The Green's function of the advection-diffusion-decay equation in an *n*-dimensional infinite domain

Eric Deleersnijder, January 8, 2008

This note is the first in a series whose objective is to provide the analytical solution of advection-diffusion-decay problems that will be used as part of the validation of SLIM's application to the Scheldt River and Estuary.

Green's function

In $\Re^n$ ($n = 1,2,3...$), consider function $G(t,t',\mathbf{x})$ that is zero if $t < t'$ and is the solution of the partial differential problem

$$\begin{cases} \dfrac{\partial G}{\partial t} + \mathbf{u} \bullet \nabla G = -\lambda G + \nabla \bullet (\mathbf{K} \bullet \nabla G) \\ \left[G(t,t',\mathbf{x}) \right]_{t=t'} = \delta(\mathbf{x} - \mathbf{0}) \end{cases}, \tag{1}$$

for $t' < t$. In the expressions above, δ denotes the Dirac function, λ is a constant, $\mathbf{u}(t)$ is a vector that depends on time t only and $\mathbf{K}$ is a tensor whose components are constants. Furthermore, tensor $\mathbf{K}$ is symmetric and positive definite. Clearly, λ, $\mathbf{u}$ and $\mathbf{K}$ may be regarded as the rate of decay, the velocity vector and the diffusivity tensor, respectively. The function $G(t,t',\mathbf{x})$ may be viewed as the Green's function of an advection-diffusion-problem.

The solution to (1) reads

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

where

$$\tau = t - t', \tag{3}$$

$$\mathbf{s}(t,t') = \int_{t'}^{t} \mathbf{u}(\xi)\, d\xi \tag{4}$$

while $\det(\mathbf{K})$ denotes the determinant of $\mathbf{K}$.

The "mass" of the solution is

$$m(t,t') \equiv \int_{\Re^n} G(t,t',\mathbf{x})\, d\mathbf{x} = e^{-\lambda\tau}. \tag{5}$$

The "centre of mass" is located at

$$\mathbf{r}(t,t') \equiv \frac{1}{m(t,t')} \int_{\Re^n} \mathbf{x}\, G(t,t',\mathbf{x})\, d\mathbf{x} = \mathbf{s}(t,t'). \tag{6}$$

The variance of the solution is

$$\sigma^2(t,t') \equiv \frac{1}{m(t,t')} \int_{\Re^n} \left| \mathbf{x} - \mathbf{r}(t,t') \right|^2 G(t,t',\mathbf{x})\, d\mathbf{x} = 2\,\mathrm{trace}(\mathbf{K})\,\tau. \tag{7}$$

Using the Green's function

In $\Re^n$ ($n = 1,2,3...$), consider function $C(t,\mathbf{x})$ that is the solution of the following partial differential problem:

$$\begin{cases} \dfrac{\partial C}{\partial t} + \mathbf{u} \bullet \nabla C = Q\delta(\mathbf{x} - \mathbf{0}) - \lambda C + \nabla \bullet (\mathbf{K} \bullet \nabla C) \\ \left[C(t,\mathbf{x})\right]_{t=0} = 0 \end{cases}, \tag{8}$$

where $Q(t)$ is the rate of release of a point-source located at $\mathbf{x}=\mathbf{0}$. The solution to this problem may be obtained with the help of the Green's function, $G(t,t',\mathbf{x})$, derived above:

$$C(t,\mathbf{x}) = \int_0^t Q(t')G(t,t',\mathbf{x})\,dt' . \tag{9}$$

One can also tackle a problem in which the source is distributed in space:

$$\begin{cases} \dfrac{\partial C}{\partial t} + \mathbf{u} \bullet \nabla C = q - \lambda C + \nabla \bullet (\mathbf{K} \bullet \nabla C) \\ \left[C(t,\mathbf{x})\right]_{t=0} = 0 \end{cases}, \tag{10}$$

where $q(t,\mathbf{x})$ is the source function. Then, the solution is

$$C(t,\mathbf{x}) = \int_0^t \int_{\Re^n} q(t',\mathbf{x}')G(t,t',\mathbf{x} - \mathbf{x}')\,d\mathbf{x}'\,dt' . \tag{11}$$

Analytical solutions for testing a model of the fate of fecal bacteria in a river

Eric Deleersnijder, January 9, 2008

Governing equations

Consider a river whose cross section is denoted $S(t,x)$, where t is time and x is the along-flow coordinate. Then, the continuity equation reads

$$\frac{\partial S}{\partial t} + \frac{\partial (Su)}{\partial x} = 0 \,, \tag{1}$$

where $u(t,x)$ is the average over the cross section of the velocity component that is normal to the latter. Now assume that vertical and lateral mixing is sufficiently intense that all of the contaminant concentrations are almost homogeneous over every cross section. As a consequence, the contaminant concentrations may be modelled by means of one-dimensional equations. For instance, the concentration $C(t,x)$ of fecal bacteria obeys the following equation

$$\frac{\partial (SC)}{\partial t} + \frac{\partial (SuC)}{\partial x} = \sum_{n=1}^{N} Q_n \, \delta(x - x_n) + q - \lambda SC + \frac{\partial}{\partial x}\left(SK \frac{\partial C}{\partial x} \right) \tag{2}$$

where λ (>0) and K (>0) denote the rate of decay of the bacteria and the relevant diffusion coefficient; δ is the Dirac function; $Q_n(t)$ is the rate of release of the point source located at $x = x_n$, while $q(t,x)$ is the lineic source term. If the concentration $C(t,x)$ is the number of bacteria per cubic metre, then $Q_n(t)$ and $q(t,x)$ are the number of bacteria released per second by the point source and the number of bacteria released per second and per metre by the lineic source, respectively.

Though the concentration $C(t,x)$ must be a continuous, its gradient is discontinuous at the location of a point source. Integrating over an arbitrarily small control volume straddling a point source yields

$$Q_n + \lim_{x \to x_n^+} \left(SK \frac{\partial C}{\partial x} \right) - \lim_{x \to x_n^-} \left(SK \frac{\partial C}{\partial x} \right) = 0 \,. \tag{3}$$

The physical interpretation of this expression is readily arrived at. The control volume being assumed to be arbitrarily small, its bacteria content is negligible and so is the contribution of the lineic source to the bacteria budget. Therefore, at any time, the incoming flux of bacteria must be equal to the outgoing flux. The former flux is

$$\left[SuC - SK \frac{\partial C}{\partial x} \right]_{x = x_n^-} + Q_i \,,$$

while the latter is

$$\left[SuC - SK \frac{\partial C}{\partial x} \right]_{x = x_n^+}$$

Prescribing that these fluxes are equal and taking into account the continuity of the concentration immediately leads to expression (3).

