

Lagrangian stochastic simulations of dispersion of gases and particles in the horizontally-uniform atmospheric surface layer

Create and execute algorithms for the zeroth-order and the first-order Lagrangian stochastic (LS) trajectory models for 1D (vertical) motion in Gaussian inhomogeneous turbulence. Apply your algorithms to the case of Project Prairie Grass Run 33 (Tables 1, 2), ie. compute the vertical profile of crosswind-integrated mean concentration $C = C(x, z)$ at a distance of 100 m downwind from a continuous source at $x = y = 0, z = h_s = 0.46$ m in the horizontally-uniform surface layer. You may treat this run as if stratification was neutral.

Modify your first-order LS model to obtain the “Settling Sticky Fluid Element” model of heavy particle trajectories, by adding a gravitational settling velocity w_g . Simulate the observed pattern of crosswind-integrated deposition $D_0(x)$ observed (Table 3) in Walker’s “Trial C” of the Suffield bead diffusion trials, for which $u_* = 0.44$ m s⁻¹, $z_0 = 0.025$ m, $L = 341$ m (effectively neutral), $z_{src} = 15$ m, settling velocity $w_g = 0.6$ m s⁻¹, and particle acceleration timescale $\tau_p = 0.06$ s.

Zeroth-order model

Assume particle position (X, Z) evolves in time with steps

$$\begin{aligned} dX &= \bar{u}(Z(t)) dt \\ dZ &= \frac{\partial K}{\partial z} dt + \sqrt{2K} d\xi \end{aligned} \quad (1)$$

where $d\xi$ is a random number drawn from a Gaussian distribution $N(0, dt)$, ie. with zero mean and variance dt , where the timestep dt should be “small”. The eddy diffusivity should be specified as

$$K = \frac{1}{S_c} k_v u_* z \quad (2)$$

where S_c is the turbulent Schmidt number.

First-order model

Assume particle position (X, Z) evolves in time with velocity (U, W) where

$$U(Z(t)) = \bar{u}(Z(t)) \quad (3)$$

and where W evolves in time according to the unique, 1-d, first-order, well-mixed model for Gaussian inhomogeneous turbulence, ie.

$$\begin{aligned} dW &= a dt + b d\xi \\ a &= -\frac{C_0 \epsilon(z)}{2\sigma_w^2(z)} W \\ b &= \sqrt{C_0 \epsilon(z)} \end{aligned} \quad (4)$$

The factor $C_0\epsilon$ should be specified according to

$$\frac{2\sigma_w^4}{C_0\epsilon} = \sigma_w^2 T_L(z) = K_\infty = \frac{1}{S_c} k_v u_* z \quad (5)$$

and the timestep should be set as a fixed proportion of the timescale, ie. $dt = \mu T_L(z)$ where $\mu \sim 0.1$. The initial vertical velocity should be a random Gaussian number with zero mean and standard deviation σ_w . Experiment with several values of the turbulent Schmidt number (including $S_c = 1$).

How is mean concentration derived from computed trajectories?

Imagine a mast or vertical axis standing at distance $x = 100$ m downwind from the source. Divide the vertical axis into layers of depth Δz , which will define the vertical resolution of your computed concentration profile. Now label your layers with index J .

Each time a particle passes $x = 100$ m, increase the count $N(J)$ in the layer it occupies. When you have computed all N_P independent trajectories, the ratio $N(J)/N_P$ is clearly the probability that a single particle released at the source crosses $x = 100$ m in layer J . Therefore $N(J)/N_P$ is related to the mean horizontal flux $\overrightarrow{F}(J)$ of particles in that layer, in fact

$$\frac{N(J)}{N_P} = \overrightarrow{F}(J) \Delta z \quad (6)$$

But since we have no horizontal fluctuations u' in our treatment, we have $\overline{F}(J) \equiv C(J) U(J)$ (the streamwise convective flux density is entirely due to the mean velocity), and so by rearrangement

$$C(J) = \frac{N(J)}{N_P \Delta z U(J)} \quad (7)$$

Don't make your bins too thin (Δz too small) or there will be a very small probability of any trajectory passing through your bins... with the result that unless you release an immense number (N_P) of trajectories, you will have a statistically unreliable (noisy, albeit high resolution) concentration profile. Probably $\Delta z \sim 0.3 - 0.5$ m is satisfactory.

Refinements for next time!

Provide flowcharts that, in conjunction with your table of symbols, unambiguously define your algorithm.

Table 1: Normalized cross-wind integrated concentration $\frac{z_0 u_* \chi}{k_v Q}$ observed at distance $x = 100m$ from the source (height $h_s = 0.46m$) in Project Prairie Grass run 33.

$z[m]$	$\frac{z_0 u_* \chi}{k_v Q}$
17.5	2.4E-6
13.5	9.04E-6
10.5	2.20E-5
7.5	5.25E-5
4.5	1.08E-4
2.5	1.73E-4
1.5	2.02E-4
1.0	2.18E-4
0.5	2.30E-4

Table 2: Micrometeorological data for Project Prairie Grass run 33.

z [m]	U [m/s]	T [C]
16	10.63	-
8	-	27.88
4	8.48	28.16
2	7.56	28.73
1	6.90	29.16
0.5	5.80	29.64
0.25	4.84	30.07
0.12	-	30.61

Table 3: Normalised cross-wind-integrated deposition density D_0 [$\text{mg g}^{-1} \text{m}^{-1}$] versus down-wind distance for Suffield Trial C.

x [m]	27.4	45.7	73.2	100.6	128	201.2	402.3	804.6
D_0	0.003	0.011	0.96	5.76	5.92	2.83	0.2	0.074