On the parameterisation of the settling flux of fecal bacteria in a depth-integated model

Eric Deleersnijder, 24 September and 15 December 2008

The objective of the present working note is to assess, by having recourse to the concept of residence time, the parameterisation of the settling flux of fecal bacteria that is commonly used in depth-averaged models of the fate of such bacteria.

Hydrodynamics

Let $\mathbf{v} = \mathbf{u} + w\mathbf{e}_z$ denote the velocity vector, where $\mathbf{u}$ and w is the horizontal velocity and the vertical velocity component, respectively. The velocity is divergence free:

$$\nabla \bullet \mathbf{u} + \frac{\partial w}{\partial z} = 0 , \tag{1}$$

where z is the vertical coordinate that is increasing upwards.

Let $H(t,\mathbf{x}) = h(\mathbf{x}) + \eta(t,\mathbf{x})$ represent the total water depth, where $h(\mathbf{x})$ and $\eta(t,\mathbf{x})$ are the reference depth and the sea surface elevation, which is positive upwards. The impermeability conditions of the surface and the bottom read

$$\left[\frac{\partial \eta}{\partial t} + \mathbf{u} \bullet \nabla \eta - w\right]_{z=\eta} = 0 \tag{2}$$

and

$$\left[\mathbf{u} \bullet \nabla h + w\right]_{z=-h} = 0 . \tag{3}$$

Integrating (1) over the water column and using (2)-(3) yield

$$\frac{\partial \eta}{\partial t} + \nabla \bullet (H\overline{\mathbf{u}}) = 0 , \tag{4}$$

where $\overline{\mathbf{u}}(t,\mathbf{x})$ is the depth-averaged horizontal velocity, i.e.

$$\overline{\mathbf{u}} = \frac{1}{H}\int_{-h}^{\eta} \mathbf{u}\, dz . \tag{5}$$

Three-dimensional fecal bacteria equation

The concentration $C(t,\mathbf{x},z)$ of fecal bacteria obeys the following advection-diffusion-production-destruction equation:

$$\frac{\partial C}{\partial t} = q - \lambda C - \nabla \bullet (\mathbf{u}C - K\nabla C) - \frac{\partial}{\partial z}\left[(w-\omega)C - \kappa\frac{\partial C}{\partial z}\right] , \tag{6}$$

where q is the source term; λ is the mortality rate; K and κ are the horizontal and vertical diffusivities, respectively; ω (>0) is the settling velocity.

There are no bacteria crossing the sea surface, implying that the following boundary condition must be enforced

$$\left[\omega C + \kappa \frac{\partial C}{\partial z}\right]_{z=\eta} = 0 \ . \tag{7}$$

The sea bed is impermeable to diffusion:

$$\left[\kappa \frac{\partial C}{\partial z}\right]_{z=-h} = 0 \ . \tag{8}$$

Therefore, the flux of bacteria settling on the bottom is

$$\phi = \left[\omega C\right]_{z=-h} \ . \tag{9}$$

Depth-averaged fecal bacteria model

The depth-averaged bacterial concentration is

$$\overline{C} = \frac{1}{H}\int_{-h}^{\eta} C \, dz \ , \tag{10}$$

while the deviation with respect to the mean is

$$\hat{C} = C - \overline{C} \ . \tag{11}$$

Integrating (6) over the water column yields

$$\frac{\partial(H\overline{C})}{\partial t} = H\overline{q} - \lambda H\overline{C} - \phi - \nabla \bullet (H\overline{\mathbf{u}}\overline{C}) - \nabla \bullet \int_{-h}^{\eta} \hat{\mathbf{u}}\hat{C} \, dz + \int_{-h}^{\eta} \nabla \bullet (K \nabla C) \, dz \ , \tag{12}$$

with

$$\overline{q} = \frac{1}{H}\int_{-h}^{\eta} q \, dz \ . \tag{13}$$

The last two terms of this equation usually are parameterized as horizontal diffusion, i.e.

$$-\nabla \bullet \int_{-h}^{\eta} \hat{\mathbf{u}}\hat{C} \, dz + \int_{-h}^{\eta} \nabla \bullet (K \nabla C) \, dz \approx \nabla \bullet (HA\nabla\overline{C}) \ , \tag{14}$$

where A is the appropriate diffusivity. The settling flux at the bottom is unknown, for the bottom concentration cannot be determined in the scope of a two-dimensional model. However, if the water column is sufficiently well-mixed, it seems reasonable to assume that

$$C(t,\mathbf{x},-h) \approx \overline{C}(t,\mathbf{x}) \ , \tag{15}$$

yielding

$$\phi \approx \omega\overline{C} \ . \tag{16}$$

Substituting (14) and (16) into (12) leads to

$$\boxed{\frac{\partial(H\overline{C})}{\partial t} = H\overline{q} - (\lambda H + \omega)\overline{C} - \nabla \bullet (H\overline{\mathbf{u}}\overline{C} - HA\nabla\overline{C})} \tag{17}$$

This equation is in conservative form. Using continuity equation (4), the convective form is readily obtained:

$$\frac{\partial \overline{C}}{\partial t} \;=\; \overline{q} \;-\; (\lambda + \omega / H)\overline{C} \;-\; \overline{\mathbf{u}} \bullet \nabla \overline{C} \;+\; \frac{1}{H} \nabla \bullet (HA \nabla \overline{C}) \;. \tag{18}$$

Assessment

The parameterisation (16) is a potential weakness of the depth-integrated equation (17). Therefore, it is necessary to assess the well-foundedness of this parameterisation. To do so, assume that the variables are horizontally homogeneous and that there is no source of bacteria. Thus, the velocity is zero. We also hypothesize that the rate of decay of the bacteria is negligible. For the sake of simplicity, we set $\eta = 0$. It is convenient to introduce a new vertical coordinate, $\xi = z + h$, with $0 \le \xi \le h$. Finally, the vertical eddy diffusivity is assumed to be time-independent.