An idealised model

Assume that S and K are positive constants and that u is a function of time, equation (2) simplifies to

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = \sum_{n=1}^{N}\frac{Q_n\,\delta(x-x_n)}{S} + \frac{q}{S} - \lambda C + K\frac{\partial^2 C}{\partial x^2}\ . \tag{4}$$

Further assume that the domain is infinite, i.e. $x \in]-\infty,+\infty[$, and the concentration at t=0 is zero, then the solution to (4) may be written with the help of Green's function $G(t,t',x)$ as follows

$$C(t,x) = \frac{1}{S}\sum_{n=1}^{N}\int_0^t Q_n(t')\,G(t,t',x-x_n)\,dt' + \frac{1}{S}\int_0^t\int_{-\infty}^{+\infty} q(t',x')\,G(t,t',x-x')\,dx'\,dt'\ . \tag{5}$$

The Green's function is zero if $t < t'$ and, for $t < t'$, is the solution of the following partial differential problem:

$$\begin{cases}\dfrac{\partial G}{\partial t} + u\dfrac{\partial G}{\partial x} = -\lambda G + K\dfrac{\partial^2 G}{\partial x^2} \\ \left[G(t,t',x)\right]_{t=t'} = \delta(x-0)\end{cases} \tag{6}$$

This yields

$$G(t,t',x) = \frac{\exp\left[-\lambda\tau - \dfrac{(x-s)^2}{4K\tau}\right]}{\sqrt{4\pi K\tau}}\ , \tag{7}$$

with $\tau = t - t'$ and

$$s(t,t') = \int_{t'}^{t} u(\xi)\,d\xi\ . \tag{8}$$

The number of bacteria $m(t)$ present in the domain of interest is independent of the transport processes and is given by

$$m(t) \equiv S\int_{-\infty}^{+\infty} C(t,x)\,dx = \int_0^t \Pi(t')e^{-\lambda(t-t')}\,dt'\ , \tag{9}$$

where $\Pi(t)$ denotes the number of bacteria that all the sources inject into the domain per second, i.e.

$$\Pi(t) = \sum_{n=1}^{N} Q_n(t) + \int_{-\infty}^{+\infty} q(t,x)\,dx\ . \tag{10}$$

Numerical implementation

The fate of bacteria is to be studied in a river influenced by tides. For testing the numerical model, it is probably sufficient to consider only one tidal component, suggesting that the velocity field be

$$u(t) = U + V\cos(\omega t + \varphi)\ , \tag{11}$$

where the constant φ is the phase angle, while U and V are constants that represent the residual velocity and the amplitude of the tidal velocity, respectively, the angular frequency of the tide being ω. Then, substituting (11) into (8) yields

$$s(t,t') = U(t-t') + \frac{V}{\omega}[\sin(\omega t+\varphi) - \sin(\omega t'+\varphi)] \ . \tag{12}$$

The Green's function above is intended for an infinite domain. Clearly, no such domain can be represented in numerical simulations; a domain having a finite length is needed. However, it is possible to select a length sufficiently large that the impact of the domain ends will remain negligible. In this respect, it is suggested that the computational domain be defined by the inequalities

$$-L < x < L \ , \tag{13}$$

and that periodicity boundary conditions be prescribed, i.e.

$$C(t,-L) = C(t,L) \quad \text{and} \quad \left[K\frac{\partial C}{\partial x}\right]_{x=-L} = \left[K\frac{\partial C}{\partial x}\right]_{x=L} \ . \tag{14}$$

Assuming that the sources of bacteria are all located in the neighbourhood of the point x=0, the length of the domain must be such that the bacteria concentration be very small at the ends of the computational domain. Therefore, the length L must be much larger that all of the length scales characterising transport and decay of the bacteria. These length scales are

$$L_t = |V|/\omega \ , \tag{15}$$

and the distances over which advection and diffusion transport bacteria during a time that is sufficient for decay to have a significant impact. Assuming that this time is λ^{-1}, the relevant advective and diffusive length scales are

$$L_a = |U|/\lambda \tag{16}$$

and

$$L_d = \sqrt{K/\lambda} \ , \tag{17}$$

respectively. Thus, the length of the computational domain must be such that

$$\max(L_t, L_a, L_d) << L \ . \tag{18}$$

Test case 1

Ignore the lineic source (q=0). Assuming that M bacteria are released at t=0 at x=0 and that there is no other injection of bacteria into the domain of interest at a later time, then $x_1 = 0$, N=1 and the single point source strength is

$$Q_1(t) = M\,\delta(t-0) \ . \tag{19}$$

Hence, according to (5) and (7-8), the bacteria concentration is

$$C(t,x) = \frac{M\exp\left[-\lambda t - \dfrac{(x-s)^2}{4Kt}\right]}{S\sqrt{4\pi K t}} \ , \tag{20}$$

with

$$s(t,0) \;=\; Ut \;+\; \frac{V}{\omega}[\sin(\omega t+\varphi)-\sin\varphi] \;. \tag{21}$$

Special cases of this solution may be considered, by setting U=0 or V=0.

The number of bacteria $m(t)$ present in the domain evolves as follows:

$$m(t) \;\equiv\; S\int_{-\infty}^{+\infty} C(t,x)\,dx \;=\; M\,e^{-\lambda t} \;. \tag{22}$$

Test case 2

Ignore the lineic source (q=0) and assume that there is only one point source that releases Θ bacteria per second into the flow at x=0. This implies that $x_1 = 0$, N=1 and $Q_1 = \Theta$, yielding the bacteria concentration

$$C(t,x) \;=\; \frac{\Theta}{S}\int_{0}^{t} G(t,t',x)\,dt' \;. \tag{23}$$

It is readily seen that the number of bacteria present in the domain tends to a constant:

$$m(t) \;\equiv\; S\int_{-\infty}^{+\infty} C(t,x)\,dx \;=\; \frac{\Theta}{\lambda}(1-e^{\lambda t}) \;. \tag{24}$$

A particularly interesting special case is obtained by neglecting the tidal velocity (V=0), yielding the following concentration

$$C(t,x) \;=\; \frac{\Theta}{S}\int_{0}^{t} \frac{e^{-\lambda t'-(x-Ut')^2/(4Kt')}}{\sqrt{4\pi K t'}}\,dt' \;. \tag{25}$$

In the limit $t\to\infty$, the concentration is amenable to a simple expression:

$$C(\infty,x) \;\equiv\; \frac{\Theta}{S}\int_{0}^{\infty} \frac{e^{-\lambda t'-(x-Ut')^2/(4Kt')}}{\sqrt{4\pi K t'}}\,dt' \;=\; \frac{\Theta\, e^{[Ux-\sqrt{4K\lambda+U^2}\,|x|]/(2K)}}{S\sqrt{4K\lambda+U^2}} \;. \tag{26}$$

Test case 3

Assume there is no point source and a lineic source is active only in the interval $-l < x < l$ with a rate of release that is independent of x. Then, the general expression (5) simplifies to

$$C(t,x) \;=\; \frac{1}{S}\int_{0}^{t} q(t')\int_{-l}^{+l} G(t,t',x-x')\,dx'\,dt' \;. \tag{27}$$

Now reduce the length l and increase the rate of release q in such a way that the product ql remains constant. In the limit $l\to 0$, the solution tends to that associated with a point-source located at x=0 that releases $2ql$ bacteria per second.

