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A depth-integrated diffusion problem in a depth-varying, unbounded domain for assessing Lagrangian schemes

Eric Deleersnijder, June 14-17, 2015

In a two-dimensional, depth-integrated tracer transport problem, if the velocity, the water column depth and the diffusivity are constant, several analytical solutions exist (e.g. Kärrnä et al. 2010), which can be used to assess Lagrangian (or Eulerian) numerical schemes. Analytical solutions are also needed that can help in deciding whether or not the bathymetry is taken into account in a satisfactory manner in a Lagrangian model. Contributing to filling this gap is the objective of the present working note, which builds on the study of Deleersnijder (2011). The analytical solution derived hereinafter exhibits counterintuitive properties, since the centre of mass of the tracer distribution and the point of maximum concentration move at the same speed in opposite directions. The centre of mass and the position variance of the particle cloud simulated by means of the Lagrangian algorithm suggested below tend to behave as their exact counterparts as the number of particles increases.

Depth-integrated diffusion problem

Let t and $\mathbf{x} = x\mathbf{e}_x + y\mathbf{e}_y$ denote the time and the horizontal position vector, with x and y representing horizontal, Cartesian coordinates; \mathbf{e}_x and \mathbf{e}_y are orthonormal vectors. The domain of interest is unbounded, i.e. $\mathbf{x} \in \mathbb{R}^2$. Now consider a passive — or inert — tracer, whose depth-averaged concentration¹ is denoted $C(t, \mathbf{x})$. The tracer particles are subject to isotropic diffusion processes that are parameterised by means of diffusivity κ ; no other transport phenomena are at work. The height of the water column is position-dependent and is denoted $h(\mathbf{x})$. Assume that a mass M of the tracer under study is suddenly released into the domain at time $t = 0$ and point $\mathbf{x} = 0$. If no tracer is present in the domain at time $t < 0$, the tracer concentration is the solution of the following partial differential equation

$$\frac{\partial(hC)}{\partial t} = \nabla \cdot (h\kappa \nabla C) , \quad (1)$$

under the initial condition

$$C(0, \mathbf{x}) = \frac{m_0}{\rho h_0} \delta(x-0) \delta(y-0) , \quad (2)$$

where $h_0 = h(0)$; the positive constant ρ represents the fluid density, while δ denotes the Dirac function.

Governing equation (1) may be rewritten as follows:

¹ The concentration used herein is defined as a mass fraction, implying that it is dimensionless. To obtain a concentration measured in kg m^{-3} , it is necessary to multiply the aforementioned concentration by the density ρ of the fluid, which is assumed to be constant (Boussinesq approximation).

$$\frac{\partial C}{\partial t} + \mathbf{v} \cdot \nabla C = \kappa \nabla^2 C, \quad (3)$$

where the equivalent velocity \mathbf{v} is defined to be

$$\mathbf{v} = -\frac{\nabla(h\kappa)}{h} \quad (4)$$

Analytical solution and its properties

There is little hope of finding an analytical solution of (3), unless the diffusivity κ and the equivalent velocity \mathbf{v} are constant. This is why the diffusivity is assumed to be constant,

$$\kappa = K, \quad (5)$$

where K is a positive constant. In addition, without any loss of generality, the water column height is prescribed to be

$$h(x, y) = h_0 e^{x/L}, \quad (6)$$

where the positive constant L is a relevant length scale. The corresponding equivalent velocity reads

$$\mathbf{v} = -\frac{K}{L} \mathbf{e}_x. \quad (7)$$

The concentration may then be seen to be

$$C(t, \mathbf{x}) = \frac{M}{4\pi\rho h_0 K t} \exp\left[-\frac{(x + Kt/L)^2 + y^2}{4Kt}\right] \quad (8)$$

Key properties of this solution are to be examined². First, the total tracer mass present in the domain, $m(t)$, remains constant:

$$m(t) \equiv \int_{\mathbb{R}^2} \rho h(\mathbf{x}) C(t, \mathbf{x}) d\mathbf{x} = \frac{M}{4\pi K t} \int_{\mathbb{R}^2} \exp\left[-\frac{(x - Kt/L)^2 + y^2}{4Kt}\right] d\mathbf{x} = M, \quad (9)$$

with $d\mathbf{x} = dx dy$.

