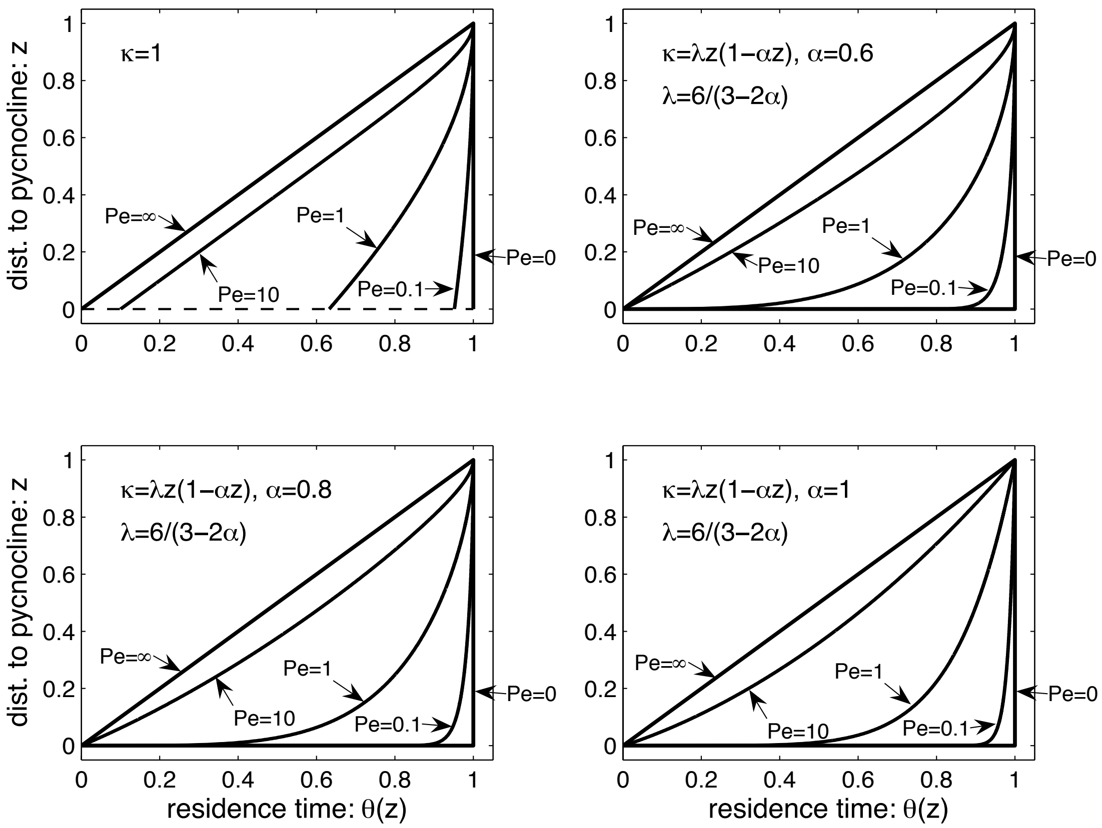


Figure 2. The residence time for various values of the Peclet number, Pe, as obtained by means of relation (22).

Selecting a constant eddy diffusivity is not entirely consistent with the main features of turbulent processes in the upper mixed layer. It is desirable that κ tend to zero as the bottom of the mixed layer is approached so as to take into account the inhibition of turbulence in the pycnocline. A simple expression is the following parabolic profile

$$\kappa(z) \;=\; \frac{6z(1-\alpha z)}{3-2\alpha} \;, \tag{24}$$

with $1/2 < \alpha \le 1$. The constant α is likely to be very close to unity, say $0.95 \le \alpha \le 1$ (Burchard, personal communication, 2005), but smaller values cannot be ruled out *a priori*. If

$$\mu \;=\; \frac{3-2\alpha}{6}\, Pe \;, \tag{25}$$

the residence time corresponding to eddy diffusivity (24) is (Figure 2)

$$\theta(z) \;=\; z \;+\; \frac{1}{\alpha}\left(\frac{\alpha z}{1-\alpha z}\right)^{\mu} B_{1-\alpha,1-\alpha z}(1+\mu, 1-\mu) \;, \tag{26}$$

where $B_{1-\alpha,1-\alpha z}(1+\mu,1-\mu)$ is a generalised incomplete beta function[1], i.e.