To assess the implementation of the lineic source term in the numerical model, having recourse to a lineic source distributed over a very short region presumably is a very demanding test. Needless to say, it is not possible in a numerical model to let l tend to zero. But, it is possible to select l in such a way that it is much smaller the length scales L_a, L_d and

L_t (if the latter in non zero). This is almost equivalent to considering the limit $l \to 0$. Then, by prescribing

$$q = \frac{M}{2l}\delta(t-0) \tag{28}$$

and

$$q = \frac{\Theta}{2l}, \tag{29}$$

the concentration must be very close to that of test case 1 and test case 2, respectively. Therefore, there is no need for specific analytical solutions for assessing the implementtion of the lineic source term; those related to point sources lead to an acceptable set of benchmarks — provided the length of the region where the lineic source is active is sufficiently small.

A two-dimensional, depth-integrated model of the fate of fecal bacteria

Eric Deleersnijder, January 10, 2008

Governing equations

Consider a shallow-water domain, e.g. a coastal zone or an estuary, whose depth is denoted $H(t,\mathbf{x})$, where t is the time and $\mathbf{x}=(x,y)$ is the position vector, x and y being horizontal Cartesian coordinates. The continuity equation reads

$$\frac{\partial H}{\partial t} + \nabla\bullet(H\mathbf{u}) = 0 , \tag{1}$$

where $\mathbf{u}(t,\mathbf{x})$ is the depth-averaged horizontal velocity. If vertical mixing is sufficiently efficient, the fate of fecal bacteria may be studied by means of a two-dimensional model. Accordingly, the depth-averaged concentration $C(t,\mathbf{x})$ satisfies the following partial differential equation:

$$\frac{\partial (HC)}{\partial t} + \nabla\bullet(H\mathbf{u}C) = \sum_{n=1}^{N} Q_n\,\delta(\mathbf{x}-\mathbf{x}_n) - \lambda HC + \nabla\bullet(H\mathbf{K}\bullet\nabla C) , \tag{2}$$

where λ (>0) denotes the rate of decay of the bacteria; $\mathbf{K}$ is the diffusivity tensor, which must be symmetric and positive definite, i.e. $\mathbf{y}\bullet\mathbf{K}\bullet\mathbf{y}>0$ for any vector $\mathbf{y}\neq\mathbf{0}$; δ is the Dirac function, with $\delta(\mathbf{x}-\mathbf{x}_n)=\delta(x-x_n)\delta(y-y_n)$; $Q_n(t)$ is the rate of release of the point source located at $\mathbf{x}=\mathbf{x}_n$. If the concentration $C(t,\mathbf{x})$ represents the number of bacteria per cubic metre, then $Q_n(t)$ is the number of bacteria released per second by the n-th point source.

Expression (2) is the bacteria budget equation in conservative form. Its convective counterpart is obtained by combining (1) and (2):

$$\frac{\partial C}{\partial t} + \mathbf{u}\bullet\nabla C = \sum_{n=1}^{N} \frac{Q_n\,\delta(\mathbf{x}-\mathbf{x}_n)}{H} - \lambda C + \frac{1}{H}\nabla\bullet(H\mathbf{K}\bullet\nabla C) . \tag{3}$$

Every segment of the boundary of the domain of interest is either open or impermeable. On the latter type of boundary, i.e. the coastline, which is denoted Γ_i, the velocity satisfies the so-called impermeability condition $\mathbf{u}\bullet\mathbf{n}=0$, where $\mathbf{n}$ denotes the outward unit normal vector to the boundary. There may exist a lineic source of bacteria on the coastline, leading to the boundary condition

$$\left[(H\mathbf{K}\bullet\nabla C)\bullet\mathbf{n}\right]_{\mathbf{x}\in\Gamma_i} = q , \tag{4}$$

where $q(t,\mathbf{x})$ ($\mathbf{x}\in\Gamma_i$) represents the number of bacteria released per second and per metre of coastline by the lineic source. Of course, in the absence of any lineic source, the rate of release q must be zero; in this case, the coastline is an impermeable boundary for the bacteria budget.

An idealised model

Assume that the domain of interest is semi-infinite and is defined by the inequalities

$$-\infty < x < +\infty , \quad 0 < y < +\infty . \tag{5}$$

Further hypothesize that the depth of the water column is constant in time and space, and that the velocity field simply is

$$\mathbf{u}(t,\mathbf{x}) \;=\; u(t)\mathbf{e}_x \;, \tag{6}$$

where $\mathbf{e}_x$ is the unit vector associated with the x-coordinate axis. Finally, as in many shallow-water models, the diffusivity tensor is taken to be diagonal, i.e.

$$\mathbf{K} \;=\; \begin{pmatrix} K_{xx} & 0 \\ 0 & K_{yy} \end{pmatrix}, \tag{7}$$

where $K_{xx}, K_{yy} > 0$. It is convenient to impose that the eddy coefficients K_{xx} and K_{yy} are constants.

Under the assumptions above, governing equation (1) and boundary condition (4) simplify to

$$\frac{\partial C}{\partial t} \;+\; u\frac{\partial C}{\partial x} \;=\; \frac{1}{H}\sum_{n=1}^{N} Q_n\,\delta(x-x_n)\delta(y-y_n) \;-\; \lambda C \;+\; K_{xx}\frac{\partial^2 C}{\partial x^2} \;+\; K_{yy}\frac{\partial^2 C}{\partial y^2} \tag{8}$$

$$\left[\frac{\partial C}{\partial y}\right]_{y=0} \;=\; \frac{q}{HK_{yy}} \;. \tag{9}$$

The solution to (8) may be written with the help of Green's function $G(t,t',x,y)$ as follows

$$\begin{aligned} C(t,x) \;=\; & \frac{1}{H}\sum_{n=1}^{N}\int_0^t Q_n(t')[G(t,t',x-x_n,y-y_n)+G(t,t',x-x_n,y+y_n)]\,dt' \\ & +\; \frac{2}{H}\int_0^t\int_{-\infty}^{+\infty} q(t',x',0)\,G(t,t',x-x',y)\,dx'\,dt' \end{aligned} \;. \tag{10}$$

The Green's function is zero if $t < t'$ and, for $t < t'$, is the solution in an infinite domain $(-\infty < x,y < +\infty)$ of the following partial differential problem:

$$\begin{cases} \dfrac{\partial G}{\partial t} \;+\; u\dfrac{\partial G}{\partial x} \;=\; -\lambda G \;+\; K_{xx}\dfrac{\partial^2 G}{\partial x^2} \;+\; K_{yy}\dfrac{\partial^2 G}{\partial y^2} \\ \left[G(t,t',x,y)\right]_{t=t'} = \delta(x-0)\delta(y-0) \end{cases} \tag{11}$$

This yields

$$G(t,t',x,y) \;=\; \frac{\exp\left[-\lambda\tau - \dfrac{(x-s)^2}{4K_{xx}\tau} - \dfrac{y^2}{4K_{yy}\tau}\right]}{4\pi\sqrt{K_{xx}K_{yy}}\,\tau} \;, \tag{12}$$

with $\tau = t - t'$ and

$$s(t,t') \;=\; \int_{t'}^{t} u(\xi)\,d\xi \;. \tag{13}$$

The number of bacteria $m(t)$ present in the domain of interest is independent of the transport processes and is given by

$$m(t) \;\equiv\; H\int_{-\infty}^{+\infty}\int_{0}^{+\infty} C(t,x,y)\,dy\,dx \;=\; \int_0^t \Pi(t')e^{-\lambda(t-t')}\,dt' \;, \tag{14}$$

where $\Pi(t)$ denotes the number of bacteria that all the sources inject into the domain per second, i.e.