Under the abovementioned assumptions, the concentration $C(t,\xi)$ of fecal bacteria is the solution of the following partial differential problem:

$$\frac{\partial C}{\partial t} \;=\; \frac{\partial}{\partial \xi}\left(\omega C + \kappa \frac{\partial C}{\partial \xi} \right) , \tag{19}$$

$$C(0,z) \;=\; C_0(\xi) \;, \tag{20}$$

$$\left[\omega C + \kappa \frac{\partial C}{\partial z} \right]_{\xi = h} = 0 \;,\; \left[\kappa \frac{\partial C}{\partial z} \right]_{\xi = 0} = 0 \;. \tag{21}$$

The following notations will turn out to be convenient:

$$\overline{C}(t) \;=\; \frac{1}{h} \int_0^h C(t,\xi)\, d\xi \;, \tag{22}$$

$$\overline{C}_0 \;=\; \overline{C}(0) \;=\; \frac{1}{h} \int_0^h C(0,\xi)\, d\xi \;, \tag{23}$$

$$C_0^{\min} \;=\; \min_{\xi} C_0(\xi) \;. \tag{24}$$

The depth-integrated counterpart of (19)-(21) is

$$\frac{d\overline{C}'}{dt} \;=\; -\frac{\omega}{h} \overline{C}' \;, \tag{25}$$

$$\overline{C}'(0) \;=\; \overline{C}_0 \;. \tag{26}$$

The solution to (23)-(24) is readily seen to be

$$\overline{C}'(t) \;=\; \overline{C}_0\, e^{-\omega t / h} \;. \tag{27}$$

It is desirable that $\overline{C}(t)$ and $\overline{C}'(t)$ be as close as possible to each other. However, it is uneasy to assess how close these two solutions are, as there is in general no closed-form solution to (19)-(21). Fortunately, an indirect approach is possible.

The mean time τ the fecal bacteria will spend in the water column — until they settle on the sea bed — is

$$\tau \;=\; \frac{1}{\overline{C}_0} \int_0^\infty \overline{C}(t)\, dt \;. \tag{28}$$

For the depth-integrated problem, this time is

$$\tau' = \frac{1}{\overline{C}_0} \int_0^\infty \overline{C}'(t)\, dt \ . \qquad (29)$$

By substituting (27) into (29), the latter timescale is readily obtained:

$$\tau' = \frac{h}{\omega} \ . \qquad (30)$$

To derive the former timescale — without knowing explicitly $\overline{C}(t)$ —, we must have recourse to the theory developed by Deleersnijder et al. (2006). Accordingly, we have

$$\tau = \frac{\int_0^h C_0(\xi)\,\theta(\xi)\, d\xi}{\int_0^h C_0(\xi)\, d\xi} \ , \qquad (31)$$

where θ is the residence time[1]

$$\theta(\xi) = \frac{\xi}{\omega} + \frac{1}{\omega}\int_\xi^h \exp\left[-\omega \int_\xi^{\xi'} [\kappa(\xi'')]^{-1}\, d\xi''\right] d\xi' \ . \qquad (32)$$

Deleersnijder et al. (2006) have demonstrated that

$$\frac{\xi}{\omega} \le \theta(\xi) \le \frac{h}{\omega} \ . \qquad (33)$$

This implies

$$\alpha\tau' \le \tau \le \tau' \ . \qquad (34)$$

with

$$\alpha = \frac{1}{h^2 \overline{C}_0} \int_0^h \xi\, C_0(\xi)\, d\xi \le 1 \ . \qquad (35)$$

Hence, one has

$$\boxed{\tau \le \tau' \le \tau/\alpha} \qquad (36)$$

Thus, having recourse to the depth-integrated model always causes an overestimation of the the time spent by bacteria in the water column. Notice that this result was obtained without knowing the evolution of the concentration profile, which is just another illustration of the power of the residence time theory.

Reference

Deleersnijder E., J.-M. Beckers and E.J.M. Delhez, 2006, The residence time of settling particles in the surface mixed layer, *Environmental Fluid Mechanics*, 6, 25-42

----

[1] The residence time $\theta(\xi)$ is defined to be the mean time that sinking particles released at a distance ξ to the sea bed spend in the water column.

A simple numerical model for assessing the parameterisation of the settling flux of fecal bacteria in a depth-integrated model

Eric Deleersnijder, October 2, 2008

The flux of bacteria leaving the water column and settling on the sea bed is the product of the settling velocity and the bacteria concentration at the bottom of the water column. In a depth-integrated model, the vertical profile of the concentration is unavailable. This is why the settling flux has to be parameterized. The most natural — and, hence, widely used — parameterisation is the product the settling velocity and the depth-averaged concentration. Setting up a simple numerical model that could help in assessing this parameterisation is the objective of the present note.

