Derivation of 1d and 2d diffusion-advection equations, and numerical solution for 1d case

Eli, APM115/ 105b

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1 Derivation of 1d diffusion equation

Consider a 1d pipe with a fluid at rest containing some contaminant with concentration $C(x,t)$. Consider the tracer budget for the short element of the pipe from $x-dx$ to $x+dx$. The equation is

$$\frac{\partial}{\partial t}(\text{total tracer}) = \text{flux in} - \text{flux out}$$

In the presence of diffusion, "Fick's law" tells us that the diffusive flux is proportional to the concentration gradient and flows from high concentration to low concentration. The incoming flux into the short segment of the pipe we are considering is therefore proportional to the gradient of the concentration at the left point, $-D\frac{\partial C}{\partial x}|_{x-dx}$, and the out flux is similarly evaluated at the right point, $D\frac{\partial C}{\partial x}|_{x+dx}$ (note the signs, can you justify them?). D is the diffusion coefficient. The above equation becomes

$$\begin{aligned}\frac{\partial}{\partial t}(2dx\,C(x,t)) &= D\left(\left.\frac{\partial C}{\partial x}\right|_{x+dx} - \left.\frac{\partial C}{\partial x}\right|_{x-dx}\right)\\ &\approx D\left.\frac{\partial^2 C}{\partial x^2}\right|_x 2dx\end{aligned}$$

where we have used the definition of a second derivative as the difference between the two first derivatives etc. The diffusion equation for C now becomes

$$\frac{\partial}{\partial t}C(x,t) = D\frac{\partial^2 C}{\partial x^2}.$$

2 Derivation of 1d advection-diffusion equation

Consider a 1d pipe with a fluid flow with velocity $u(x,t)$ containing some contaminant (tracer) with concentration $C(x,t)$. Consider the tracer budget for the short element of the pipe from $x-dx$ to $x+dx$. The equation is

$$\frac{\partial}{\partial t}(\text{total tracer}) = \text{flux in} - \text{flux out}$$

Diffusion: In the presence of diffusion, "Fick's law" tells us that the diffusive flux is proportional to the concentration gradient and flows from high concentration to low concentration. The incoming flux due to diffusion into the short segment of the pipe we are considering is therefore proportional to the gradient of the concentration at the left point, $-D\frac{\partial C}{\partial x}|_{x-dx}$, and the out flux is similarly evaluated at the right point, $D\frac{\partial C}{\partial x}|_{x+dx}$ (note the signs, can you justify them?). D is the diffusion coefficient.

Advection: the fluid flow also leads to flux into and our of the segment. The flux in is $u(x-dx)C(x-dx,t)$ and the flux out is $u(x+dx)C(x+dx,t)$.

The above equation now becomes

$$\begin{aligned}\frac{\partial}{\partial t}(2dx\,C(x,t)) = {} & D\left(\left.\frac{\partial C}{\partial x}\right|_{x+dx} - \left.\frac{\partial C}{\partial x}\right|_{x-dx}\right)\\ & + u(x+dx)C(x+dx,t) - u(x-dx)C(x-dx,t)\\ \approx {} & D\left.\frac{\partial^2 C}{\partial x^2}\right|_x 2dx - \frac{\partial}{\partial x}(uC)\,2dx\end{aligned}$$

where we have used the definition of a second derivative as the difference between the two first derivatives etc. The advection-diffusion equation for C now becomes

$$\frac{\partial}{\partial t}C(x,t) + \frac{\partial}{\partial x}(uC) = D\frac{\partial^2 C}{\partial x^2}.$$

3 Scaling

Let U be a typical scale for the velocity, L for the spatial scale, and τ for time. Starting from

$$\frac{\partial}{\partial t}C(x,t) + \frac{\partial}{\partial x}(uC) = D\frac{\partial^2 C}{\partial x^2},$$

the different terms may be crudely estimated as

$$\frac{\delta C}{\tau} + U\frac{\delta C}{L} = D\frac{\delta C}{L^2}.$$

If diffusion is dominant and advection negligible, we find that the time it takes a tracer perturbation to be carried by diffusion to a distance L is given by

$$\tau \sim L^2/D.$$

If advection is dominant, we find,

$$\tau \sim L/U.$$

Equivalently, note that the distance traveled by the perturbation due to diffusion is proportional to the square root of time, while in the case of advection it is linear in time.

4 Derivation of 2d diffusion equation

Consider a 2d domain pipe with a fluid at rest containing some contaminant with concentration $C(x,y,t)$. Consider the tracer budget for the small area element $x-dx$ to $x+dx$ and $y-dy$ to $y+dy$. The budget equation for the small square area element

$$\frac{\partial}{\partial t}(\text{total tracer}) = \text{flux in} - \text{flux out}$$

The total tracer is simply given by $2dx2dyC(x,y,t)$.

In the presence of diffusion, "Fick's law" tells us that the diffusive flux is proportional to the concentration gradient and flows from high concentration to low concentration. The incoming flux in the x direction into the small square area element we are considering is therefore proportional to the gradient of the concentration at the left point times its extent in the y direction, $F^{(x,in)}(x-dx,y) = -2dyD\frac{\partial C}{\partial x}|_{x-dx}$, where D is the diffusion coefficient. The out flux in the x direction is similarly evaluated at the right edge of the small square, $F^{(x,out)}(x+dx,y) = -2dy\frac{\partial C}{\partial x}|_{x+dx}$. The fluxes into and out of the small area element in the y direction are similarly given by $F^{(y,in)}(x,y-dy) = -2dxD\frac{\partial C}{\partial y}|_{y-dy}$ and $F^{(y,out)}(x,y+dy) = -2dx\frac{\partial C}{\partial y}|_{y+dy}$

The above equation therefore becomes

$$\begin{aligned}
\frac{\partial}{\partial t}(2dx2dyC(x,y,t)) &= F^{(x,in)}(x-dx,y) - F^{(x,out)}(x+dx,y) \\
&+ F^{(y,in)}(x,y-dy) - F^{(y,out)}(x,y+dy) \\
&= (2dy)D\left(\left.\frac{\partial C}{\partial x}\right|_{x+dx} - \left.\frac{\partial C}{\partial x}\right|_{x-dx}\right) \\
&+ (2dx)D\left(\left.\frac{\partial C}{\partial y}\right|_{y+dy} - \left.\frac{\partial C}{\partial y}\right|_{y-dy}\right) \\
&\approx D\left(\left.\frac{\partial^2 C}{\partial x^2}\right|_{x,y} + \left.\frac{\partial^2 C}{\partial y^2}\right|_{x,y}\right) 2dx2dy
\end{aligned}$$

were we have used the definition of a second derivative as the difference between the two first derivatives etc. Dividing by the area of the small square, the diffusion equation for C now becomes

$$\frac{\partial}{\partial t}C(x,y,t) = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right).$$

This may be written in vector form as

$$\frac{\partial}{\partial t}C = D\nabla^2 C.$$

which is easily extended to 3d and to other coordinate systems.

5 Numerical solution

Start from the diffusion equation

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}.$$

Discretize in space (center difference, location denoted by subscript i) and time (Euler forward, time denoted by superscript n),

$$(C_i^{n+1} - C_i^n)/\Delta t = D(C_{i+1}^n - 2C_i^n + C_{i-1}^n)/(\Delta x)^2,$$

so that we can solve for C_i^{n+1} in terms of the concentration at n.