The point where the concentration reaches its maximum value is located on the x -axis at

$$\begin{cases} x_m(t) = -\frac{Kt}{L} \\ y_m(t) = 0 \end{cases} \quad (10)$$

Thus, the point of maximum concentration moves towards the shallower part of the domain at speed K/L . The maximum of the concentration is readily seen to be

$$C_m(t) \equiv C[t, x_m(t), 0] = C(t, -Kt/L, 0) = \frac{M}{4\pi\rho h_0 K t} \quad (11)$$

Remarkably, the centre of mass, $\mathbf{r}_c(t)$, moves at the same speed in the opposite direction (i.e. toward the deeper part of the domain):

² To establish the key properties of the solution (8), it is necessary to evaluate somewhat intricate integrals, which may be achieved with the help of the following expressions (e.g. Gradshteyn and Ryzhik 2007):

$$\int_0^\infty e^{-a\zeta^2} d\zeta = \sqrt{\frac{\pi}{4a}}, \quad \int_0^\infty \zeta^2 e^{-a\zeta^2} d\zeta = \sqrt{\frac{\pi}{16a^3}}, \quad a > 0.$$

$$\begin{aligned}
\mathbf{r}_c(t) &= \frac{1}{M} \int_{\mathfrak{R}^2} \rho h(\mathbf{x}) C(t, \mathbf{x}) \mathbf{x} d\mathbf{x} \\
&= \frac{1}{4\pi Kt} \int_{\mathfrak{R}^2} \exp\left[-\frac{(x - Kt/L)^2 + y^2}{4Kt}\right] \mathbf{x} d\mathbf{x} = \frac{Kt}{L} \mathbf{e}_x
\end{aligned} \tag{12}$$

Upon defining the components $\mathbf{r}_c(t)$ as follows $\mathbf{r}_c(t) = x_c(t)\mathbf{e}_x + y_c(t)\mathbf{e}_y$, (12) is obviously equivalent to

$$\begin{cases} x_c(t) = \frac{Kt}{L} \\ y_c(t) = 0 \end{cases} \tag{13}$$

The centre of mass of the tracer patch moves at velocity K/L along the x -axis though the velocity appearing in (3) has the same magnitude but the opposite sign. In other words, the velocity in advection-diffusion equation (3) is \mathbf{v} , which is the velocity of the point of maximum concentration, but the velocity of the centre of mass is $-\mathbf{v}$. This key property may seem to be counterintuitive if one considers only equation (3). However, if the centre of mass were moving at velocity \mathbf{v} , it would imply that the tracer particles would concentrate in the shallower part of the domain, which is also somewhat counterintuitive.

A quantity that is also of interest is the vertical inventory, $J(t, \mathbf{x}) \equiv \rho h(\mathbf{x}) C(t, \mathbf{x})$, which represents the mass per unit area — in the horizontal plane. As a consequence, the vertical inventory may be expressed in kg m^{-2} . Combing (6) and (8), this variable is readily seen to be

$$J(t, \mathbf{x}) \equiv \rho h(\mathbf{x}) C(t, \mathbf{x}) = \frac{M}{4\pi Kt} \exp\left[-\frac{(x - Kt/L)^2 + y^2}{4Kt}\right]. \tag{14}$$

It is readily seen that the maximum of the vertical inventory is located at the same point as the centre of mass of the tracer distribution, i.e. $\mathbf{r}_c(t) = (Kt/L)\mathbf{e}_x$.

Finally, the position variance of the tracer distribution, which is defined to be

$$\sigma^2(t) \equiv \frac{1}{M} \int_{\mathfrak{R}^2} \rho h(\mathbf{x}) C(t, \mathbf{x}) |\mathbf{x} - \mathbf{r}_c(t)|^2 d\mathbf{x}, \tag{15}$$

is worth calculating, for $\sigma(t)$ may be regarded as a measure of the width of the tracer patch. This leads to the unsurprising result

$$\sigma^2(t) = \frac{1}{4\pi Kt} \int_{\mathfrak{R}^2} \exp\left[-\frac{(x - Kt/L)^2 + y^2}{4Kt}\right] \left[\left(x - \frac{Kt}{L}\right)^2 + y^2\right] d\mathbf{x} = 4Kt \tag{16}$$