A one-dimensional model and its depth-integrated counterpart

Let the constant w represent the settling velocity of bacteria. Assuming horizontal homogeneity, the concentration $C(t,z)$ of fecal bacteria is the solution of the following partial differential problem:

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

(2) $$C(0,z) = C_0(z) ,$$

(3) $$\left[wc + \kappa \frac{\partial C}{\partial z}\right]_{z=h} = 0 ,$$

(4) $$\left[\kappa \frac{\partial C}{\partial z}\right]_{z=0} = 0 ,$$

where z is the vertical coordinate, which is zero at the sea bed and is equal to h at the sea surface; $\kappa(z)$ is the eddy diffusivity; $q(t,z)$ is the source of bacteria; λ is the motality rate.

The depth-integrated counterpart to this model is

(5) $$\frac{d\overline{C}'}{dt} = \overline{q} - (\lambda + w/h)\overline{C}' ,$$

$$(6) \qquad \overline{C}'(0) \; = \; \overline{C}_0 \; ,$$

where $\overline{C}'(t)$ is the depth-averaged bacteria concentration and

$$(7) \qquad \overline{q}(t) \; = \; \frac{1}{h}\int_0^h q(t,z)\, dz \; ,$$

$$(8) \qquad \overline{C}_0 \; = \; \frac{1}{h}\int_0^h C_0(z)\, dz \; .$$

Dimensionless variables

It is convenient to introduce dimensionless variables. For the one-dimensional model, we take

$$(9) \qquad \tilde{t} = \frac{t}{h/w} \; , \quad \tilde{z} = \frac{z}{h} \; , \quad \tilde{C} = \frac{C}{\mathcal{C}} \; , \quad \tilde{q} = \frac{q}{Q} \; , \quad \tilde{\lambda} = \frac{\lambda}{w/h} \; , \quad \tilde{\kappa} = \frac{\kappa}{\overline{\kappa}} \; ,$$

with

$$(10) \qquad \overline{\kappa} \; = \; \frac{1}{h}\int_0^h \kappa(z)\, dz \; ,$$

$$(11) \qquad Pe \; = \; \frac{wh}{\overline{\kappa}} \; ,$$

where Pe denotes the Peclet number. The characteristic concentration $\mathcal{C}$ may be taken to be Qh/w, where Q is the typical value of the source term q. If there is no source, then it is probably natural to set $\mathcal{C} = \overline{C}_0$.

From here on, only dimensionless variables will be used. Therefore, in order to simplify the notations, the tildes will be dropped. Accordingly, the one-dimensional partial differential problem to be solved reads

$$(12) \qquad \begin{cases} \dfrac{\partial C}{\partial t} \; = \; q \; - \; \lambda C \; + \; \dfrac{\partial}{\partial z}\left(C + \dfrac{\kappa}{Pe}\dfrac{\partial C}{\partial z} \right) \\[2ex] C(0,z) = C_0(z) \; , \quad \left[C + \dfrac{\kappa}{Pe}\dfrac{\partial C}{\partial z} \right]_{z=1} = 0 \; , \quad \left[\dfrac{\kappa}{Pe}\dfrac{\partial C}{\partial z} \right]_{z=0} = 0 \end{cases}$$

In dimensionless variables, one has

(13) $$\int_0^h \kappa(z)\, dz \;=\; 1$$

and

(14) $$\overline{C}(t) \;=\; \int_0^1 C(t,z)\, dz \;.$$

In dimensionless variables, the depth-integrated problem reads

(15) $$\begin{cases} \dfrac{d\overline{C}'}{dt} \;=\; \overline{q} \;-\; (\lambda+1)\overline{C}' \\ \overline{C}'(0) \;=\; \overline{C}(0) \end{cases}$$

The solution thereof is

(16) $$\overline{C}'(t) \;=\; \overline{C}_0\, e^{-(\lambda+1)t} \;+\; \int_0^t \overline{q}(\zeta) e^{-(\lambda+1)(t-\zeta)}\, d\zeta \;.$$

Numerical implementation

The solution to (15) may be obtained by evaluating — analytically or numerically — the integral appearing in the right-hand side of (16). Alternatively, one may discretize (15). If $\overline{C}'_n = \overline{C}'(n\Delta t)$ and $\overline{q}_n = \overline{q}(n\Delta t)$ with n=0,1,2..., a simple discretisation of the depth-integrated equation (15) is

(17) $$\frac{\overline{C}'_{n+1} - \overline{C}'_n}{\Delta t} \;=\; \overline{q}_n \;-\; (\lambda+1)\overline{C}'_{n+1} \;.$$

This Patankar-like scheme (Patankar 1980) is readily seen to be positive-definite, for (17) may be rewritten as

(18) $$\overline{C}'_{n+1} \;=\; \frac{\overline{C}'_n + \overline{q}_n \Delta t}{1 + (\lambda+1)\Delta t} \;,$$

an expression which is positive for any value of the time increment Δt — provided $\overline{C}'_n$ is positive. The corresponding settling flux is

$$(19) \quad \phi'_n = \overline{C}'_{n+1} .$$

To discretize the one-dimensional problem, it is appropriate to introduce first the following notations

$$(20) \quad \begin{cases} C_k^n = C[n\Delta t,(k-1/2)\Delta z] \ , \quad q_k^n = q[n\Delta t,(k-1/2)\Delta z] \ , \quad \kappa_{k-1/2} = \kappa[(k-1)\Delta z] \\ n = 0,1,2,\ldots \qquad k = 1,2,\ldots K \qquad \Delta z = 1/K \end{cases}$$

