Polluted River

SF2520

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Contents

Discretization

We solve the PDE

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial y}(\frac{u}{w}) + \eta\frac{\partial^2 u}{\partial y^2} + \psi \tag{1}$$

with initial conditon $u(t, y) = 0$ and boundary conditions

$$\eta\frac{\partial u}{\partial y}(t, 0) = \bar{a}u(t, 0), \qquad u(t, 1) = 0. \tag{2}$$

This leads to the discretization, for inner points,

$$\frac{du}{dt}(t, x_j) \approx u_{t,j+1}(\frac{1}{2hw(x_j)} + \frac{\eta}{h^2}) + u_{t,x_j}(\frac{-2}{h^2}\eta - \frac{w'(x_j)}{w(x_j)^2}) + u_{t,j-1}(\frac{-1}{w(x_j)2h} + \frac{\eta}{h^2}). \tag{3}$$

Let the constants be c_j, b_j and a_j in order. For $j = 0$ we have

$$\frac{du}{dt}(t, 0) \approx u_{t,1}(\frac{1}{2hw(0)} + \frac{\eta}{h^2}) + u_{t,0}(\frac{-2}{h^2}\eta - \frac{w'(0)}{w(0)^2}) + u_{t,-1}(\frac{-1}{w(x_j)2h} + \frac{\eta}{h^2}). \tag{4}$$

Where we use the BC 2, e.g

$$\begin{aligned} \bar{a}u_{t,0} &= \eta\frac{u_{t,1} - u_{t,-1}}{2h} \\ \implies u_{t,-1} &= u_{t,1} - \frac{2h\bar{a}u_{t,0}}{\eta}. \end{aligned}$$

So that for $j = 0$ we have the discretization

$$\frac{du}{dt}(t, 0) \approx u_{t,1}(\frac{1}{2hw(0)} + \frac{\eta}{h^2}) + u_{t,0}(\frac{-2}{h^2}\eta - \frac{w'(0)}{w(0)^2}) + (u_{t,1} - \frac{2h\bar{a}u_{t,0}}{\eta})(\frac{-1}{w(0)2h} + \frac{\eta}{h^2}).$$

or after grouping terms

$$\frac{du}{dt}(t, 0) \approx u_{t,1}(c_0 + a_0) + u_{t,0}(b_0 - \frac{2h\bar{a}}{\eta}a_0).$$

Lastly at the point $j = N - 1$ we have

$$\frac{du}{dt}(t, x_{N-1}) \approx u_{t,N}(\frac{1}{2hw(x_{N-1})} + \frac{\eta}{h^2}) + u_{t,N-1}(\frac{-2}{h^2}\eta - \frac{w'(x_{N-1})}{w(x_{N-1})^2}) + u_{t,N-2}(\frac{-1}{w(x_{N-1})2h} + \frac{\eta}{h^2}).$$

Since $u_{i,N} = 0$ by 2 we get

$$\frac{du}{dt}(t, x_{N-1}) \approx +u_{t,N-1}(\frac{-2}{h^2}\eta - \frac{w'(x_{N-1})}{w(x_{N-1})^2}) + u_{t,N-2}(\frac{-1}{w(x_{N-1})2h} + \frac{\eta}{h^2}) = u_{i,N-1}b_{N-1} + u_{i,N-2}a_{N-1}.$$

This gives a tridagonal matrix

$$\mathbf{A} = \begin{pmatrix} b_0 - a_0\frac{2h\bar{a}}{\eta} & a_0 + c_0 & 0 & \dots & & & \\ a_1 & b_1 & c_2 & & & & \\ 0 & a_2 & b_2 & c_2 & & & \\ 0 & 0 & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & a_{N-1} & b_{N-1} & 0 \end{pmatrix} \tag{5}$$

Note that $\mathbf{A} \in \mathbb{R}^{N\times N}$.

Non-dimensionalizing

The original PDE is

$$\frac{\partial C}{\partial t} - \frac{\partial(VC)}{\partial x} = D\frac{\partial^2 C}{\partial x^2} + \Psi. \tag{6}$$

With substitutions $C = uC_0, t = \tau T$ and $x = yL$ where C_0 and T are TBD. From this we have

$$\frac{\partial}{\partial t} = T^{-1}\frac{\partial}{\partial \tau}, \qquad \frac{\partial}{\partial x} = L^{-1}\frac{\partial}{\partial y}.$$

Simply substituting this into 6 we get

$$\frac{\partial u}{\partial \tau}\frac{C_0}{T} - \frac{\partial(Vu)}{\partial y}\frac{C_0}{L} = \frac{DC_0}{L^2}\frac{\partial^2 u}{\partial y^2} + \Psi.$$

Since $V = V(x) = \frac{V_0W_0}{W(X)} = \frac{V_0}{w(\frac{x}{L})}$. We can write

$$\frac{\partial u}{\partial \tau}\frac{C_0}{T} - \frac{\partial}{\partial y}(\frac{u}{w})\frac{C_0V_0}{L} = \frac{DC_0}{L^2}\frac{\partial^2 u}{\partial y^2} + \Psi. \tag{7}$$

Moving appropriate terms to the RHS and multiplying with $\frac{T}{C_0}$ we now have

$$\frac{\partial u}{\partial \tau} = \frac{\partial}{\partial y}(\frac{u}{w})\frac{TV_0}{L} + \frac{DT}{L^2}\frac{\partial^2 u}{\partial y^2} + \frac{T}{C_0}\Psi.$$

This gives

$$\begin{cases} \frac{TV_0}{L} = 1 \implies T = \frac{L}{V_0}, \\ \eta = \frac{DT}{L^2} \implies \eta = \frac{D}{LV_0}. \end{cases}$$

