I. K-Theory

1. Derivation of Equations

6 Jun 79

a. K-Theory (Gradient Diffusion)

What is concen. in BL as fnT of time & dist. ?

From our derivations earlier:

$$\frac{d\bar{c}}{dt} = -\frac{\partial \overline{w'c'}}{\partial z} + \dot{S} \qquad \text{II.E.4.2}$$

where $\dot{S}$ is a source or loss term due to chem. reactions, radioactive decay, etc.

This describes the avg. concentration in a turbulent BL.

But $\overline{w'c'}$ is unknown (Closure Problem)

so Make the simplifying assumption that the flux flows down gradient,

Ex/ Heat flows from hot to cold
Pollutants flow from high to low concentration.

This is a very poor assumption because we are modeling the turbulent properties of the flow analogous to the molecular properties of the fluid.

$$\text{Assume} \quad \boxed{\overline{w'c'} = -K \frac{\partial \bar{c}}{\partial z}} \qquad \text{IV.B.2.1}$$

where K = eddy diffusivity, (L^2/T)

This is known as $\boxed{\text{K - Theory}}$ - bad because often there is no vertical gradient within ML
or Gradient Transport

Thus

$$\frac{d\bar{c}}{dt} = \frac{\partial}{\partial z}\left(K \frac{\partial \bar{c}}{\partial z}\right) + \dot{S}$$

(see eq 9.6c of Dobbins)

If $K \neq fct(z)$ then

$$\boxed{\frac{d\bar{c}}{dt} = K \frac{\partial^2 c}{\partial z^2} + \dot{S}}$$ parabolic IV.B.2.2

b. Fickian Diffusion in 3-D

(const. K)

"del squared" or Laplacian

$$\boxed{\frac{d\bar{c}}{dt} = K \nabla^2 \bar{c} + \dot{S}}$$

Diffusion Eq.

Heat Cond. Eq. IV.B.2.3

Same as eq 9.7 of Dobbins

Cartesian Coordinates: with no $\dot{S}$:

$$\boxed{\frac{d\bar{c}}{dt} = K \left[\frac{\partial^2 \bar{c}}{\partial x^2} + \frac{\partial^2 \bar{c}}{\partial y^2} + \frac{\partial^2 \bar{c}}{\partial z^2} \right]}$$ IV.B.2.4

Small-eddy assumption for K-theory to work.

∴ K-theory fails during the initial spread of the puff when the eddies are larger than the puff.

a. Instantaneous ~~Puff Diffusion~~ Point Source (Puff)

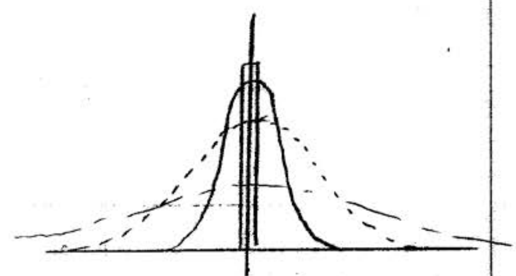
1) Diffusion of 1-D Puff

Look at 1-D problem (c = mass / dist)

$$\frac{d\bar{c}}{dt} = K \frac{\partial^2 \bar{c}}{\partial x^2} \quad \text{parabolic}$$

Neglect advection

$$\frac{\partial \bar{c}}{\partial t} = K \frac{\partial^2 \bar{c}}{\partial x^2}$$



Special Solution;

Problem: Find concentration as a fnt of time & dist. as diffused from an instantaneous point source of strengt Q (Q = total grams)

Like a bomb exploding, or puff of smoke.

IC: $\bar{c} = 0$ @ $t = 0$ all x except $x=0$

B.C.; 1) $\int_{-\infty}^{\infty} \bar{c}\, dx = Q$ conservation of pollutants

B.C. 2) $\bar{c} \to 0$ @ $x \to \infty$

See solution in Dobbins section 9.2.1

Q = mass
c = mass/length

Solution

$$\boxed{\bar{c} = \frac{Q}{(4\pi K t)^{1/2}} e^{-\left(\frac{x^2}{4Kt}\right)}} \quad \text{IV.B.3.1}$$

Let $\boxed{\sigma_t = \sqrt{2Kt}}$

But $\sigma(t) = \sigma_v \sqrt{2T_L t}$ from Taylor at large t

$\therefore \boxed{K = \sigma_v^2 T_L}$

$$\bar{c} = \frac{Q}{\sqrt{2\pi}\,\sigma_t} e^{-\frac{x^2}{2\sigma_t^2}}$$

Answer: Proof that Gaussian is solution to Diffusion Eq.

$$c = \frac{Q}{(4\pi K)^{1/2}\, t^{1/2}} \exp\left(\frac{-x^2}{4Kt}\right)$$

$$\frac{\partial c}{\partial t} = \frac{Q}{(4\pi K)^{1/2}}\left[-\frac{1}{2}t^{-3/2}\cdot \exp\left(\frac{-x^2}{4Kt}\right) + t^{-1/2}\exp\left(\frac{-x^2}{4Kt}\right)\cdot \frac{x^2}{4K}t^{-2}\right]$$

$$= \left\{\frac{Q}{(4\pi K t)^{1/2}} \exp\left(\frac{-x^2}{4Kt}\right)\cdot \frac{1}{t}\left[\frac{x^2}{4Kt} - \frac{1}{2}\right]\right\}$$

$$\frac{\partial c}{\partial x} = \frac{-Q}{(4\pi K t)^{1/2}} \exp\left(\frac{-x^2}{4Kt}\right)\cdot \frac{2x}{4Kt}$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{-Q}{(4\pi K t)^{1/2}}\left[\exp\left(\frac{-x^2}{4Kt}\right)\cdot\frac{1}{2Kt} - \exp\left(\frac{-x^2}{4Kt}\right)\left(\frac{x}{2Kt}\right)^2\right]$$

$$= \left\{\frac{Q}{(4\pi K t)^{1/2}} \exp\left(\frac{-x^2}{4Kt}\right)\cdot \frac{1}{t}\left[\frac{x^2}{4Kt} - \frac{1}{2}\right]\right\}\frac{1}{K}$$

$$\therefore \frac{\partial c}{\partial t} = K\frac{\partial^2 c}{\partial x^2} \quad \checkmark$$