Then, using a first-order upwind discretisation of the advective term, the Patankar-like discretisation of the governing equation is

$$(21) \quad \frac{C_k^{n+1} - C_k^n}{\Delta t} = q_k^n - \lambda C_k^{n+1} + \frac{\left(C_{k+1}^n + \frac{\kappa_{k+1/2}}{Pe} \frac{C_{k+1}^{n+1} - C_k^{n+1}}{\Delta z} \right) - \left(C_k^n + \frac{\kappa_{k-1/2}}{Pe} \frac{C_k^{n+1} - C_{k-1}^{n+1}}{\Delta z} \right)}{\Delta z}$$

while that of the boundary conditions conditions is

$$(22) \quad \frac{\kappa_{1/2}}{Pe} \frac{C_1^{n+1} - C_0^{n+1}}{\Delta z} = 0 \ ,$$

$$(23) \quad C_{K+1}^n + \frac{\kappa_{K+1/2}}{Pe} \frac{C_{K+1}^{n+1} - C_K^{n+1}}{\Delta z} = 0 \ .$$

This scheme is inspired by Deleersnijder et al. (1997). Accordingly, I am convinced it is stable and positive definite for any value of the parameters, but the formal demonstration thereof has yet to be performed. In other words, it is believed that the numerical algorithm is very robust.

Discrete expressions (21)-(23) may be combined, yielding the following tridiagonal system of linear algebraic equations

$$(24) \quad \begin{cases} (1 + \lambda \Delta t + \mu_{3/2}) C_1^{n+1} - \mu_{3/2} C_2^{n+1} = C_1^n + q_1^n \Delta t + \frac{\Delta t}{\Delta z} \left(C_2^n - C_1^n \right) \\ -\mu_{k-1/2} C_{k-1}^{n+1} + (\mu_{k-1/2} + 1 + \lambda \Delta t + \mu_{k+1/2}) C_k^{n+1} - \mu_{k+1/2} C_{k+1}^{n+1} = C_k^n + q_k^n \Delta t + \frac{\Delta t}{\Delta z} \left(C_{k+1}^n - C_k^n \right) \ , \quad k = 2,3,\ldots K-1 \\ -\mu_{K-1/2} C_{K-1}^{n+1} + (\mu_{K-1/2} + 1 + \lambda \Delta t) C_K^{n+1} = C_K^n + q_K^n \Delta t - \frac{\Delta t}{\Delta z} C_K^n \end{cases}$$

with

(25) $$\mu_{k\pm 1/2} = \frac{\kappa_{k\pm 1/2}\,\Delta t}{Pe\,\Delta z^2}\ .$$

The first-order upwind treatment of the advective term is highly diffusive (e.g. Roache 1972), unless the Courant number[1] is equal to unity. In the latter case, assuming production, mortality and diffusion to be negligible, the governing equation reduces to an advection equation, whose exact solution, $C(t+\Delta t, z) = C(t, z+\Delta t)$, is provided by the numerical scheme, i.e. $C_k^{n+1} = C_{k+1}^n$. Therefore, we set $\Delta t = \Delta z$, and the system (24) simplifies to

(26) $$\begin{cases} (1+\lambda\Delta t+\mu_{3/2})C_1^{n+1} \; - \; \mu_{3/2}C_2^{n+1} \; = \; q_1^n\Delta t \; + \; C_2^n \\ -\mu_{k-1/2}C_{k-1}^{n+1} \; + \; (\mu_{k-1/2}+1+\lambda\Delta t+\mu_{k+1/2})C_k^{n+1} \; - \; \mu_{k+1/2}C_{k+1}^{n+1} \; = \; q_k^n\Delta t \; + \; C_{k+1}^n \ , \quad k = 2,3,\ldots K-1 \\ -\mu_{K-1/2}C_{K-1}^{n+1} \; + \; (\mu_{K-1/2}+1+\lambda\Delta t)C_K^{n+1} \; = \; q_K^n\Delta t \end{cases}$$

The tridiagonal system (26) may be solved by means of the following algorithm (Dahlquist and Bjorck 1974):

Example 5.4.3

The special case when $p = q = 1$—i.e., when A is **tridiagonal**—arises frequently. If the LU-decomposition exists, then it can be written as

$$\begin{pmatrix} a_1 & c_1 & & & \\ b_2 & a_2 & c_2 & & \\ & \cdot & \cdot & \cdot & \\ & \cdot & \cdot & \cdot & \\ & \cdot & \cdot & \cdot & \\ & & b_{n-1} & a_{n-1} & c_{n-1} \\ & & & b_n & a_n \end{pmatrix} = \begin{pmatrix} 1 & & & & \\ \beta_2 & 1 & & & \\ & \beta_3 & & & \\ & & \cdot & \cdot & \\ & & & \cdot & \cdot \\ & & & \cdot & \cdot \\ & & & \beta_n & 1 \end{pmatrix} \begin{pmatrix} \alpha_1 & c_1 & & & \\ & \alpha_2 & c_2 & & \\ & & \cdot & \cdot & \\ & & \cdot & \cdot & \\ & & \cdot & \cdot & \\ & & & & c_{n-1} \\ & & & & \alpha_n \end{pmatrix}.$$

