

Eulerian Simulation of Dispersion

Write a program to calculate the mean concentration field $C = C(x, z)$ down-wind from a continuous crosswind line source¹ at $x = 0, z = h_s = 0.46$ m in the horizontally-uniform, neutrally-stratified atmospheric surface layer. Assume C is the solution of the advection-diffusion equation

$$\frac{\partial}{\partial x} [U(z) C] = \frac{\partial}{\partial z} \left[K(z) \frac{\partial C}{\partial z} \right] \quad (1)$$

with mean windspeed and eddy diffusivity profiles

$$U(z) = \frac{u_*}{k_v} \ln \frac{z}{z_0}, \quad (2)$$

$$K(z) = \frac{k_v}{S_c} u_* z \quad (3)$$

($k_v = 0.4$ is the von Karman constant and S_c is the turbulent Schmidt number).

Discretize using grid-lengths $\Delta x \sim 0.5$ m, $\Delta z \sim 0.2$ m. For two choices $S_c = (1, 0.63)$ of the Schmidt number, compare your calculated solution $C(100, z)$ at $x = 100$ m with the observations (Table 1) of Project Prairie Grass run 57, for which the meteorological situation was $u_* = 0.50$ m s⁻¹, $z_0 = 0.0058$ m. (Note: to compare with Table 1, you'll need to scale your computed concentrations the same way, that is, you multiply by $z_0 u_* / k_v$.)

Method

The algorithm derived in class for this class of problem has the form

$$A_J^N C_{I,J+1} + A_J^C C_{I,J} + A_J^S C_{I,J-1} = B_{I,J}, \quad J = 1..J_{mx} \quad (4)$$

¹The field of C is the analog of the crosswind integrated concentration $\chi = \chi(x, z)$ due to a steady point source, and Project Prairie Grass provided field measurements of the latter.

where the A_J 's are the centre (C), north (N) and south (S) “neighbour coefficients”, and $C_{I,J}$ [or $C(I, J)$] is the concentration matrix. The term $B_{I,J}$ contains information (only) from the upstream column at $I - 1$, so we can regard it as a known. Thus we may frame our problem of finding the vertical column of values of C at downstream location I (given the column at $I - 1$) as a matrix problem,

$$\mathbf{M} \mathbf{C} = \mathbf{B} \quad (5)$$

where \mathbf{M} is the coefficient matrix, and is tridiagonal. Thus we may find the unknown column (i.e. $C_{I,J} \forall J$) as

$$\mathbf{C} = \mathbf{M}^{-1} \mathbf{B} \quad (6)$$

This is a marching problem, implicit along the J (vertical)-axis. We need only once compute \mathbf{M}^{-1} , and we use it repeatedly to step down the I axis. Each time we get a new \mathbf{C} column matrix we recompute \mathbf{B} , and repeat the operation. Each step gives us \mathbf{C} at a column further down the x -axis by a distance Δx .

Upper and lower boundary conditions

Set the top of your domain $z(J_{max})$ sufficiently high (say, at least 30 m) that $C(J_{max}) = 0$. Then your coefficients at $J = J_{max}$ are

$$\begin{aligned} A_{J_{max}}^C &= 1 \\ A_{J_{max}}^N &= \text{not used} \\ A_{J_{max}}^S &= 0 \\ B_{J_{max}} &= 0 \end{aligned} \quad (7)$$

If we presume our gas does not react with the ground, we want zero flux to ground, which is assured by requiring $C(I, 1) \equiv C(I, 2)$. Thus at $J = 1$ the needed coefficients are

$$\begin{aligned}
A_1^C &= 1 \\
A_1^N &= -1 \\
A_1^S &= \text{not used} \\
B_1 &= 0
\end{aligned}
\tag{8}$$

Inlet boundary condition

How is your solution going to “know” there is a source? Let J_h be the height index of the cell the physical source will lie within, and let the streamwise index value $I = 0$ (or $I = 1$ if you prefer) correspond to a column of gridpoints aligned at the source location. The easiest approach is to set the inlet or inflow concentration profile as

$$C(0, J) = \begin{cases} 0 & \text{if } J \neq J_h, \\ 1/(U(J_h) \Delta z) & \text{if } J = J_h \end{cases}
\tag{9}$$

which guarantees that the total mass flux across the first interior plane $I = 1$ will be

$$Q = \sum_J C(0, J) U(J) \Delta z = 1
\tag{10}$$

Adding interest to your report

Its a good bet that, having eventually squashed all bugs, each student will get the correct numeric solution. That being the case, scores are going to revolve around effectiveness of the assignment report. Elsewhere some tips have been given. YOu want to be creative, and interesting. For example rather than just graph the concentration profile at $x = 100$ m, you might show a contour plot of the C field in two dimensions, i.e. $C(x, z)$. You could experiment with

the sensitivity of the computed concentration profile to gridlengths Δx , Δz . What is the order of the Truncation Error of the algorithm used (i.e. is it proportional to Δx or Δx^2 , etc.)? Do deviations of your computed solution from the experimental data scale in the expected way with Δx , Δz ? What would happen if you changed the boundary condition at ground to enforce $C = 0$ (absorption boundary condition)?

Table 1: Normalized concentration $z_0 u_* C / (k_v Q)$ observed at distance $x = 100$ m from the source (height $h_s = 0.46$ m) in Project Prairie Grass run 57.

z [m]	$z_0 u_* C / (k_v Q)$
17.5	1.5E-6
13.5	6.6E-6
10.5	1.56E-5
7.5	3.51E-5
4.5	7.9E-5
2.5	1.25E-4
1.5	1.53E-4
1.0	1.62E-4
0.5	1.70E-4