$$B_{1-\alpha,1-\alpha z}(1+\mu,1-\mu) \;=\; \int_{1-\alpha}^{1-\alpha z} \sigma^{\mu}\,(1-\sigma)^{-\mu}\,d\sigma\ . \tag{27}$$

If the eddy diffusivity is asymptotic to z^a ($a \geq 0$) in the limit $z \to 0$, then the value of the residence time at the lower boundary of the domain (Deleersnijder et al. 2006):

$$\lim_{z\to 0} \theta(z) \;=\; \begin{cases} 0 & \text{if } \ a \geq 1 \\ >0 & \text{if } \ a < 1 \end{cases}\ . \tag{28}$$

So, the residence time in the vicinity of the pycnocline crucially depends on how "fast" the diffusivity tends to zero.

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[1] The software *Mathematica* is able to deal with the generalised incomplete beta function as is defined and used here. Unfortunately, there are commercial softwares that resort to another definition of this function — while retaining the same name!

An analytical solution of a two-dimensional iso- and dia-pycnal diffusion problem

Eric Deleersnijder, 24 January 2006

If advective processes can be neglected, the concentration $C(t,\mathbf{x})$ of a passive tracer obeys the following equation:

$$\frac{\partial C}{\partial t} = \nabla \bullet (\mathbf{K} \bullet \nabla C) \ , \tag{1}$$

where $\mathbf{K}$ denotes the diffusivity tensor, which must be symmetric and positive definite. For large-scale ocean diffusion problems, the diffusion tensor depends on two diffusivities, K_i and K_d, which are the isopycnal and diapycnal eddy coefficients, respectively. If homogeneity can be assumed along one horizontal coordinates, a two-dimensional problem is to be dealt with. In the principal axes, the diffusivity tensor reads

$$\mathbf{K} = \begin{pmatrix} K_i & 0 \\ 0 & K_d \end{pmatrix} . \tag{2}$$

The first principal axis is parallel to the isopycnal direction, while the other is orthogonal to it. If θ denotes the angle between the horizontal and the isopycnal direction, in the horizontal-vertical coordinates (x,z), the diffusivity tensor is (Redi 1982, Beckers et al. 1998)

$$\mathbf{K} = \begin{pmatrix} \cos^2\theta K_i + \sin^2\theta K_d & \sin\theta\cos\theta(K_i - K_d) \\ \sin\theta\cos\theta(K_i - K_d) & \sin^2\theta K_i + \cos^2\theta K_d \end{pmatrix} . \tag{3}$$

The domain of interest is assumed to be infinite,

$$-\infty < x < \infty \ , \ -\infty < z < \infty \ , \tag{4}$$

and the initial concentration is a Dirac impulse, i.e.

$$C(0,\mathbf{x}) = \delta(\mathbf{x} - 0) = \delta(x - 0)\delta(z - 0) \ . \tag{5}$$

It is useful to introduce dimensionless variables. The time and space coordinate are transformed as follows:

$$t' = \frac{t}{T} \ , \ x' = \frac{x}{L_h} \ , \ z' = \frac{z}{L_v} \ , \tag{6}$$

where T, L_h and L_v denote the appropriate timescale, horizontal length scale and vertical length scale. It is convenient to define the latter in such a way that

$$T = \frac{L_h^2}{K_i} = \frac{L_v^2}{K_d} \ . \tag{7}$$

The ratio of the vertical length scale to the horizontal one, i.e. the aspect ratio, is

$$\alpha = \frac{L_v}{L_h} \ . \tag{8}$$

The concentration is scaled as follows:

$$C' = \frac{C}{1/(L_h L_v)} \ . \tag{9}$$

The equation to be solved now reads

$$\frac{\partial C'}{\partial t'} \;=\; \frac{\partial}{\partial x'}\left(K'_{xx}\frac{\partial C'}{\partial x'} + K'_{xz}\frac{\partial C'}{\partial z'} \right) \;+\; \frac{\partial}{\partial z'}\left(K'_{zx}\frac{\partial C'}{\partial x'} + K'_{zz}\frac{\partial C'}{\partial z'} \right) , \qquad (10)$$

with

$$K'_{xx} \;=\; \frac{K_{xx}}{L_h^2/T} \;=\; \cos^2\theta \;+\; \alpha^2\sin^2\theta \;, \qquad (11)$$

$$K'_{xz} \;=\; \frac{K_{xz}}{L_h L_v/T} \;=\; (\alpha^{-1}-\alpha)\sin\theta\cos\theta \;, \qquad (12)$$

$$K'_{zx} \;=\; \frac{K_{zx}}{L_v L_h/T} \;=\; (\alpha^{-1}-\alpha)\sin\theta\cos\theta \;, \qquad (12)$$

$$K'_{zz} \;=\; \frac{K_{zz}}{L_v^2/T} \;=\; \cos^2\theta \;+\; \alpha^{-2}\sin^2\theta \;. \qquad (13)$$