$$\Pi(t) = \sum_{n=1}^{N} Q_n(t) + \int_{-\infty}^{+\infty} q(t,x,0)\,dx \ . \tag{15}$$

Particularly interesting solutions

The fate of bacteria is to be studied in a domain influenced by tides. For testing the numerical model, it is probably sufficient to consider only one tidal component, suggesting that the velocity field be

$$u(t) = U + V\cos(\omega t + \varphi) \ , \tag{16}$$

where the constant φ is the phase angle, while U and V are constants that represent the residual velocity and the amplitude of the tidal velocity, respectively, the angular frequency of the tide being ω. Then, substituting (16) into (13) yields

$$s(t,t') = U(t-t') + \frac{V}{\omega}[\sin(\omega t + \varphi) - \sin(\omega t' + \varphi)] \ . \tag{17}$$

Sudden pointwise release of bacteria. Ignore the lineic source (q=0). Assuming that M bacteria are released at t=0 at $(x,y) = (0,Y)$, with $Y \geq 0$, and that there is no other injection of bacteria into the domain of interest at a later time, then $x_1 = 0$, $y_1 = Y$, N=1 and the single point source strength is

$$Q_1(t) = M\,\delta(t-0) \ . \tag{18}$$

Hence, according to (10) and (12-13), the bacteria concentration is

$$C(t,x,y) = \frac{M\exp\left[-\lambda t - \dfrac{(x-s)^2}{4K_{xx}t}\right]\left\{\exp\left[-\dfrac{(y-Y)^2}{4K_{yy}t}\right] + \exp\left[-\dfrac{(y+Y)^2}{4K_{yy}t}\right]\right\}}{4\pi H\sqrt{K_{xx}K_{yy}}\,t} \ , \tag{19}$$

with

$$s(t,0) = Ut + \frac{V}{\omega}[\sin(\omega t + \varphi) - \sin\varphi] \ . \tag{20}$$

Special cases of this solution may be considered, by setting U=0 or V=0.

The number of bacteria $m(t)$ present in the domain evolves as follows:

$$m(t) = M\,e^{-\lambda t} \ . \tag{21}$$

Continuous pointwise release of bacteria. Ignore the lineic source (q=0) and assume that there is only one point source that releases Θ bacteria per second into the flow at $(x,y) = (0,Y)$, with $Y \geq 0$. This implies that $x_1 = 0$, $y_1 = Y$, N=1 and $Q_1 = \Theta$, yielding the bacteria concentration

$$C(t,x,y) = \frac{\Theta}{H}\int_0^t [G(t,t',x,y-Y) + G(t,t',x,y+Y)]\,dt' \ . \tag{22}$$

It is readily seen that the number of bacteria present in the domain tends to a constant:

$$m(t) = \frac{\Theta}{\lambda}(1-e^{\lambda t}) . \tag{23}$$

A particularly interesting special case is obtained by neglecting the tidal velocity (V=0), yielding the following concentration

$$C(t,x,y) = \frac{\Theta}{H}\int_0^t \frac{e^{-\lambda t'-(x-Ut')^2/(4K_{xx}t')}\,[e^{-(y-Y)^2/(4K_{yy}t')}+e^{-(y+Y)^2/(4K_{yy}t')}]}{4\pi\sqrt{K_{xx}K_{yy}}\,t'}\,dt' . \tag{24}$$

In the limit $t\to\infty$, the concentration is amenable to a relatively simple expression:

$$C(\infty,x,y) = \frac{\Theta\, e^{Ux/(2K_{xx})}\,[K_0(\zeta_-)+K_0(\zeta_+)]}{2\pi H\sqrt{K_{xx}K_{yy}}} . \tag{25}$$

where K_0 is a modified Bessel function of the second kind and

$$\zeta_\pm = \sqrt{\frac{4\lambda K_{xx}+U^2}{4K_{xx}^2K_{yy}}[K_{yy}x^2+K_{xx}(y\pm Y)^2]} . \tag{26}$$

In a one-dimensional representation, the concentration is finite at the location of a point source. In a multi-dimensional problem, however, the concentration is singular. Indeed, expression (25) admits the following asymptotic expansion in the vicinity of the point source:

$$C(\infty,x,y) \sim \frac{-\Theta\log\zeta_-}{2\pi H\sqrt{K_{xx}K_{yy}}} , \quad \zeta_-\to 0 . \tag{27}$$

Lineic source of bacteria. Assume there is no point source and a lineic source is active only in the interval $-l<x<l$ with a rate of release that is independent of x. Then, the general expression (10) simplifies to

$$C(t,x) = \frac{2}{H}\int_0^t q(t')\int_{-l}^{+l} G(t,t',x-x',y)\,dx'\,dt' . \tag{28}$$

Now reduce the length l and increase the rate of release q in such a way that the product ql remains constant. In the limit $l\to 0$, the solution tends to that associated with a point-source located at $(x,y)=(0,0)$ that releases $2ql$ bacteria per second. Then, by prescribing

$$q = \frac{M}{2l}\delta(t-0) \tag{29}$$

and

$$q = \frac{\Theta}{2l} , \tag{30}$$

the concentration must be very close to that derived for the sudden and continuous pointwise releases of bacteria.

An idealised model of the fate of fecal bacteria in a two-dimensional channel flow

Eric Deleersnijder, January 15, 2008

An idealised channel model

Consider an infinitely-long channel in which vertical mixing is sufficiently strong for a depth-integrated model to be relevant. Let x and y be the along-channel and cross-channel Cartesian coordinates, respectively. Then, the domain of interest is defined by the inequalities

$$-\infty < x < +\infty \ , \quad 0 < y < W \ , \tag{1}$$

where the constant W denotes the width of the channel. The depth H of the water column is assumed to be constant. The velocity in the channel is taken to be of the form

$$\mathbf{u} \ = \ u(t)\mathbf{e}_x \ . \tag{2}$$

The depth-averaged concentration of fecal bacteria $C(t,\mathbf{x})$ satisfies the following partial differential equation:

$$\frac{\partial C}{\partial t} \ + \ u\frac{\partial C}{\partial x} \ = \ \frac{1}{H}\sum_{n=1}^{N} Q_n \, \delta(x-x_n)\delta(y-y_n) \ - \ \lambda C \ + \ K_{xx}\frac{\partial^2 C}{\partial x^2} \ + \ K_{yy}\frac{\partial^2 C}{\partial y^2} \ , \tag{3}$$

where λ (>0) denotes the rate of decay of the bacteria; the constants K_{xx} (>0) and K_{yy} (>0) are the relevant eddy diffusivities; δ is the Dirac function; $Q_n(t)$ is the rate of release of the point source located at $(x,y)=(x_n,y_n)$. If the concentration $C(t,\mathbf{x})$ represents the number of bacteria per cubic metre, then $Q_n(t)$ is the number of bacteria released per second by the n-th point source. On the boundaries of the channel, there may exist lineic sources:

$$\left[HK_{yy}\frac{\partial C}{\partial y}\right]_{y=0} = q(t,x,0) \ , \quad \left[HK_{yy}\frac{\partial C}{\partial y}\right]_{y=W} = -q(t,x,W) \ , \tag{4}$$

where $q(t,x,0)$ and $q(t,x,W)$ represents the number of bacteria released per second and per metre of coastline by the lineic sources. Of course, in the absence of any lineic source, the rate of release q must be zero; in this case, the coastline is an impermeable boundary for the bacteria budget equation.