By equating elements we find that $\alpha_1, \alpha_2, \ldots, \alpha_n$ and $\beta_2, \beta_3, \ldots, \beta_n$ can be determined by

$$\alpha_1 = a_1, \qquad \beta_k = \frac{b_k}{\alpha_{k-1}}, \qquad \alpha_k = a_k - \beta_k c_{k-1}, \qquad k = 2, 3, \ldots, n.$$

Then, the solution to a system $\boldsymbol{Ax} = \boldsymbol{f}$ is found by forward and back substitution:

$$g_1 = f_1, \qquad g_i = f_i - \beta_i g_{i-1}, \quad i = 2, 3, \ldots, n,$$

$$x_n = \frac{g_n}{\alpha_n}, \qquad x_i = \frac{g_i - c_i x_{i+1}}{\alpha_i}, \quad i = n-1, \ldots, 2, 1.$$

With the scheme above, the flux of bacteria settling on the sea bed is

[1] Using dimensional variables, the Courant number is $w\Delta t/\Delta z$. The dimensionless counterpart of the latter is $\Delta t/\Delta z$.

(27) $\phi_n = C_1^n$,

which will have to be compared with its counterpart in the depth-integrated model, i.e. expression (19).

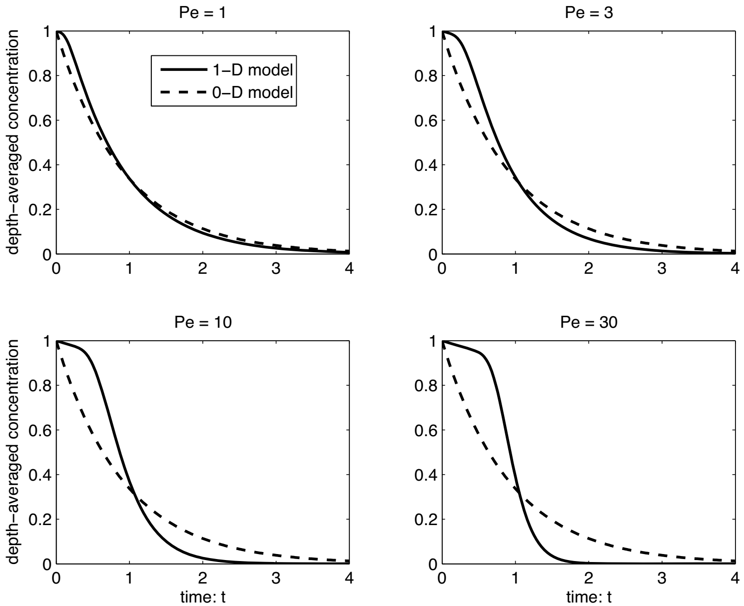
It is instructive to write the mass balance of the discretized equations, i.e. that of the depth-integrated model,

(28) $\overline{C}'_{n+1} = \overline{C}'_n + \underbrace{\overline{q}_n \Delta t}_{source} - \underbrace{\lambda \overline{C}'_{n+1} \Delta t}_{mortality} - \underbrace{\overline{C}'_{n+1} \Delta t}_{settling\ \ flux}$,

as well as that of the one-dimensional model

(29) $\overline{C}_{n+1} = \overline{C}_n + \underbrace{\overline{q}_n \Delta t}_{source} - \underbrace{\lambda \overline{C}_{n+1} \Delta t}_{mortality} - \underbrace{C_1^n \Delta t}_{settling\ \ flux}$.

These expressions look very similar; the only difference lies in the expression of the settling flux. This seemingly minor discrepancy may significantly impact the approximate solutions, especially if the Peclet number is high, i.e. when settling proceeds much faster than vertical mixing. This is illustrated in the figure below, which was obtained for $q = 0$, $\lambda = 0.1$, $\kappa(z) = 6z(1-z)$, $K = 50$ and $C(0,z) = \delta(z-1)$, where δ denotes the Dirac function.



References

Dahlquist G. and A. Bjorck, 1974, *Numerical Methods*, Prentice-Hall, 573 pp.

Deleersnijder E., J.-M. Beckers, J.-M. Campin, M. El Mohajir, T. Fichefet and P. Luyten, 1997, Some mathematical problems associated with the development and use of marine models, in: *The Mathematics of Models for Climatology and Environment*, J.I. Diaz (ed.), NATO ASI Series, Vol. I 48, Springer-Verlag, pp.39-86

Patankar S.V., 1980, *Numerical Heat Transfer and Fluid Flow*, Hemisphere, 197 pp

Roache P.J., 1972, On artificial viscosity, *Journal of Computational Physics*, 10, 169-184

Positivity and stability of a 1D numerical scheme for simulating the fate of fecal bacteria

Eric Deleersnijder, October 5, 2008

In the previous note[1], I discretized a partial differential problem modelling the fate of fecal bacteria in a water column. This led to the following algorithm:

$$(1) \quad \begin{cases} (1+\lambda\Delta t+\mu_{3/2})C_1^{n+1} \; - \; \mu_{3/2}C_2^{n+1} \; = \; q_1^n\Delta t \; + \; C_2^n \\ -\mu_{k-1/2}C_{k-1}^{n+1} \; + \; (\mu_{k-1/2}+1+\lambda\Delta t+\mu_{k+1/2})C_k^{n+1} \; - \; \mu_{k+1/2}C_{k+1}^{n+1} \; = \; q_k^n\Delta t \; + \; C_{k+1}^n \; , \quad k=2,3,...K-1 \\ -\mu_{K-1/2}C_{K-1}^{n+1} \; + \; (\mu_{K-1/2}+1+\lambda\Delta t)C_K^{n+1} \; = \; q_K^n\Delta t \end{cases}$$

The objective of the present note is to demonstrate that this algorithm is unconditionally positive and stable.