Lagrangian approach

If one opts for a Lagrangian representation, then N particles are to be released into the domain at $t=0$ and $\mathbf{x}=\mathbf{0}$. The mass of every particle is M/N . The position vector of the n -th particle is denoted $\mathbf{r}_n(t)$ ($n=1,2,..N$). The centre of mass and the position variance of the particle distribution are defined as

$$\tilde{\mathbf{r}}_c(t) = \frac{1}{N} \sum_{n=1}^N \mathbf{r}_n(t) \quad (17)$$

and

$$\tilde{\sigma}^2(t) = \frac{1}{N} \sum_{n=1}^N |\mathbf{r}_n(t) - \tilde{\mathbf{r}}_c(t)|^2, \quad (18)$$

respectively.

The simplest Lagrangian scheme is of the Euler forward type in the sense of the definitions presented in Gräwe et al. (2012), for instance. For the transport problem under consideration, this scheme reads (e.g. Heemink 1990, Spagnol et al. 2002)

$$\mathbf{r}_n(t + \Delta t) = \mathbf{r}_n(t) - \mathbf{v} \Delta t + \frac{\sqrt{2K\Delta t}}{\mu} \mathbf{R}_n(t) \quad (19)$$

where Δt is a suitable time increment and $\mathbf{R}_n = R_{x,n} \mathbf{e}_x + R_{y,n} \mathbf{e}_y$ is a horizontal vector whose components are random numbers having zero mean and a variance equal to μ^2 . In other words, the aforementioned random vector satisfies

$$\lim_{N \rightarrow \infty} \left(\frac{1}{N} \sum_{n=1}^N \mathbf{R}_n \right) = \mathbf{0}, \quad (20)$$

$$\lim_{N \rightarrow \infty} \left(\frac{1}{N} \sum_{n=1}^N |\mathbf{R}_n|^2 \right) = \lim_{N \rightarrow \infty} \left(\frac{1}{N} \sum_{n=1}^N (R_{x,n}^2 + R_{y,n}^2) \right) = 2\mu^2. \quad (21)$$

Whatever the number N of particles, the Lagrangian schemes conserves mass. This is trivial. In the limit $N \rightarrow \infty$ (i.e. the number of particles is arbitrarily large), the movement of the centre of mass of the particle cloud and the rate of increase of its position variance should be similar to those of exact solution of the problem. Demonstrating that these properties are satisfied by a Lagrangian scheme is not trivial — even for the simple, Euler forward algorithm suggested above.

Combining (17) and (19) leads to

$$\lim_{N \rightarrow \infty} \tilde{\mathbf{r}}_c(t + \Delta t) = \lim_{N \rightarrow \infty} \tilde{\mathbf{r}}_c(t) - \mathbf{v} \Delta t + \frac{\sqrt{2K\Delta t}}{\mu} \underbrace{\left[\lim_{N \rightarrow \infty} \left(\frac{1}{N} \sum_{n=1}^N \mathbf{R}_n(t) \right) \right]}_{=\mathbf{0}, \text{ see (19)}}, \quad (22)$$

which, using (7), simplifies to

$$\lim_{N \rightarrow \infty} \tilde{\mathbf{r}}_c(t + \Delta t) = \lim_{N \rightarrow \infty} \tilde{\mathbf{r}}_c(t) + \frac{K \Delta t}{L} \mathbf{e}_x \quad (23)$$

At $t = 0$, since the particles are all located at $\mathbf{x} = \mathbf{0}$, the position of the centre of mass of the particle obviously is $\tilde{\mathbf{r}}_c(0) = \mathbf{0}$. Therefore, (23) leads to

$$\lim_{N \rightarrow \infty} \tilde{\mathbf{r}}_c(t) = -\mathbf{v} t = \frac{K t}{L} \mathbf{e}_x \quad (24)$$

which is equivalent to (12), as expected.