For obtaining the solution of (3) under the boundary conditions (4), it is convenient to somewhat modify the formulation of the problem by assuming that the boundaries of the channel are now impermeable, implying that the lineic source terms must be introduced into equation (3)[1]. Accordingly, the latter transforms to

$$\begin{aligned} \frac{\partial C}{\partial t} \ + \ u\frac{\partial C}{\partial x} \ &= \ \frac{1}{H}\sum_{n=1}^{N} Q_n \, \delta(x-x_n)\delta(y-y_n) \\ &+ \ \frac{1}{H}\left[q(t,x,0)\delta(y-0^+) + q(t,x,W)\delta(y-W^-)\right] \ - \ \lambda C \ + \ K_{xx}\frac{\partial^2 C}{\partial x^2} \ + \ K_{yy}\frac{\partial^2 C}{\partial y^2} \end{aligned} \tag{5}$$

The boundary conditions to be enforced now read

[1] It is common knowledge that using a flux boundary condition is equivalent to putting an equivalent source at an arbitrarily-small distance to the boundary while imposing that the flux through the boundary is zero. Nonetheless, a good reference thereon is badly needed...

$$\left[HK_{yy}\frac{\partial C}{\partial y}\right]_{y=0^-} = 0 \ , \ \left[HK_{yy}\frac{\partial C}{\partial y}\right]_{y=W^+} = 0 \ . \tag{6}$$

A generic solution

Let $\psi_k(y)$ represent the k-th solution to the following Sturm-Liouville problem:

$$\begin{cases} K_{yy}\dfrac{d^2\psi_k}{dy^2} + \mu_k\psi_k = 0 \\ \left[\dfrac{d\psi_k}{dy}\right]_{y=0,W} = 0 \end{cases} \tag{7}$$

The eigenfuctions of the above operator are orthogonal. They may be normalised as follows:

$$\frac{1}{W}\int_0^W \psi_k(y)\psi_{k'}(y)\,dy = \begin{cases} 1 \ , & \text{if } k = k' \\ 0 \ , & \text{if } k \neq k' \end{cases} . \tag{8}$$

Then, it is readily seen that the functions $\psi_k(y)$ and the eigenvalues μ_k are

$$\begin{cases} \psi_0(y) = 1 \ , \ \mu_0 = 0 \\ \psi_k(y) = \sqrt{2}\cos(k\pi y/W) \ , \ \mu_k = k^2\pi^2 K_{yy}/W^2 \ , \ k = 1,2,3... \end{cases} \tag{9}$$

Using the eigenfunctions defined above, the fecal bacteria concentration may be written as follows

$$C(t,x,y) = \sum_{k=0}^{\infty} a_k(t,x)\psi_k(y) \ , \tag{10}$$

where the functions $a_k(t,x)$ satisfy the one-dimensional partial differential equations

$$\frac{\partial a_k}{\partial t} + u\frac{\partial a_k}{\partial x} = \frac{1}{HW}\sum_{n=1}^{N} Q_{n,k}\,\delta(x-x_n) + \frac{q_k}{HW} - \gamma_k a_k + K_{xx}\frac{\partial^2 a_k}{\partial x^2} \ , \tag{11}$$

with

$$Q_{n,k}(t) = \begin{cases} Q_n(t) \ , \ k = 0 \\ \sqrt{2}\,Q_n(t)\cos(k\pi y_n/W) \ , \ k = 1,2,3... \end{cases} , \tag{12}$$

$$q_k(t) = \begin{cases} q(t,x,0) + q(t,x,W) \ , \ k = 0 \\ \sqrt{2}\,[q(t,x,0) + (-1)^k q(t,x,W)] \ , \ k = 1,2,3... \end{cases} , \tag{13}$$

$$\gamma_k = \lambda + \mu_k \ . \tag{14}$$

The equation (11) is similar to that one had to tackle in the one-dimensional river model presented in a previous working note (Note2.pdf). Therefore, all of the results established therein will be of use to solve the present problem. Then, assuming that the concentration is zero at the initial instant, i.e. $C(0,x,y) = 0$, the functions $a_k(t,x)$ are readily seen to be

$$a_k(t,x) = \frac{1}{HW}\sum_{n=1}^{N}\int_0^t Q_{n,k}(t')G_k(t,t',x-x_n)\,dt' + \frac{1}{HW}\int_0^t\int_{-\infty}^{+\infty} q_k(t',x')G_k(t,t',x-x')\,dx'\,dt' \tag{15}$$

where the Green's function $G_k(t,t',x)$ is zero if $t < t'$ and, for $t' < t$, is

$$G_k(t,t',x) = \frac{\exp\left[-\gamma_k\tau - \dfrac{(x-s)^2}{4K_{xx}\tau}\right]}{\sqrt{4\pi K_{xx}\tau}}\ , \tag{16}$$

with $\tau = t - t'$ and

$$s(t,t') = \int_{t'}^{t} u(\xi)\,d\xi\ . \tag{17}$$

The number of bacteria $m(t)$ present in the domain of interest is independent of the transport processes and is given by

$$m(t) \equiv H\int_{-\infty}^{+\infty}\int_0^W C(t,x,y)\,dy\,dx = \int_0^t \Pi(t')e^{-\lambda(t-t')}\,dt'\ , \tag{18}$$

where $\Pi(t)$ denotes the number of bacteria that all the sources inject into the domain per second, i.e.

$$\Pi(t) = \sum_{n=1}^{N} Q_n(t) + \int_{-\infty}^{+\infty}[q(t,x,0) + q(t,x,W)]\,dx\ . \tag{19}$$

Numerical implementation

The fate of bacteria is to be studied in a domain influenced by tides. For testing the numerical model, it is probably sufficient to consider only one tidal component, suggesting that the velocity field be

$$u(t) = U + V\cos(\omega t + \varphi)\ , \tag{20}$$

where the constant φ is the phase angle, while U and V are constants that represent the residual velocity and the amplitude of the tidal velocity, respectively, the angular frequency of the tide being ω. Then, substituting (20) into (17) yields

$$s(t,t') = U(t-t') + \frac{V}{\omega}[\sin(\omega t + \varphi) - \sin(\omega t' + \varphi)]\ . \tag{21}$$