Positivity

Let the integer i be defined as follows:

$$(2) \quad C_i^{n+1} \; = \; \min_k C_k^{n+1} \; , \quad k=1,2,...\; K \; .$$

Then, according to whether i=1, $2 \le i \le K-1$ or i=K, (1) may be transformed to

$$(3) \quad \begin{cases} (1+\lambda\Delta t+\mu_{3/2})C_i^{n+1} \; - \; \mu_{3/2}C_2^{n+1} \; = \; q_1^n\Delta t \; + \; C_2^n \; , \quad i=1 \\ -\mu_{i-1/2}C_{i-1}^{n+1} \; + \; (\mu_{i-1/2}+1+\lambda\Delta t+\mu_{i+1/2})C_i^{n+1} \; - \; \mu_{i+1/2}C_{i+1}^{n+1} \; = \; q_i^n\Delta t \; + \; C_{i+1}^n \; , \quad 2 \le i \le K-1 \\ -\mu_{K-1/2}C_{K-1}^{n+1} \; + \; (\mu_{K-1/2}+1+\lambda\Delta t)C_i^{n+1} \; = \; q_K^n\Delta t \; , \quad i=K \end{cases}$$

which leads to

[1] Deleersnijder E., 2008, A simple numerical model for assessing the parameterisation of the settling flux of fecal bacteria in a depth-integrated model, *Note2*, 7 pp.

$$(4)\quad \begin{cases} (1+\lambda\Delta t)C_i^{n+1} \;\geq\; q_1^n\Delta t \;+\; C_2^n \;, \quad i=1 \\ (1+\lambda\Delta t)C_i^{n+1} \;\geq\; q_i^n\Delta t \;+\; C_{i+1}^n \;, \quad 2\leq i\leq K-1 \\ (1+\lambda\Delta t)C_i^{n+1} \;\geq\; q_K^n\Delta t \;, \quad i=K \end{cases}$$

So, if $C_k^n \geq 0$, then

$$(5)\quad \min_k C_k^{n+1} \;\geq\; 0 \;.$$

Therefore, if the concentration at the initial time is positive ($C_k^0 \geq 0$), the concentration will be positive at any later time ($C_k^n \geq 0,\ n>0$). QED.

Stability

Let the integer *j* be defined as follows:

$$(6)\quad C_j^{n+1} \;=\; \max_k C_k^{n+1} \;, \quad k=1,2,\ldots\; K \;.$$

Then, according to whether *j*=1, $2\leq j\leq K-1$ or *j*=*K*, (1) may be transformed to

$$(7)\quad \begin{cases} (1+\lambda\Delta t+\mu_{3/2})C_j^{n+1} \;-\; \mu_{3/2}C_2^{n+1} \;=\; q_1^n\Delta t \;+\; C_2^n \;, \quad j=1 \\ -\mu_{j-1/2}C_{j-1}^{n+1} \;+\; (\mu_{j-1/2}+1+\lambda\Delta t+\mu_{j+1/2})C_j^{n+1} \;-\; \mu_{j+1/2}C_{j+1}^{n+1} \;=\; q_j^n\Delta t \;+\; C_{j+1}^n \;, \quad 2\leq j\leq K-1 \\ -\mu_{K-1/2}C_{K-1}^{n+1} \;+\; (\mu_{K-1/2}+1+\lambda\Delta t)C_j^{n+1} \;=\; q_K^n\Delta t \;, \quad j=K \end{cases}$$

which leads to

$$(8)\quad \begin{cases} (1+\lambda\Delta t)C_j^{n+1} \;\leq\; q_1^n\Delta t \;+\; C_2^n \;, \quad j=1 \\ (1+\lambda\Delta t)C_j^{n+1} \;\leq\; q_j^n\Delta t \;+\; C_{j+1}^n \;, \quad 2\leq j\leq K-1 \\ (1+\lambda\Delta t)C_j^{n+1} \;\leq\; q_K^n\Delta t \;, \quad j=K \end{cases}$$

which implies

$$(9)\quad \max_k C_k^{n+1} \;\leq\; \frac{\max_k q_k^n\,\Delta t \;+\; \max_k C_k^n}{1+\lambda\Delta t}$$

Thus, as was seen in the previous section, the concentration of bacteria will remain positive and, if there is no source of bacteria, the concentration will not increase. We can regard this property as equivalent to stability. QED.

Fecal bacteria concentration in a steady-state, water column model

Eric Deleersnijder, October 27, 2008

The one-dimensional model for the fecal bacteria concentration developed in previous working notes is considered herein under the assumption that all variables are time-independent. Therefore, the dimensionless fecal bacteria concentration $C(z)$ is the solution of the following dimensionless ordinary differential problem

$$\begin{cases} \dfrac{d}{dz}\left(\kappa \dfrac{dC}{dz} + C\right) - \lambda C + q = 0 , \quad 0 < z < 1 \\ \left[\kappa \dfrac{dC}{dz}\right]_{z=0} = 0 , \quad \left[\kappa \dfrac{dC}{dz} + C\right]_{z=1} = 0 \end{cases} \tag{1}$$

The depth-averaged concentration is

$$\overline{C} = \int_0^1 C(z)\, dz . \tag{2}$$

It must be borne in mind that that the — dimensionless — depth-averaged diffusivity must be equal to unity, i.e.