After some calculations, the position variance of the particle cloud may be seen to obey

$$\lim_{N \rightarrow \infty} \tilde{\sigma}^2(t + \Delta t) = \lim_{N \rightarrow \infty} \tilde{\sigma}^2(t) + \frac{2K\Delta t}{\mu^2} \underbrace{\left[\lim_{N \rightarrow \infty} \left(\frac{1}{N} \sum_{n=1}^N |\mathbf{R}_n(t)|^2 \right) \right]}_{=2\mu^2, \text{ see (20)}}, \quad (25)$$

which transforms to

$$\lim_{N \rightarrow \infty} \tilde{\sigma}^2(t + \Delta t) = \lim_{N \rightarrow \infty} \tilde{\sigma}^2(t) + 4K\Delta t \quad (26)$$

Since all the particles are located at the same point at the initial instant, the initial value of their position variance is $\tilde{\sigma}^2(0) = 0$, implying

$$\lim_{N \rightarrow \infty} \tilde{\sigma}^2(t) = 4Kt \quad (27)$$

According to the above theoretical developments, in the limit $N \rightarrow \infty$ (number of particles arbitrarily large), the centre of mass of the particle cloud and the associated position variance exhibit a behaviour that is equivalent to that of the exact solution of the transport problem under consideration. In other words, in the limit $N \rightarrow \infty$, the centre of mass of the particle cloud moves toward the deeper part of the domain at speed K/L , whilst the position variance increases linearly in time and is equal to $4Kt$.

Illustration

To illustrate the solution of the present diffusion problem and some of its properties, it is convenient to introduce dimensionless space coordinates and time,

$$(\eta, \xi) = \frac{(x, y)}{L}, \quad \tau = \frac{t}{L^2 / K}, \quad (28)$$

as well as the following scaling of the concentration

$$\gamma(\tau, \eta, \xi) = \frac{4\pi\rho h_0 L^2}{M} C(t, x, y). \quad (29)$$

Then, using the normalised variables, the solution and its properties may be re-written without any dimensionless parameter. In other words, the expressions below contain all of the solution of the problem under study.

Combining (28) and (29), the normalised concentration is readily seen to be

$$\gamma(\tau, \eta, \xi) = \frac{1}{\tau} \exp \left[-\frac{(\eta + \tau)^2 + \xi^2}{4\tau} \right]. \quad (30)$$

This concentration and some of its properties are illustrated in Figures 1 and 2.

The following scaling of the vertical inventory of the tracer under study is worth introducing

$$\vartheta(\tau, \eta, \xi) = \frac{4\pi L^2}{M} J(t, x, y). \quad (31)$$

Then, combining (14), (28) and (31) yields

$$\vartheta(\tau, \eta, \xi) = \frac{1}{\tau} \exp \left[-\frac{(\eta - \tau)^2 + \xi^2}{4\tau} \right]. \quad (32)$$

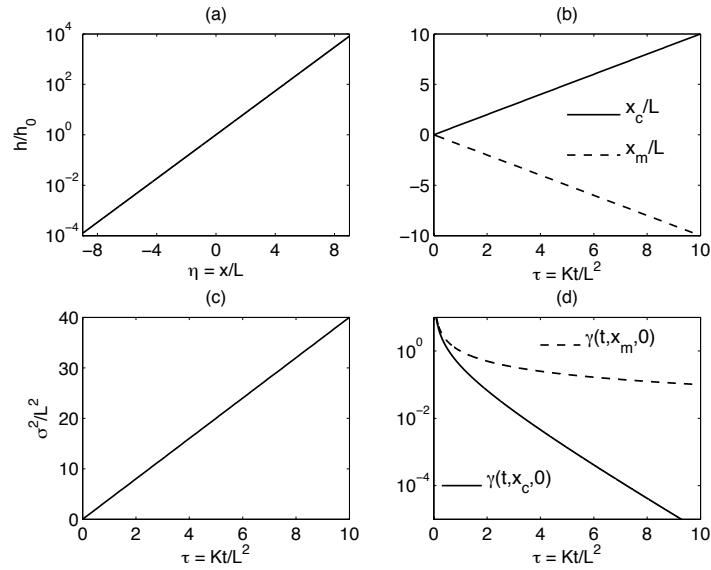


Figure 1. Panel (a) displays the water column depth as a function of the space coordinate η . As may be seen in panel (b), the centre of mass, $x_c(t)$ (solid curve), and the point of maximum concentration, $x_m(t)$ (dashed curve), move in opposite directions at the same speed. The position variance is proportional to the elapsed time (panel (c)). Panel (d) displays the evolution of the maximum of the normalised concentration (dashed curve) and the concentration at the centre of mass (solid curve).