The initial condition is

$$C'(0,\mathbf{x}) \;=\; \delta(\mathbf{x}'-0) \;=\; \delta(x'-0)\delta(z'-0) \;. \qquad (14)$$

From here on, only dimensionless variables quantities will be dealt with. So, for the sake of simplicity, *the primes will be dropped.*

The general form of the solution to the differential problem (10)-(14) is

$$C(t,\mathbf{x}) \;=\; \frac{\exp\left[-\dfrac{\mathbf{x}\bullet\mathbf{K}^{-1}\bullet\mathbf{x}}{4t}\right]}{4\pi t\sqrt{\det\mathbf{K}}} \;. \qquad (15)$$

It is readily seen that the determinant of $\mathbf{K}$ is equal to unity, i.e.

$$\det\mathbf{K} \;=\; 1 \;, \qquad (16)$$

while its inverse simply is

$$\mathbf{K}^{-1} \;=\; \begin{pmatrix} \cos^2\theta+\alpha^2\sin^2\theta & -(\alpha^{-1}-\alpha)\sin\theta\cos\theta \\ -(\alpha^{-1}-\alpha)\sin\theta\cos\theta & \cos^2\theta+\alpha^{-2}\sin^2\theta \end{pmatrix} . \qquad (17)$$

Using all of the developments above, the domain of interest, the problem to be solved and its solution may be rewritten as follows:

$$\boxed{\begin{gathered}
0 \le t \;,\; -\infty < x < +\infty \;,\; -\infty < z < +\infty \\
\frac{\partial C}{\partial t} \;=\; \frac{\partial}{\partial x}\left(K_{xx}\frac{\partial C}{\partial x} + K_{xz}\frac{\partial C}{\partial z} \right) \;+\; \frac{\partial}{\partial z}\left(K_{zx}\frac{\partial C}{\partial x} + K_{zz}\frac{\partial C}{\partial z} \right) \\
\begin{pmatrix} K_{xx} & K_{xz} \\ K_{zx} & K_{zz} \end{pmatrix} \;=\; \begin{pmatrix} \cos^2\theta+\alpha^2\sin^2\theta & (\alpha^{-1}-\alpha)\sin\theta\cos\theta \\ (\alpha^{-1}-\alpha)\sin\theta\cos\theta & \cos^2\theta+\alpha^{-2}\sin^2\theta \end{pmatrix} \\
C(0,x,z) \;=\; \delta(x-0)\delta(z-0) \\
C(t,x,z) \;=\; \frac{1}{4\pi t}\exp\left[\frac{-(\cos\theta\, x+\alpha\sin\theta\, z)^2-(\cos\theta\, z-\alpha^{-1}\sin\theta\, x)^2}{4t}\right]
\end{gathered}}$$

In the ocean, the slope of the isopycnal surfaces and the aspect ratio is usually small — which is why Cox (1987) suggested a simplified version of the isopycnal diffusivity tensor.

For numerical experiments, I would suggest using the following values (Mathieu and Deleersnijder 1998):

$$\theta \approx 10^{-3} \approx \alpha \, . \tag{18}$$

Needless to say, *representing iso- and dia-pycnal diffusion in a Lagrangian framework using random walks is a way to avoid some of the problems faced by the corresponding Eulerian solvers, chiefly their lack of monotonicity* (Beckers et al. 1998, Mathieu and Deleersnijder 1998, Beckers et al. 2000).

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Test cases for assessing the Ito and Ito backward methods

Eric Deleersnijder, 28 January 2007

Daria Spivakovskaya used Lagrangian methods to reproduce the analytical solutions of Deleersnijder et al. (2006). The Ito method naturally lead to the residence time $\tau(z,0^+)$, while the Ito backward approach yielded $\tau(z,0^-)$. This is worth being explained in detail in a publication. However, in the aforementioned problem, the discontinuity of the diffusivity lies on one of the boundaries of the domain of interest. This situation may be regarded as too peculiar to provide a sufficiently convincing illustration. Another type of problem also needs to be tackled, in which the discontinuity in the eddy diffusivity is located inside the domain of interest. In this respect, inspiration may be found in the one-dimensional idealized problems dealt with in Delhez et al. (2004) and Delhez and Deleersnijder (2006).