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

The depth-integrated counterpart to this model is

$$-\overline{C}' - \lambda \overline{C}' + \overline{q} = 0 , \tag{4}$$

with

$$\overline{q} = \int_0^1 q(z)\, dz . \tag{5}$$

The first, second and third terms in (3) represent the settling flux to the seabed, the mortality and the source, respectively.

It is rather natural to assume that the source of fecal bacteria is pointwise and located at the top of the water column, i.e. the sea surface. Without any loss of generality, the rate of release of the source may be prescribed to be unity. Thus, one has

$$q(z) = \delta(z-1) , \tag{6}$$

where δ denotes the Dirac function. Therefore, the depth-averaged release rate of the source is

$$\overline{q} = 1 , \tag{7}$$

implying that the concentration in the zero-dimensional model is

$$\overline{C}' = \frac{1}{1+\lambda} . \tag{8}$$

This result was obtained by substituting (7) into (4).

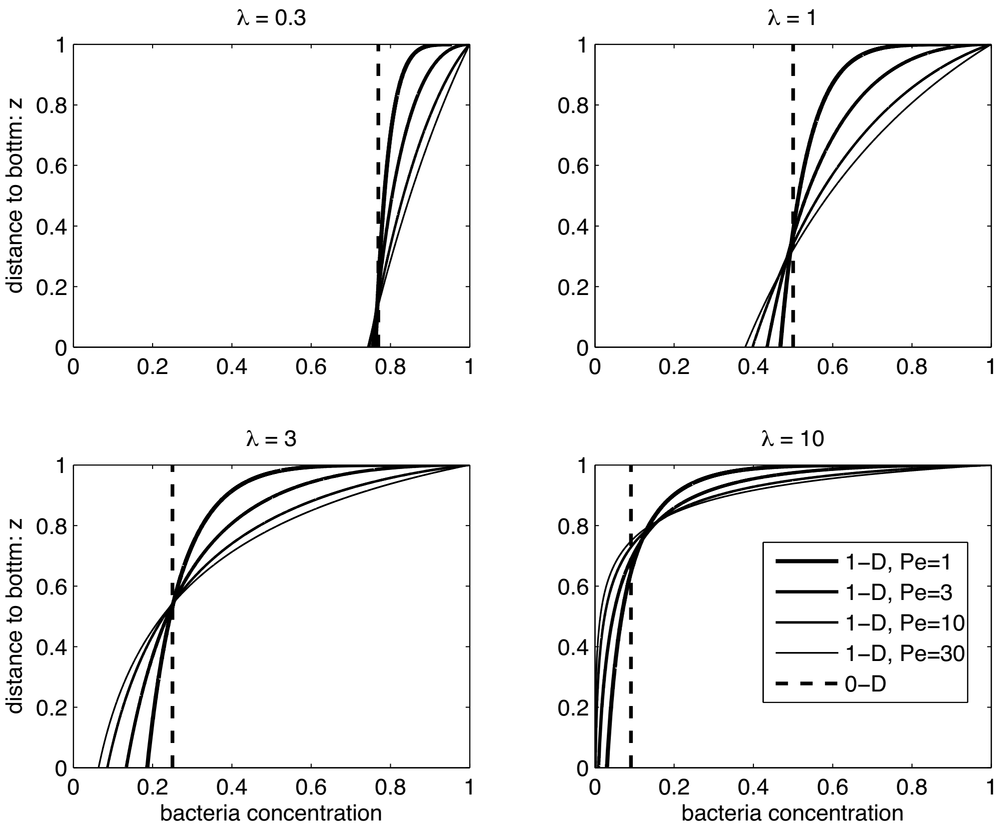


Figure1. Concentration profiles $C(z)$ ensuing from the one-dimensional model (14)-(15) for various values of the of the Peclet number Pe and the mortality rate λ. The corresponding value of the concentration in the zero-dimensional model $\overline{C}'$ is also displayed; this concentration is independent of z and Pe.

For the present study, the eddy diffusivity is taken to be

$$\kappa(z) = 6z(1-z) \ . \tag{9}$$

The impact of the source located at the sea surface may be investigated by integrating the equation governing the concentration on the arbitrarily small interval $[1^-,1^+]$:

$$\int_{1^-}^{1^+} \left[\frac{d}{dz}\left(\kappa \frac{dC}{dz} + C \right) - \lambda C + \delta(z-1) \right] dz = 0 \ . \tag{10}$$

This yields

$$\left[\kappa \frac{dC}{dz} + C \right]_{z=1^+} - \left[\kappa \frac{dC}{dz} \right]_{z=1^-} - \left[C(z) \right]_{z=1^-} - \int_{1^-}^{1^+} \lambda C \, dz + \int_{1^-}^{1^+} \delta(z-1) \, dz = 0 \ . \tag{11}$$