The Green's function above is intended for an infinite domain. Clearly, no such domain can be represented in numerical simulations; a domain having a finite length is needed. However, it is possible to select a length sufficiently large that the impact of the domain ends will remain negligible. In this respect, it is suggested that the computational domain be defined by the inequalities

$$-L < x < L\ , \tag{22}$$

and that periodicity boundary conditions be prescribed, i.e.

$$C(t,-L) = C(t,L) \quad \text{and} \quad \left[K\frac{\partial C}{\partial x}\right]_{x=-L} = \left[K\frac{\partial C}{\partial x}\right]_{x=L} . \tag{23}$$

Assuming that the sources of bacteria are all located in the neighbourhood of the point x=0, the length of the domain must be such that the bacteria concentration be very small at the ends of the computational domain. Therefore, the length L must be much larger that all of the length scales characterising transport and decay of the bacteria. These length scales are

$$L_t = |V|/\omega , \tag{24}$$

and the distances over which advection and diffusion transport bacteria during a time that is sufficient for decay to have a significant impact. Assuming that this time is

$$\max_k \gamma_k^{-1} = \gamma_0^{-1} = \lambda^{-1} , \tag{25}$$

the relevant advective and diffusive length scales are

$$L_a = |U|/\lambda \tag{26}$$

and

$$L_d = \sqrt{K/\lambda} , \tag{27}$$

respectively. Thus, the length of the computational domain must be such that

$$\max(L_t, L_a, L_d) << L . \tag{28}$$

Test case 1

Ignore the lineic source (q=0). Assuming that M bacteria are released at t=0 at $(x,y) = (0,Y)$, with 0<Y<W, and that there is no other injection of bacteria into the domain of interest at a later time, then $x_1 = 0$, $y_1 = Y$, N=1 and the single point source intensity is

$$Q_1(t) = M\,\delta(t-0) . \tag{29}$$

Hence, according to (15-16) and (21), the bacteria concentration is

$$C(t,x,y) = \frac{M\,e^{-\lambda t-(x-s)^2/(4K_{xx}t)}}{HW\sqrt{4\pi K_{xx}t}}\left[1 + 2\sum_{k=1}^{\infty}\cos(k\pi Y/W)\,e^{-\mu_k t}\cos(k\pi y/W)\right], \tag{30}$$

with

$$s(t,0) = Ut + \frac{V}{\omega}[\sin(\omega t+\varphi) - \sin\varphi] . \tag{31}$$

Special cases of this solution may be considered, by setting U=0 or V=0.

The number of bacteria $m(t)$ present in the domain evolves as follows:

$$m(t) \equiv H\int_{-\infty}^{+\infty}\int_{0}^{W} C(t,x,y)\,dy\,dx = M\,e^{-\lambda t} . \tag{32}$$

Test case 2

Ignore the lineic source (q=0) and assume that there is only one point source that releases Θ bacteria per second into the flow at $(x,y)=(0,Y)$, with $0<Y<W$. This implies that $x_1=0$, $y_1=Y$, N=1 and $Q_1=\Theta$, yielding the bacteria concentration

$$C(t,x,y) \;=\; \frac{\Theta}{HW}\int_0^t \left[G_0(t,t',x) + 2\sum_{k=1}^{\infty} \cos(k\pi Y/W)\, G_k(t,t',x) \cos(k\pi y/W) \right] dt' \;. \qquad (33)$$

It is readily seen that the number of bacteria present in the domain tends to a constant:

$$m(t) \;\equiv\; H\int_{-\infty}^{+\infty}\int_0^W C(t,x,y)\, dy\, dx \;=\; \frac{\Theta}{\lambda}(1-e^{\lambda t}) \;. \qquad (34)$$

A particularly interesting special case is obtained by neglecting the tidal velocity (V=0), yielding the following concentration

$$C(t,x,y) \;=\; \frac{\Theta}{HW}\int_0^t \frac{e^{-\lambda t'-(x-Ut')^2/(4K_{xx}t')}}{\sqrt{4\pi K_{xx}t'}} \left[1 + 2\sum_{k=1}^{\infty} \cos(k\pi Y/W)\, e^{-\mu_k t'} \cos(k\pi y/W) \right] dt' \;. \qquad (35)$$

In the limit $t\to\infty$, the concentration is amenable to the following series:

$$\begin{aligned} C(\infty,x,y) \;&\equiv\; \frac{\Theta}{HW}\int_0^{\infty} \frac{e^{-\lambda t'-(x-Ut')^2/(4K_{xx}t')}}{\sqrt{4\pi K_{xx}t'}} \left[1 + 2\sum_{k=1}^{\infty} \cos(k\pi Y/W)\, e^{-\mu_k t'} \cos(k\pi y/W) \right] dt' \\ &=\; \frac{\Theta\, e^{[Ux-\sqrt{4K_{xx}\lambda+U^2}\,|x|]/(2K_{xx})}}{HW\sqrt{4K_{xx}\lambda+U^2}} \;+\; \frac{2\Theta}{HW}\sum_{k=1}^{\infty} \cos(k\pi Y/W)\, \frac{e^{[Ux-\sqrt{4K_{xx}\gamma_k+U^2}\,|x|]/(2K_{xx})}}{\sqrt{4K_{xx}\gamma_k+U^2}} \cos(k\pi y/W) \end{aligned} \qquad (36)$$

Test case 3

Assume there is no point source and a lineic source is active only in the interval $-l<x<l$ on one side of the channel, at y=0 say, with a rate of release q that is independent of x. Then, the general expression (15) leads to

$$\begin{aligned} C(t,x,y) \;&=\; \frac{1}{HW}\int_0^t q(t')\int_{-l}^{+l} G_0(t,t',x-x')\, dx'\, dt' \\ &\quad+\; \frac{2}{HW}\int_0^t q(t')\int_{-l}^{+l}\sum_{k=1}^{\infty} G_k(t,t',x-x')\cos(k\pi y/W)\, dx'\, dt' \end{aligned} \qquad (37)$$

Now reduce the length l and increase the rate of release q in such a way that the product ql remains constant. In the limit $l\to 0$, the solution tends to that associated with a point-source located at $(x,y)=(0,0)$ that releases $2ql$ bacteria per second.

To assess the implementation of the lineic source term in the numerical model, having recourse to a lineic source distributed over a very short region presumably is a very demanding test. Needless to say, it is not possible in a numerical model to let l tend to zero. But, it is possible to select l in such a way that it is much smaller the length scales L_a, L_d and L_t (if the latter in non zero). This is almost equivalent to considering the limit $l\to 0$. Then, by prescribing

$$q = \frac{M}{2l}\delta(t-0) \tag{38}$$

and

$$q = \frac{\Theta}{2l}\,, \tag{39}$$

the concentration must be very close to that of test case 1 and test case 2, respectively. Therefore, there is no need for specific analytical solutions for assessing the implementtion of the lineic source term; those related to point sources lead to an acceptable set of benchmarks — provided the length of the region where the lineic source is active is sufficiently small.