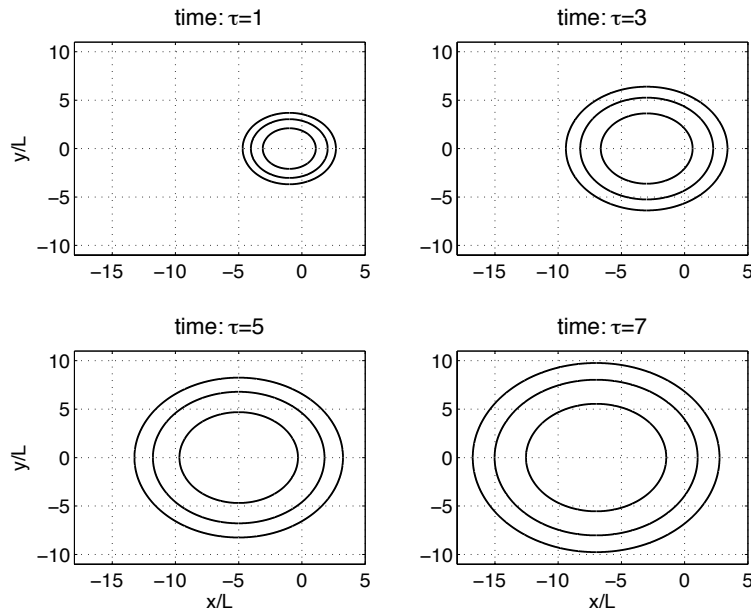


Figure 2. Iso-lines of the concentration at different instants. The values of the concentration related to these iso-lines are $C[t, x_m(t), 0]/3$, $C[t, x_m(t), 0]/10$, and $C[t, x_m(t), 0]/30$. The iso-lines are circles, but appear as ellipses in the graphs above, since their aspect ratio is not equal to unity. These graphs clearly illustrate the motion of the point of maximum concentration toward the shallower part of the domain and the progressive widening of the concentration distribution.

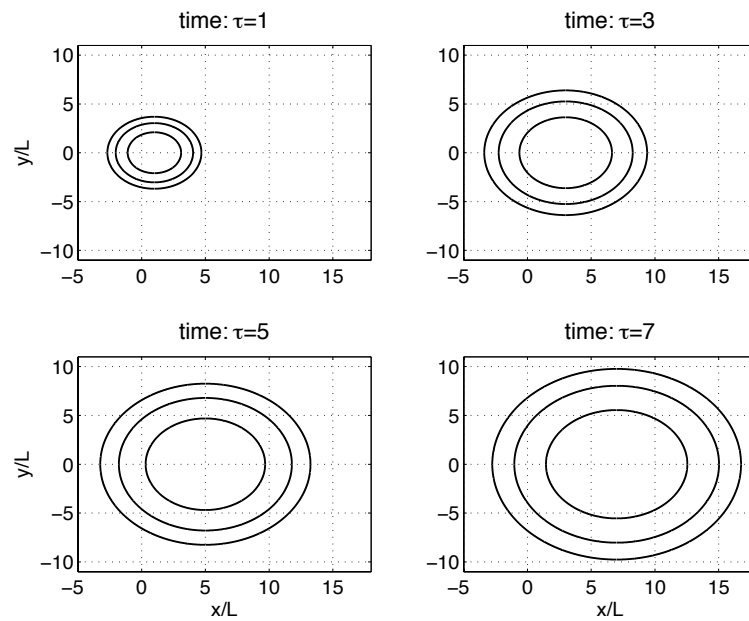


Figure 3. Iso-lines of the vertical inventory at different instants. The values of the vertical inventory related to these iso-lines are $J[t, x_c(t), 0]/3$, $J[t, x_c(t), 0]/10$, and $J[t, x_c(t), 0]/30$. The iso-lines are circles, but appear as ellipses in the graphs above, since their aspect ratio is not equal to unity. These graphs clearly illustrate the motion of the point of maximum vertical inventory toward the deeper part of the domain and the progressive widening of the distribution of the vertical inventory.

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