Numerical Solver Method

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The function titled `CrankNicolson` is the solver method intended for use, and explained here. The other functions use different schemes.

Problem

The PDE this solver numerically approximates is,

$$\frac{\partial c_g}{\partial t} = D_e \frac{\partial^2 c_g}{\partial z^2} - V_e \frac{\partial c_g}{\partial z} - \lambda c_g$$

where c_g is the concentration of the tracer in the gas phase, z is the depth under the surface, D_e is the effective diffusion constant, V_e is the effective velocity, λ is the decay constant, and t is time. The boundary at the surface, $c_g(t,\ z = 0)$, is the measured atmospheric concentration of the tracer gas. The initial boundary, $c_g(t = 0,\ z)$, and the boundary at the max depth of 200 meters, $c_g(t,\ z = 200)$, are both assumed to be zero.

Solution

The PDE is approximated using a scheme similar to the Crank Nicolson method, an implicit finite difference scheme. Let u_j^m be the approximation of $c_g(t, z)$ at $t = m\Delta t$ and $z = j\Delta z$. The partial with respect to time is approximated using the forward difference approximation,

$$\frac{\partial c_g}{\partial t} \approx \frac{u_j^{m+1} - u_j^m}{\Delta t},$$

The partials with respect to depth are approximated using central differences averaged between the $(m + 1)$th time step and the mth time step,

$$\frac{\partial^2 c_g}{\partial z^2} \approx \frac{1}{2}\left(\frac{u_{j+1}^{m+1} - 2u_j^{m+1} + u_{j-1}^{m+1}}{\Delta x^2} + \frac{u_{j+1}^{m} - 2u_j^{m} + u_{j-1}^{m}}{\Delta x^2}\right),$$

and

$$\frac{\partial c_g}{\partial z} \approx \frac{1}{2}\left(\frac{u_{j+1}^{m+1} - u_{j-1}^{m+1}}{2\Delta x} + \frac{u_{j+1}^{m} - u_{j-1}^{m}}{2\Delta x}\right).$$

The decay term is approximated with an average between the concentrations at the $(m+1)$th time step and the mth time step,

$$c_g \approx \frac{1}{2}\left(u_j^{m+1} + u_j^m\right).$$

When substituted into the original equation these approximations yield the equation,

$$\begin{aligned}\frac{u_j^{m+1} - u_j^m}{\Delta t} =& \frac{1}{2}\left(D_e \frac{u_{j+1}^{m+1} - 2u_j^{m+1} + u_{j-1}^{m+1} + u_{j+1}^{m} - 2u_j^{m} + u_{j-1}^{m}}{\Delta x^2} - \right.\\ & \left. V_e \frac{u_{j+1}^{m+1} - u_{j-1}^{m+1} + u_{j+1}^{m} - u_{j-1}^{m}}{2\Delta x} - \lambda(u_j^{m+1} + u_j^m)\right).\end{aligned}$$

This can be and rearranged into the equation,

$$\begin{aligned}(-2D_e - V_e\Delta x)u_{j-1}^{m+1} + \left(4\frac{\Delta x^2}{\Delta t} + 4D_e + \lambda\right)u_j^{m+1} + (-2D_e + V_e\Delta x)u_{j+1}^{m+1} = \\ (2D_e + V_e\Delta x)u_{j-1}^{m} + \left(4\frac{\Delta x^2}{\Delta t} - 4D_e - \lambda\right)u_j^{m} + (2D_e - V_e\Delta x)u_{j+1}^{m}.\end{aligned} \tag{1}$$

This gives a system of equations that may be solved using a tridiagonal matrix.

Accuracy

The depth approximations are both central differences, which are second order, so their error is $O(\Delta x^2)$. The time approximation is a forward difference which is only first order, but because the depth approximations are averaged over the $(m+1)$th and the mth time steps the error in time is $O(\Delta t^2)$. Thus the approximation is second order in the time and depth steps.

Stability

To use von Neumann stability we will make the substitution,

$$u_j^m = Q^m e^{ij\Delta xk},$$

where Q^m is the magnitude at the mth time step, k is frequency, and i is $\sqrt{-1}$.

Substituting this into the equation (1),

$$\begin{aligned}(-2D_e - V_e\Delta x)Q^{m+1}e^{i(j-1)k} + \left(4\frac{\Delta x^2}{\Delta t} + 4D_e + \lambda\right)Q^{m+1}e^{ijk} + (-2D_e + V_e\Delta x)Q^{m+1}e^{i(j+1)k} = \\ (2D_e + V_e\Delta x)Q^{m}e^{i(j-1)k} + \left(4\frac{\Delta x^2}{\Delta t} - 4D_e - \lambda\right)Q^{m}e^{ijk} + (2D_e - V_e\Delta x)Q^{m}e^{i(j+1)k}.\end{aligned}$$

This can be simplified into,

$$Q^{m+1} = Q^m a,$$

where a is the amplification factor,

$$a = \frac{(2D_e + V_e\Delta x)e^{-i\Delta xk} + (2D_e - V_e\Delta x)e^{i\Delta xk} + 4\frac{\Delta x^2}{\Delta t} - 4D_e - \lambda}{(-2D_e - V_e\Delta x)e^{-i\Delta xk} + (-2D_e + V_e\Delta x)e^{i\Delta xk} + 4\frac{\Delta x^2}{\Delta t} + 4D_e + \lambda}.$$

Now we can reduce this further using Euler's formula to,

$$a = \frac{4D_e\cos\Delta xk - 2V_e\Delta xi\sin\Delta xk + 4\frac{\Delta x^2}{\Delta t} - 4D_e - \lambda}{-4D_e\cos\Delta xk + 2V_e\Delta xi\sin\Delta xk + 4\frac{\Delta x^2}{\Delta t} + 4D_e + \lambda}$$

and finally to,

$$a = \frac{1 - \lambda\frac{\Delta t}{\Delta x^2} - D_e\frac{\Delta t}{\Delta x^2}(1-\cos\Delta xk)}{1 + \lambda\frac{\Delta t}{\Delta x^2} + D_e\frac{\Delta t}{\Delta x^2}(1-\cos\Delta xk)} - i.$$

Since the imaginary term is always -1 for the magnitude of a to be less than 1 the real part must be zero. This is not feasibly possible, so the method is unstable.