The first, second and fourth terms in the relation above are zero because the surface bondary condition prescribes that the flux through the surface is zero, the diffusivity is zero at the upper boundary of the domain and the integration interval is arbitrarily small. The fifth term is equal to unity, by virtue of the definition of the Dirac function. Therefore, (11) transforms to

$$\left[C(z) \right]_{z=1^-} = 1 \ . \tag{12}$$

The differential problem (1) is discretized as follows

$$\begin{cases} \dfrac{\kappa_{3/2}\dfrac{C_2 - C_1}{\Delta z} + C_2 - C_1}{\Delta z} - \lambda C_1 = 0 \\ \dfrac{\kappa_{k+1/2}\dfrac{C_{k+1} - C_k}{\Delta z} + C_{k+1} - \kappa_{k-1/2}\dfrac{C_k - C_{k-1}}{\Delta z} - C_k}{\Delta z} - \lambda C_k = 0 , \quad k = 2,3...K-1 \\ \dfrac{-\kappa_{K-1/2}\dfrac{C_K - C_{K-1}}{\Delta z} - C_K}{\Delta z} - \lambda C_K = \dfrac{1}{\Delta z} \end{cases} \tag{13}$$

with $K = 1/\Delta z$. Thus, one has to solve a tri-diagonal system of algebraic equtions

$$\begin{cases} (-\Delta z^{-1} - \lambda - \xi_{3/2})C_1 + (\xi_{3/2} + \Delta z^{-1})C_2 = 0 \\ \xi_{k-1/2}C_{k-1} + (-\xi_{k-1/2} - \Delta z^{-1} - \lambda - \xi_{k+1/2})C_k + (\xi_{k+1/2} + \Delta z^{-1})C_{k+1} = 0 , \quad k = 2,3...K-1 \\ \xi_{K-1/2}C_{K-1} + (-\xi_{K-1/2} - \Delta z^{-1} - \lambda)C_K = \Delta z^{-1} \end{cases} \tag{14}$$

where

$$\xi_{k\pm1/2} = \frac{\kappa_{k\pm1/2}}{\Delta z^2} . \tag{15}$$

The notations used above are essentially those of the previous working notes.

The numerical solutions of Figure 1 suggest that there is a boundary layer adjacent to the upper boundary of the water column. In this regions, it seems that the concentration gradient increases as the mortality increases or the Peclet number decreases. In an attempt to properly resolve the boundary layer, the number of grid points K was taken to be rather large, i.e. 20×10^3. The mathematics and the physics of this boundary layer are poorly understood.

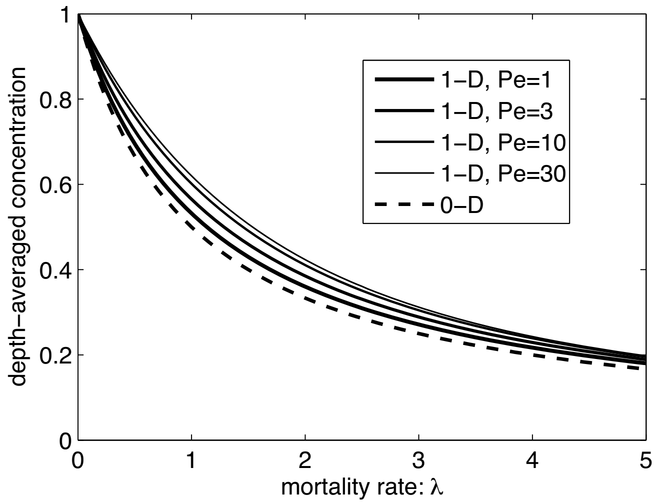


Figure 2. The depth-averaged concentrations $\overline{C}$ and $\overline{C}'$ as a function of the mortality rate λ for various values of the Peclet number.

As the Peclet number decreases, the depth-mean concentration obtained from the one-dimensional model, $\overline{C}$, tends to that derived from the depth-integrated model, $\overline{C}'$ (Figure 2). This is no surprise as, the smaller the Peclet number, the larger the impact of diffusive processes, which tend to reduce vertical contrasts. It is not known why $\overline{C}'$ seems to be always smaller than $\overline{C}$.

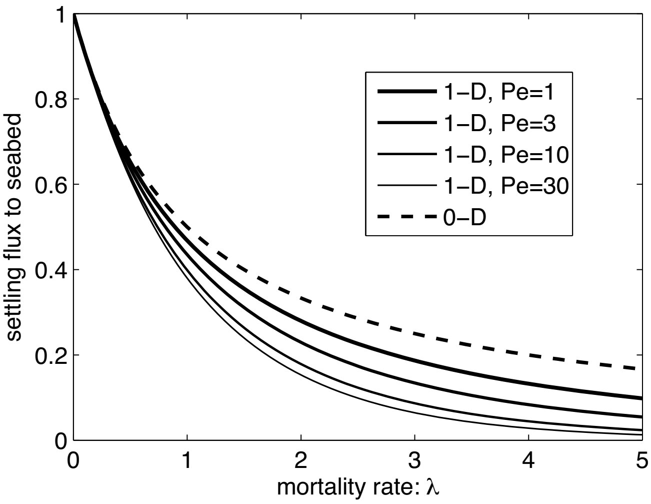


Figure 3. The settling flux to the seabed in the one-dimensional and the zero-dimensional models.

The bacteria flux reaching the seabed may exhibit significant differences according to whether it is estimated by means of the one-dimensional model or the zero-dimensional one (Figure 3).