For the Ψ term we now have (by definition)

$$\frac{T}{C_0}\Psi = \frac{T\Psi_0}{T_0\Delta a C_0}g(\frac{t}{T_0}, \frac{x-a}{\Delta a}) = \frac{\Psi_0}{\tau_0 \Delta a C_0}g(\frac{\tau}{\tau_0}, \frac{y-\hat{a}}{\Delta \hat{a}}).$$

We now need

$$\frac{\Psi_0}{\tau_0\Delta a C_0} = \frac{1}{\tau_0 \Delta\hat{a}} = \frac{1}{\tau_0\frac{\Delta a}{L}} = \frac{L}{\tau_0\Delta a}$$

i.e

$$C_0 = \frac{\Psi_0\tau_0\Delta a}{\tau_0\Delta a L} = \frac{\Psi_0}{L}.$$

Boundary Conditions

The BC for 6 is

$$D\frac{\partial C}{\partial x}(t,0) = \alpha C(t,0).$$

So substituting again we have

$$\frac{DC_0}{L}\frac{\partial u}{\partial y}(\tau T, 0) = \alpha C_0 u(\tau T, 0)$$

or

$$\frac{D}{L}\frac{\partial u}{\partial y}(\tau T, 0) = \alpha u(\tau T, 0).$$

We also have

$$\alpha = \sqrt{\frac{V(0)^2}{4} + \alpha_0^2} - \frac{V(0)}{2} = \sqrt{\frac{1}{4}(\frac{V_0W_0}{W_0w(\frac{x}{L})})^2 + \alpha_0^2} - \frac{1}{2}\frac{V_0W_0}{W_0w(\frac{x}{L})} = \sqrt{\frac{1}{4}\frac{V_0^2}{w(\frac{x}{L})^2} + \alpha_0^2} - \frac{V_0}{2w(\frac{x}{L})}.$$

So,

$$\frac{D}{L}\frac{\partial u}{\partial y}(\tau T, 0) = (\sqrt{\frac{1}{4}\frac{V_0^2}{w(\frac{x}{L})^2} + \alpha_0^2} - \frac{V_0}{2w(\frac{x}{L})})u(\tau T, 0).$$

Dividing by V_0 and noticing that $\frac{x}{L} = y = 0$ we have

$$\frac{D}{LV_0}\frac{\partial u}{\partial y}(\tau T, 0) = (\sqrt{\frac{1}{4w(0)} + (\frac{a_0}{V_0})^2}) - \frac{1}{2w(0)})u(\tau T, 0).$$

This gives $\beta_0 = \frac{a_0}{V_0}$. So finally we have with $\eta = \frac{D}{LV_0}$ as before

$$\eta\frac{\partial u}{\partial y}(\tau, 0) = (\sqrt{\frac{1}{4w(0)} + \beta_0^2} - \frac{1}{2w(0)})u(\tau, 0) = \bar{a}u(\tau, 0).$$

Fish Death

The maximum concentration over time is

$$c_\infty(x) = \frac{1}{R_\infty}\max_{t>0} C_v(t,x) = \frac{1}{R_\infty}\max_{t>0}\frac{C(t,x)}{W_0w(\frac{x}{L})D_p} = \frac{1}{R_\infty W_0 D_p}\max_{t>0}\frac{C(t,x)}{w(\frac{x}{L})}.$$

Making the substitutions we now have

$$u_\infty(y) = \frac{C_0}{R_\infty W_0 D_p}\max_{\tau>0}\frac{u(\tau,y)}{w(y)}$$

This gives $\gamma_\infty = \frac{C_0}{R_\infty W_0 D_p}$.

The total volume concentration exposure time

Now for

$$c_{tot} = \frac{1}{R_{tot}}\int_0^\infty \frac{C(t,x)}{W_0w(\frac{x}{L})D_p}dt = \frac{1}{R_{tot}W_0D_p}\int_0^\infty \frac{C(t,x)}{w(\frac{x}{L})}dt.$$

We know that $dt = Td\tau$ so we get

$$u_{tot}(y) = \frac{C_0T}{R_{tot}W_0D_p}\int_0^\infty \frac{u(\tau,y)}{w(y)}d\tau$$

which implies

$$\gamma_{tot} = \frac{C_0T}{R_{tot}W_0D_p}.$$

Experiments

Fixing all parameters on default and changing $\Delta\hat{a}$ we get the following table for fish death. Wish makes sense, if

	p_{\infty}	p_{tot}
\hat{a}=0.9	0.2778	0.4102
\hat{a}=0.8	0.2581	0.3701
\hat{a}=0.5	0.1900	0.2749

we put the pestcide in the river at later stages, fewer fish will be contaminated with the poison.

Keeping all other parameters constant (default) and varying τ_0 we get.

	p_{\infty}	p_{tot}
\tau_0=0.01	0.2889	0.3869
\tau_0=0.05	0.2654	0.3713
\tau_0=0.07	0.2581	0.3701
\tau_0=0.1	0.2471	0.3692
\tau_0=1	0.0747	0.3665

Note that not all pesticide has left in the last one and $T = 2$.

Lastly, varying $\Delta\hat{a}$ and keeping all other constant (default).

	p_{\infty}	p_{tot}
\Delta hat{a}=0.002	0.2581	0.3701
\Delta hat{a}=0.009	0.2581	0.3702
\Delta hat{a}=0.1	0.2467	0.3737
\Delta hat{a}=1	0.0957	0.2535

Now for η we get,

	p_inf	p_tot
eta=0.01	0.2581	0.3701
eta=0.05	0.1738	0.3770
eta=0.1	0.1465	0.3492
eta=1	0.0644	0.1089
eta=0.001	0.4119	0.3653