Properties of one-dimensional tracer transport in a river

Eric Deleersnijder, February 8 & February 20, 2011

Consider a infinitely-long river whose cross-sectional area is denoted $A(t,x)$, where t and x are the time and the along-river coordinate $(-\infty < x < \infty)$. The one-dimensional continuity equation reads

$$\frac{\partial A}{\partial x} + \frac{\partial (Au)}{\partial x} = 0 \,, \tag{1}$$

where $u(t,x)$ is the section-averaged longitudinal velocity. The section-averaged concentration $C(t,x)$ of a tracer undergoing a first-order reaction obeys the following equation

$$\frac{\partial (AC)}{\partial t} + \frac{\partial (AuC)}{\partial x} = -\lambda AC + \frac{\partial}{\partial x}\left(AK \frac{\partial C}{\partial x} \right) , \tag{2}$$

where $K(t,x)$ is the longitudinal diffusivity, which is positive (>0); the positive constant λ (>0) denotes the rate of decay[1] of the tracer[2] under study. At t=0, a patch of tracer is present in the river; the corresponding concentration, which is denoted

$$C(0,x) = C_0(x) \,, \tag{3}$$

obeys

$$\forall \alpha \geq 0, \ \forall \beta > 0 : \ \lim_{x \to \pm\infty} |x|^{\alpha} [C_0(x)]^{\beta} = 0 \,. \tag{4}$$

Therefore, a similar relation holds true at any time, i.e.

$$\forall \alpha \geq 0, \ \forall \beta > 0 : \ \lim_{x \to \pm\infty} |x|^{\alpha} [C(t,x)]^{\beta} = 0 \,. \tag{5}$$

The objective of the present note is to establish properties of the tracer concentration field $C(t,x)$ that is the solution of the partial differential equation (2) under the constraints (1) and (3)-(5). This may be of use to assess and understand numerical results, such as those obtained by means of SLIM in the Scheldt tidal river network.

Mass budget

The amount of tracer present in the river at time t is

$$m(t) = \int_{-\infty}^{\infty} A(t,x) C(t,x) \, dx \,. \tag{6}$$

Then, integrating (2) over the domain of interest yields

[1] If λ is zero, then the tracer is passive.

[2] Equation (2) is generally unsuitable for representing the fate of fecal bacteria. In an idealised approach, it is common practice to assume that the settling velocity and the mortality rate are constant. However, assuming that the water depth is constant is an assumption that, herein, is unacceptable in general. Hence, the settling term cannot be represented by means of a constant decay rate; the latter must be a function of time and location.

$$\frac{dm}{dt} \;=\; -\lambda m \;+\; \underbrace{\left[-AuC + AK\frac{\partial C}{\partial c}\right]_{x=-\infty}^{x=\infty}}_{=0,\ \text{by virtue of (5)}} \;=\; -\lambda m \;, \tag{7}$$

implying that the amount of tracer contained in the river decreases exponentially in time, i.e.

$$\boxed{m(t) \;=\; m_0\, e^{-\lambda t}} \tag{8}$$

with $m_0 = m(0)$.

The decay rate being constant, it is convenient to introduce the modified concentration

$$\tilde{C}(t,x) \;=\; e^{\lambda t}\, C(t,x) \;, \tag{9}$$

which satisfies the following equation

$$\frac{\partial(A\tilde{C})}{\partial t} \;+\; \frac{\partial(Au\tilde{C})}{\partial x} \;=\; \frac{\partial}{\partial x}\left(AK\frac{\partial \tilde{C}}{\partial x}\right) \;, \tag{10}$$

and the initial distribution $\tilde{C}(0,x) = C_0(x)$. Therefore, $\tilde{C}(t,x)$ is the concentration of a passive tracer. The amount of the latter contained in the domain is equal to m_0 at any time.

Centre of mass

The location $X_c(t)$ of the centre of mass of the tracer distribution is defined by

$$\int_{-\infty}^{\infty} (x - X_c)\, AC\, dx \;=\; 0 \;, \tag{11}$$

hence

$$\boxed{X_c(t) \;=\; \frac{1}{m_0}\int_{-\infty}^{\infty} x\, A(t,x)\tilde{C}(t,x)\, dx} \tag{12}$$

Therefore, the location of the centre of mass is independent of the decay phenomena.

Combining (10) and (12), one obtains after some calculations

$$\begin{aligned}\frac{dX_c}{dt} \;&=\; -\frac{1}{m_0}\underbrace{\left[(xAu + AK)\tilde{C} - xAK\frac{\partial \tilde{C}}{\partial x}\right]_{x=-\infty}^{x=\infty}}_{=0,\ \text{by virtue of (5)}} \;+\; \frac{1}{m_0}\int_{-\infty}^{\infty}\left[Au + \frac{\partial(AK)}{\partial x}\right]\tilde{C}\, dx \\ &=\; \frac{1}{m_0}\int_{-\infty}^{\infty}\left[Au + \frac{\partial(AK)}{\partial x}\right]\tilde{C}\, dx\end{aligned} \tag{13}$$

Therefore, if the velocity u and the product AK are independent of x, the evolution of the location of the centre of mass depends only on the velocity:

$$\frac{dX_c}{dt} \;=\; u \;, \tag{14}$$

implying that

$$X_c(t) \;=\; X_c(0) \;+\; \int_0^t u(t')\, dt' \;. \tag{15}$$

Variance of the distribution

To measure the spreading of the patch of tracer, the variance of the concentration distribution may be resorted to. The latter is defined to be

$$\mu \;=\; \frac{1}{m}\int_{-\infty}^{\infty}(x-X_c)^2\,AC\,dx\;. \tag{16}$$

Then, using (8) and (9), it is readily seen that (16) may be simplified to

$$\boxed{\mu(t) \;=\; \frac{1}{m_0}\int_{-\infty}^{\infty}[x-X_c(t)]^2\,A(t,x)\tilde{C}(t,x)\,dx} \tag{17}$$

As expected, decay has no impact of the variance of the concentration distribution.

Combining (10) and (17) yields after some calculations

$$\begin{aligned}\frac{d\mu}{dt} \;=\; -\frac{1}{m_0}\underbrace{\left[[(x-X_c)^2\,Au+2(x-X_c)AK]\tilde{C}-(x-X_c)^2\,AK\frac{\partial\tilde{C}}{\partial x}\right]_{x=-\infty}^{x=\infty}}_{=0,\text{ by virtue of (5)}}\\ +\;\frac{2}{m_0}\int_{-\infty}^{\infty}(x-X_c)\left[Au+\frac{\partial(AK)}{\partial x}\right]\tilde{C}\,dx\;+\;\frac{2}{m_0}\int_{-\infty}^{\infty}AK\,\tilde{C}\,dx \qquad (18)\\ =\;\frac{2}{m_0}\int_{-\infty}^{\infty}(x-X_c)\left[Au+\frac{\partial(AK)}{\partial x}\right]\tilde{C}\,dx\;+\;\frac{2}{m_0}\int_{-\infty}^{\infty}AK\,\tilde{C}\,dx\end{aligned}$$

If the velocity u and the product AK are independent of x, the first integral in the right-hand side of (18) vanishes, implying that the variance grows monotonically as time progresses. Further assuming that K is independent of the space coordinate, (18) reduces to

$$\frac{d\mu}{dt} \;=\; 2K\;, \tag{19}$$

so that

$$\mu(t) \;=\; \mu(0)\;+\;2\int_0^t K(t')\,dt'\;. \tag{20}$$

In this case, the growth of the variance only depends on the diffusivity. Needless to say, if the diffusivity is constant, the diffusivity obeys the well-known formula $\mu(t)=\mu(0)+2Kt$.