The direct and adjoint problems for the residence time

Let t and x denote time and a space coordinate, respectively. In the domain $-L \le x \le L$, the advection-diffusion Green function $G(t,x,x_0)$ obeys the following partial differential problem

$$\frac{\partial G}{\partial t} = -\frac{\partial}{\partial x}\left(uG - \kappa\frac{\partial G}{\partial x}\right) , \tag{1}$$

$$G(0,x,x_0) = \delta(x - x_0) \ , \ -L < x_0 < L \ , \tag{2}$$

$$G(t,\pm L,x_0) = 0 \ , \tag{3}$$

where δ is the Dirac function; the positive constant u is the fluid velocity, while $\kappa(x) > 0$ denotes the eddy diffusivity. The residence time in the domain of interest of the tracer whose concentration obeys the partial differential problem (1)-(3) is (Delhez et al. 2004)

$$\theta(x_0) = \int_0^\infty \int_{-L}^{L} G(t,x,x_0)\, dx\, dt \ . \tag{5}$$

In principle this value may be evaluated for any admissible value of x_0. The ensuing function may then be recast as a function of x, *i.e.* $\theta(x)$. However, obtaining the analytical solution of the direct problem (1)-(3) is usually considered as difficult. Fortunately, it is much easier to obtain the residence time by solving the adjoint problem (Delhez et al. 2004, Delhez and Deleersnijder 2006):

$$\frac{d}{dx}\left(\kappa\frac{d\theta}{dx} + u\theta\right) = -1 \ , \tag{6}$$

$$\theta(\pm L) = 0 \ . \tag{7}$$

For the purposes of the present study, the eddy diffusivity must exhibit a discontinuity inside the domain of the interest. The simplest expression that satisfies this constraint probably is the following piecewise constant function

$$\kappa(x_0) = \begin{cases} \kappa^+ \ , & 0 < x_0 \le L \\ \kappa^- \ , & -L \le x_0 < 0 \end{cases} , \tag{8}$$

where κ^+ and κ^- are positive constants. Therefore, at x=0, the residence time must satisfy two matching conditions:

$$\left[\theta(x)\right]_{x=0^-}^{x=0^+} = 0 , \tag{9}$$

$$\left[\kappa\frac{d\theta}{dx} + u\theta\right]_{x=0^-}^{x=0^+} = 0 . \tag{10}$$

In the developments below, the residence time at x=0 will be denoted θ_0. In other words, the latter satisfies the equalities

$$\theta(0^-) = \theta_0 = \theta(0^+) . \tag{11}$$

The zero advection case

If the advection is zero (u=0), then it is appropriate to introduce the dimensionless parameter $\mu = \kappa^+/\kappa^-$ and variables

$$t' = \frac{t}{L/(\kappa^-)^2} , \; (x', x_0') = \frac{(x, x_0)}{L} , \; \kappa' = \frac{\kappa}{\kappa^-} , \; G' = \frac{G}{1/L} , \; (\theta', \theta_0') = \frac{(\theta, \theta_0)}{L/(\kappa^-)^2} . \tag{12}$$

Hence, the dimensionless diffusivity is

$$\kappa'(x') = \begin{cases} \mu , & 0 < x' \le 1 \\ 1 , & -1 \le x' < 0 \end{cases} . \tag{13}$$

Dropping the primes, it is readily seen that the direct problem to solve reads

$$\frac{\partial G}{\partial t} = \frac{\partial}{\partial x}\left(\kappa\frac{\partial G}{\partial x}\right) , \tag{14}$$

$$G(0, x, x_0) = \delta(x - x_0) , \quad G(t, \pm 1, x_0) = 0 , \tag{15}$$

$$\theta(x_0) = \int_0^\infty \int_{-1}^1 G(t, x, x_0)\, dx\, dt , \tag{16}$$

The corresponding adjoint problem consists of the following expressions:

$$\frac{d}{dx}\left(\kappa\frac{d\theta}{dx}\right) = -1 , \tag{17}$$

$$\theta(\pm 1) = 0 . \tag{18}$$

After some calculations, the residence time is obtained:

