

Eulerian Simulation of Dispersion in the stably-stratified hhASL

Write a program to calculate the mean concentration field $C = C(x, z)$ downwind from a continuous line source¹ at $x = 0, z = h_s$ in the horizontally-uniform, stably-stratified atmospheric surface layer. Assume C is the solution of

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

and that the surface layer mean windspeed and eddy diffusivity profiles are

$$U(z) = \frac{u_*}{k_v} \left[\ln \frac{z}{z_0} + \beta \frac{z - z_0}{L} \right] \quad (2)$$

$$K(z) = \frac{(k_v/S_c) u_* z}{1 + \beta z/L} \quad (3)$$

where the Obukhov length $L > 0$, $k_v = 0.4$ is the von Karman constant, the empirical factor $\beta = 5$, and S_c is the turbulent Schmidt number.

Discretize using grid-lengths $\Delta x \sim \Delta z \sim 0.1$ m. For two choices $S_c = (0.63, 1.0)$ 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 59, for which source height $h_s = 0.46$ m, and the meteorological situation was: $u_* = 0.14$ m s⁻¹, $L = 7$ m, $z_0 = 0.005$ m. Alongside your solution, plot also the solution for $|L| = \infty$ (neutral stratification).

¹By symmetry, this is identical to the crosswind-integrated concentration at the same distance downwind from a continuous point source. This is the situation for which we have experimental data, viz., Project Prairie Grass.

Method

The algorithm suggested in class is of the form:

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

where the $A_{I,J}$ are the centre (C), north (N) and south (S) “neighbour coefficients”, and $C_{I,J}$ is the concentration matrix. But in fact since our neighbour coefficient vectors $A_{I,J}^C, A_{I,J}^N, A_{I,J}^S$ do not change with I we can simplify the notation to

$$A_J^C C(I, J) = A_J^N C(I, J + 1) + A_J^S C(I, J - 1) + B_{I,J}, \quad J = 1..J_{max} \quad (5)$$

This is a marching problem, implicit along the J (vertical)-axis. You will need to use a Tridiagonal Matrix Inversion Algorithm, eg. that given in *Numerical Recipes* or the one in the Appendix at the end of this document.

Upper and lower boundary conditions

Set the top of your domain $z(J_{max})$ sufficiently high (say, at least 15 m) that $C(J_{max}) = 0$. Then (using the terminology of the TDMA subroutine given in the Appendix), your coefficients at $J = J_{max}$ are

$$\begin{aligned} a(J_{max}) &= A_{J_{max}}^C = 1 \\ b(J_{max}) &= A_{J_{max}}^N = 0 \\ c(J_{max}) &= A_{J_{max}}^S = 0 \\ d(J_{max}) &= 0 \end{aligned} \quad (6)$$

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 $J = 1$ your coefficients are

$$\begin{aligned} a(1) &= 1 \\ b(1) &= 1 \\ c(1) &= 0 \\ d(1) &= 0 \end{aligned} \tag{7}$$

Inlet boundary condition

Now note that the governing equation is homogeneous... 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 1 if you prefer) correspond to gridpoints aligned at the source location. The easiest approach is to set the inlet or inflow concentration profile as

$$C(0, J) = \begin{cases} 0 & \text{if } J \neq J_h, \\ 1/(U(J_h) \Delta z) & \text{if } J = J_h \end{cases} \tag{8}$$

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

$$Q = \sum_J C(0, J) U(J) \Delta z = 1 \tag{9}$$

Last words

Provide a flowchart that, in conjunction with your table of symbols, unambiguously defines your algorithm. Experiment with the sensitivity of the computed concentration profile to gridlengths Δx , Δz .

Before solving the diffusion problem, make sure your implementation of the matrix inversion program correctly solves a simple test problem; eg. suppose the problem is of form $\mathbf{M} \mathbf{S} = \mathbf{R}$ where the coefficient matrix is $\mathbf{M} = \begin{pmatrix} 3 & -1 \\ 2 & 1 \end{pmatrix}$ and $\mathbf{R} = \begin{pmatrix} 7 \\ 3 \end{pmatrix}$... you should be able to apply TDMA to determine that $\mathbf{S} = \begin{pmatrix} 2 \\ -1 \end{pmatrix}$.

Table 1: Normalized, crosswind-integrated 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 59.

z [m]	$z_0 u_* C / (k_v Q)$
7.5	7 E-7
4.5	2.1E-5
2.5	1.05E-4
1.5	1.75E-4
1.0	2.14E-4
0.5	2.40E-4

Appendix: TDMA algorithm

```
c
  subroutine tdma(m,n,a,b,c,t,d)
c
c   structure is:  a(j) t(j) = b(j) t(j+1) + c(j) t(j-1) + d(j)
c
c   where vector t(j), j=m..n is the solution we compute from
c   our neighbour coefficients (a=centre, b=north or upper
c                               c=south or lower) and from our
c   and the coefficient vector that depends on the solution
c   "behind our back", d(j)
c
c   don't confuse the local coefficient c(j) with the
c   concentration field C(I,J) that we are seeking !
c
  implicit none
  integer nx,ny,nz,span
  parameter (span=125)          ! adjust as appropriate
  integer j,k,m,n
  real denom
  real a(span),b(span),c(span),d(span),t(span)
  double precision p(span),q(span)
  p(m)=b(m)/a(m)
  q(m)=d(m)/a(m)
  do j=m+1,n
    denom=a(j)-c(j)*p(j-1)
    p(j)=b(j)/denom
    q(j)=(d(j)+c(j)*q(j-1))/denom
  end do
  t(n)=q(n)
  do k=1,n-m
    j=n-k
    t(j)=p(j)*t(j+1)+q(j)
  end do
  return
end
```

c