1.020 Ecology II: Engineering for Sustainability
Spring 2008

1.020 Ecology II: Engineering for Sustainability

Lectures 08_12 & 08_13 Outline: Mass Transport, Diffusion, Air Quality

---

Motivation/Objective

Develop a model to examine spatial variations in the concentration of a chemical plume emitted from a line source (e.g. vehicles traveling on a road).

Approach

1. Generalize bulk system concept to provide for spatial variability. Define particles, identify source, emission rate, diffusion/dispersion process.
2. Construct rule for particle transport over time and space.
3. Relate chemical concentration to particle density.
4. Simulate transport in MATLAB and plot particles and concentrations.
5. Examine impact of emissions rate, mean velocity and dispersion coefficient.

Concepts and Definitions Needed:

Define point particles, each identified with a small fixed mass (*m*) of chemical and described by its changing spatial coordinates $\boldsymbol{x}_n^i = [x_{1,n}^i, x_{2,n}^i, x_{3,n}^i]$ (particle *i*, time step *n*)

Particles move with fluid that contains them (advection). Fluid velocity = $\boldsymbol{V}_n$

Particles move randomly within fluid due to molecular motion (diffusion) and small variations in fluid velocity not included in $\boldsymbol{V}_n$ (dispersion).

Random particle displacement $\boldsymbol{\omega}_n = [\omega_{1,n}^i, \omega_{2,n}^i, \omega_{3,n}^i]$

Mean($\omega_{j,n}^i$)=0, Variance$(\omega_{j,n}^i) = 1$, all $\omega_{j,n}^i$ uncorrelated

Particle transport eq. describes changes in particle coords. over time Δt:

$$x_{1,n+1}^i = x_{1,n}^i + V_{1,n}\Delta t + d_1\omega_{1,n}^i,\ x_{2,n+1}^i = x_{2,n}^i + V_{2,n}\Delta t + d_2\omega_{2,n}^i,\ x_{3,n+1}^i = x_{3,t}^i + V_{3,n}\Delta t + d_3\omega_{3,n}^i$$

$d_j = \sqrt{2D_j\Delta t}$ = Dispersion distance coord. *j*, (m), D_j = Dispersion coef. coord. *j* (m^2 sec^{-1})

Spatial characteristics of sources: point vs distributed sources
Temporal characteristics of sources: pulse vs continuous sources
Bulk properties of the plume can be described by its first and second spatial moments.
For point source, constant $\boldsymbol{V}_n$ (see attached supplement for 1 dimensional derivation):

First moment (plume center):

$$x_{1,n+1} = V_1 t, \quad x_{2,,n+1} = V_2 t, \quad x_{3,n+1} = V_3 t, \quad t = n\Delta t$$

Second moment (plume length/width/height):

$$S_{1,n} = \sigma_{\omega 1}^2 t = 2D_1 t, \quad S_{2,,n} = \sigma_{\omega 2}^2 t = 2D_2 t, \quad x_{3,n} = \sigma_{\omega 3}^2 t = 2D_3 t$$

Concentration computed from particles in specified volumes:

$$C_{np} \approx \frac{mN_{np}}{V_p}$$ gm m^{-3} = approximate chemical concentration in cell (pixel) *p* at time *t*

Modeling Example -- Air Quality

Note how particle spreading depends on dispersion coefficient and mean velocity. Plot spatial moments vs. time.

Supplement: Derivation of spatial moments for point source in one dimension (x_1):

Assumptions:

1) Point source at origin: $x_{1,0}^i = 0$

2) Mean($\omega_{1,n}^i$) = $\overline{\omega}_{1,n} = \frac{1}{P}\sum_{i=1}^{P}\omega_{1,n}^i = 0$

3) Uncorrelated $\omega_{1,n}^i$: Correlation = $\sum_{i\neq j \text{ or } m\neq n}(\omega_{1,m}^i - \overline{\omega}_{1,m})(\omega_{1,n}^j - \overline{\omega}_{1,n}) = 0$

4) Constant $\boldsymbol{V_{1n}} = V_1$ (same for every particle at all times

5) Variance($\omega_{1,n}^i$) = $\sigma_\omega^2 = \frac{1}{P}\sum_{i=1}^{P}[(\omega_{1,n}^i - \overline{\omega}_{1,n})^2 = \frac{1}{P}\sum_{i=1}^{P}[(\omega_{1,n}^i)^2 = 1$

If ω is distributed uniformly betweeen $-\omega_{\max}$ and $+\omega_{\max}$ **,** $\omega_{\max} = \sqrt{3}$ gives $\sigma_\omega^2 = 1$

First and second moments are derived from the solution to the particle transport equation:

$$x_{1,n+1}^i = x_{1,n}^i + V_1\Delta t + d_1\omega_{1,n}^i \quad \to \quad x_{1,n}^i = V_1 n\Delta t + d_1 \sum_{1\ m=1}^{n}\omega_{1,m}^i$$

First spatial moment, invoke Assumption 2 :

$$\overline{x}_{1,n} = \frac{1}{P}\sum_{i=1}^{P}x_{1,n}^i = V_1 n\Delta t + \frac{d_1}{P}\sum_{i=1}^{P}\left[\sum_{m=1}^{n}\omega_{1,m}^i\right] = V_1 n\Delta t + d_1\sum_{m=1}^{n}\left[\frac{1}{P}\sum_{i=1}^{P}\omega_{1,m}^i\right] = V_1 n\Delta t = V_1 t$$

Second spatial moment:

$$S_{1,n} = \frac{1}{P}\sum_{i=1}^{P}(x_{1,n}^i - \overline{x}_{1,n})^2 =$$

$$\frac{1}{P}\sum_{i=1}^{P}(V_1 n\Delta t + d_1\sum_{m=1}^{n}\omega_{1,m}^i - V_1 n\Delta t)^2 = \frac{d_1^2}{P}\sum_{i=1}^{P}\left[\sum_{m=1}^{n}\omega_{1,m}^i\right]^2 = \frac{d_1^2}{P}\sum_{i=1}^{P}\sum_{l=1}^{n}\sum_{m=1}^{n}\omega_{1,l}^i\omega_{1,m}^j$$

Separate terms of final summation into 2 parts, invoke Assumption 3:

$$S_{1,n} = \frac{d_1^2}{P}\sum_{i=1}^{P}\sum_{l=1}^{n}\sum_{m=1}^{n}\omega_{1,l}^i\omega_{1,m}^j = \frac{d_1^2}{P}\sum_{i=1}^{P}\sum_{m=1}^{n}\left[\omega_{1,m}^i\right]^2 + \frac{d_1^2}{P}\sum_{i=1}^{P}\left[\sum_{i\neq j \text{ or } m\neq n}\omega_{1,m}^i\omega_{1,n}^j\right] = \frac{nd_1^2}{P}\sum_{i=1}^{P}\left[\omega_{1,m}^i\right]^2 = 2nD_1\Delta t = 2D_1 t$$

Plume characteristic "size" is square root of second moment: $L_1 = \sqrt{S_{1,n}} = \sqrt{2D_1 t}$