$$\theta(x) = \begin{cases} -\dfrac{x^2}{2\mu} - \dfrac{2\mu\theta_0 - 1}{2\mu}x + \theta_0 , & 0 < x \le 1 \\ -\dfrac{x^2}{2} + \dfrac{2\theta_0 - 1}{2}x + \theta_0 , & -1 \le x < 0 \end{cases} , \tag{19}$$

with

$$\theta_0 = \frac{1}{1+\mu} . \tag{20}$$

For the sake of completeness, we also consider the case in which there is no discontinuity in the eddy diffusivity. Then, the parameter μ is equal to unity and solution (19) becomes

$$\theta(x) \;=\; \frac{1-x^2}{2} \;. \tag{21}$$

The advection-diffusion case

If advection is present ($u > 0$), then it is appropriate to introduce the following dimensionless parameters and variables:

$$t' = \frac{t}{L/u} \;,\; (x', x_0') = \frac{(x, x_0)}{L} \;,\;\; Pe^{\pm} = \frac{uL}{\kappa^{\pm}} \;,\;\; G' = \frac{G}{1/L} \;,\;\; (\theta', \theta_0') = \frac{(\theta, \theta_0)}{L/u} \;. \tag{22}$$

It is also useful to define a piecewise constant Peclet number:

$$Pe(x) \;=\; \begin{cases} Pe^{+} \;,\;\; 0 < x \le L \\ Pe^{-} \;,\;\; -L \le x < 0 \end{cases} . \tag{23}$$

Dropping the primes, the direct problem to solve reads

$$\frac{\partial G}{\partial t} \;=\; -\frac{\partial}{\partial x}\left(G - \frac{1}{Pe}\frac{\partial G}{\partial x} \right) , \tag{24}$$

$$G(0, x, x_0) = \delta(x - x_0) \;,\;\; G(t, \pm 1, x_0) = 0 \;, \tag{25}$$

$$\theta(x_0) \;=\; \int_0^{\infty}\int_{-1}^{1} G(t, x, x_0)\, dx\, dt \;, \tag{26}$$

The corresponding adjoint problem is

$$\frac{d}{dx}\left(\frac{1}{Pe}\frac{d\theta}{dx} + \theta \right) \;=\; -1 \;, \tag{27}$$

$$\theta(\pm 1) \;=\; 0 \;. \tag{28}$$

After some calculations the residence time is obtained:

$$\theta(x) \;=\; \begin{cases} a^{+} - x + b^{+} e^{-Pe^{+} x} \;,\;\; 0 < x \le 1 \\ a^{-} - x + b^{-} e^{-Pe^{-} x} \;,\;\; -1 \le x < 0 \end{cases} , \tag{29}$$

with

$$a^{\pm} = \frac{e^{\mp Pe^{\pm}}\theta_0 \mp 1}{e^{\mp Pe^{\pm}} - 1} \;,\;\; b^{\pm} = \frac{\pm 1 - \theta_0}{e^{\mp Pe^{\pm}} - 1} \;\;, \tag{30}$$

and

$$\theta_0 \;=\; \frac{Pe^{+} - Pe^{-}}{Pe^{+} Pe^{-}} \frac{(e^{-Pe^{+}} - 1)(e^{Pe^{-}} - 1)}{e^{-Pe^{+}} - e^{Pe^{-}}} \;-\; \frac{e^{-Pe^{+}} + e^{Pe^{-}} - 2}{e^{-Pe^{+}} - e^{Pe^{-}}} \;. \tag{31}$$

For the sake of completeness, the situation in which the eddy diffusivity is continuous — and constant — is also considered. Then, we have $Pe^{+} = Pe = Pe^{-}$ and the residence time is

$$\theta(x) \;=\; \frac{e^{Pe} - e^{-Pe}}{e^{Pe} + e^{-Pe}} \;-\; x \;-\; \frac{2 e^{-Pe\, x}}{e^{Pe} + e^{-Pe}} \;\;. \tag{32}$$

Final remark

If, for testing the Ito backward method, the advection is not absolutely necessary, then it may thought to be appropriate to concentrate on the zero advection case only. However, one might object that in most marine problems advection is present, and is often the dominant transport process. As a consequence, it is not unlikely that an idealized problem devoid of advection may be regarded as inappropriate. So, unless there are very strong arguments that allow for neglecting advection, the second version of the test case — that includes advection — should be taken into account, no matter if the zero advection version is also implemented or not.

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