The simplifying assumptions resorted to for establishing (20) are rather stringent. As a consequence, in most cases, the variance does not grow monotonically.

Maximum of the concentration

Let $C_{max}(t)$ denote the maximum of the tracer concentration, i.e.

$$C_{max}(t) \;=\; \max_x C(t,x)\;. \tag{21}$$

The maximum concentration is located at coordinate $X_{max}(t)$, where the following relations obviously hold true

$$C[t, X_{max}(t)] \;=\; C_{max}(t)\;, \tag{22a}$$

$$\left[\frac{\partial C}{\partial x}\right]_{x=X_{max}} \;=\; 0 \tag{22b}$$

and

$$\left[\frac{\partial^2 C}{\partial x^2}\right]_{x=X_{max}} \;\leq\; 0\;. \tag{22c}$$

Combining (1) and (2), the convective form of the tracer budget equation is obtained:

$$\frac{\partial C}{\partial t} \;+\; \left[u - \frac{1}{A}\frac{\partial (AK)}{\partial x}\right]\frac{\partial C}{\partial x} \;=\; -\lambda C \;+\; K\frac{\partial^2 C}{\partial x^2}\;. \tag{23}$$

At $x = X_{max}$, this equation may be transformed to

$$\left[\frac{\partial C}{\partial t} \;+\; \frac{dX_{\max}}{dt}\frac{\partial C}{\partial x}\right]_{x=X_{\max}} \;=\; \underbrace{\left[\left(-u + \frac{dX_{\max}}{dt} + \frac{1}{A}\frac{\partial (AK)}{\partial x}\right)\frac{\partial C}{\partial x}\right]_{x=X_{\max}}}_{=0,\ \text{by virtue of (22b)}} \;+\; \underbrace{\left[-\lambda C \;+\; K\frac{\partial^2 C}{\partial x^2}\right]_{x=X_{\max}}}_{\leq 0,\ \text{by virtue of (22c)}}\;, \tag{24}$$

yielding

$$\boxed{\left[\frac{\partial C}{\partial t} \;+\; \frac{dX_{\max}}{dt}\frac{\partial C}{\partial x}\right]_{x=X_{\max}} \;\leq\; 0} \tag{25}$$

Therefore, the maximum of the concentration does not increase. Similar developments apply to the associated passive tracer whose concentration is $\tilde{C}(t,x)$. The latter is governed by the convective-form equation

$$\frac{\partial \tilde{C}}{\partial t} \;+\; \left[u - \frac{1}{A}\frac{\partial (AK)}{\partial x}\right]\frac{\partial \tilde{C}}{\partial x} \;=\; K\frac{\partial^2 \tilde{C}}{\partial x^2}\;, \tag{26}$$

so that

$$\left[\frac{\partial \tilde{C}}{\partial t} \;+\; \frac{dX_{\max}}{dt}\frac{\partial \tilde{C}}{\partial x}\right]_{x=X_{\max}} \;\leq\; 0, \tag{27}$$

implying that the maximum of $\tilde{C}(t,x)$ does not increase.

Another measure of spreading

As was seen above, the variance does not always grow monotonically. In addition, in most cases, the variance will not obey an analytical expression. Therefore, the variance is not well suited for assessing a numerical solution. Checking whether or nor the concentration maximum of the discrete solution decays is relevant, but this is a local test that ignores most of the concentration distribution. Therefore, a global measure of spreading well suited for assessing a numerical solution has yet to be suggested. As will be seen, the latter may be the normalised integral over the domain of the square of the concentration, i.e.

$$\xi(t) \;=\; \frac{m_0}{m^2}\int_{-\infty}^{\infty} AC^2\,dx\;. \tag{28}$$

Substituting (8)-(9) into (28) leads to

$$\boxed{\xi(t) \;=\; \frac{1}{m_0}\int_{-\infty}^{\infty} A\tilde{C}^2\,dx} \tag{29}$$

By manipulating (26), one obtains

$$\frac{d\xi}{dt} \;=\; -\frac{2}{m_0}\underbrace{\int_{-\infty}^{\infty} AK\left(\frac{\partial\tilde{C}}{\partial x}\right)^2 dx}_{>0} \;-\; \frac{1}{m_0}\underbrace{\left[Au\tilde{C}^2 - 2\tilde{C}AK\frac{\partial\tilde{C}}{\partial x}\right]_{x=-\infty}^{x=\infty}}_{=0,\ \text{by virtue of (5)}}\;, \tag{30}$$

i.e.

$$\frac{d\xi}{dt} \;=\; -\frac{2}{m_0}\int_{-\infty}^{\infty} AK\left(\frac{\partial\tilde{C}}{\partial x}\right)^2 dx \;<\; 0\;. \tag{31}$$

Therefore, the integral measure of the square of the concentration decreases monotonically as time progresses. It is desirable that a numerical approximation to the solution of the present tracer transport problem satisfy this property.

An analytical solution

To illustrate some of the concepts introduced above, consider an infinite channel whose section is given by

$$A(x) \;=\; A_0\,e^{\gamma x}\;. \tag{32}$$

Without any loss of generality, it may be assumed that $\gamma \geq 0$; if one sets $\gamma = 0$, then the cross-sectional area of the channel is constant. At t=0, an amount m_0 of a tracer is released at location x=0, implying that the initial concentration is

$$C_0(x) \;=\; \frac{m_0}{A_0}\delta(x-0)\;. \tag{33}$$

where δ denotes the Dirac function. Let λ denote the decay rate of the tracer under consideration. Then, the tracer concentration is

$$\boxed{C(t,x) \;=\; \frac{m_0}{A_0\sqrt{4\pi Kt}}\exp\left[-\lambda t - \frac{(x+\gamma Kt)^2}{4Kt}\right]} \tag{34}$$

The amount of tracer present in the channel decreases exponentially:

$$m(t) \;=\; m_0\,e^{-\lambda t}\;. \tag{35}$$

The location of the concentration maximum moves at constant speed in the direction in which the section decreases,

$$X_{max}(t) \;=\; -\gamma Kt\;, \tag{36}$$

while the center of mass of the concentration distribution moves in the opposite direction with the same speed

$$X_c(t) = \gamma K t \ . \tag{37}$$

The variance grows monotonically with a growth rate that, surprisingly, is independent of the section variation of the channel:

$$\mu(t) = 2Kt \ . \tag{38}$$

The measure $\xi(t)$ of the square of the concentration decreases monotonically

$$\xi(t) = \frac{m_0 \, e^{-\gamma^2 Kt/2}}{A_0 \sqrt{8\pi K t}} \ , \tag{39}$$

but the rate of decay crucially depends on the rate at which the cross-sectional area of the channel varies. If the section is constant ($\gamma = 0$), the rate of decay of $\xi(t)$ is slowest.