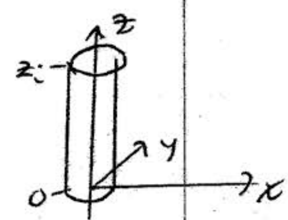
B. From Gaussian Puff to Gaussian Plume

2) Similarly, for a 2-D puff:

$$\boxed{c = \frac{Q}{4\pi K t} e^{-\left(\frac{x^2+y^2}{4Kt}\right)}} \quad \text{IV.B.3.2}$$

Q = mass
c = mass/area
$K_x = K_y$

Special case: cylindrical puff trapped within ML of height z_i



$$\boxed{c = \frac{Q/z_i}{4\pi K t} e^{-\left(\frac{x^2+y^2}{4Kt}\right)}} \quad \text{IV.B.3.3}$$

Q = mass
c = mass/vol

3) Similarly, for a 3-D puff:

$$\boxed{c = \frac{Q}{(4\pi K t)^{3/2}} e^{-\left(\frac{r^2}{4Kt}\right)}} \quad \text{IV.B.3.4}$$

Eq 9.17 of Dobbins

Q = mass
c = mass/vol
$r^2 = x^2+y^2+z^2$
$K_x = K_y = K_z$
(isotropic)

Special case: non-isotropic 3-D puff

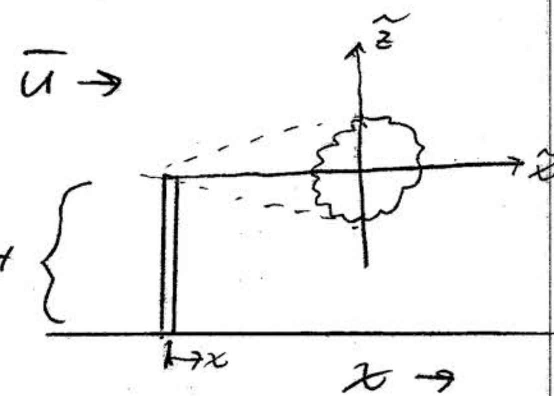
$K_x \neq K_y \neq K_z$

$$\boxed{c = \frac{Q}{\left[(4\pi t)^3 K_x K_y K_z\right]^{1/2}} \exp\left[-\frac{1}{4t}\left(\frac{x^2}{K_x} + \frac{y^2}{K_y} + \frac{z^2}{K_z}\right)\right]}$$

IV. B. 3. 5

4) 3-D Puff emitted into mean Wind from stack top

In a non-accelerating coordinate system moving with the puff, emitted at height H



Same as before:

$$c = \frac{Q}{\left[(4\pi t)^3 K_x K_y K_z\right]^{1/2}} \exp\left[-\frac{1}{4t}\left(\frac{\tilde{x}^2}{K_x} + \frac{y^2}{K_y} + \frac{\tilde{z}^2}{K_z}\right)\right]$$

But $\tilde{z} = z - H$

$\tilde{x} = x - \bar{u}t$ using Taylor's Hypothesis

Thus, relative the a point on the ground (below source)

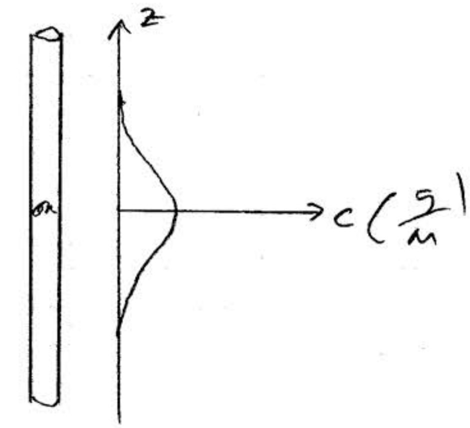
$$\boxed{c = \frac{Q}{\left[(4\pi t)^3 K_x K_y K_z\right]^{1/2}} \exp\left[-\frac{1}{4t}\left(\frac{(x-\bar{u}t)^2}{K_x} + \frac{y^2}{K_y} + \frac{(z-H)^2}{K_z}\right)\right]}$$

IV.B.36

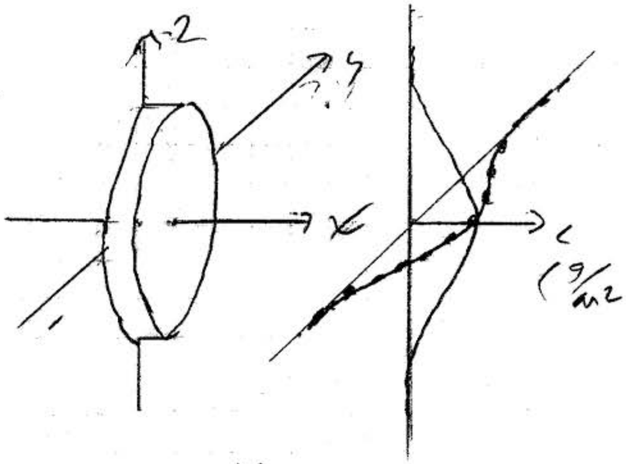
where we choose the x-direction parallel to the mean wind for simplicity.

Summary so far

1-D

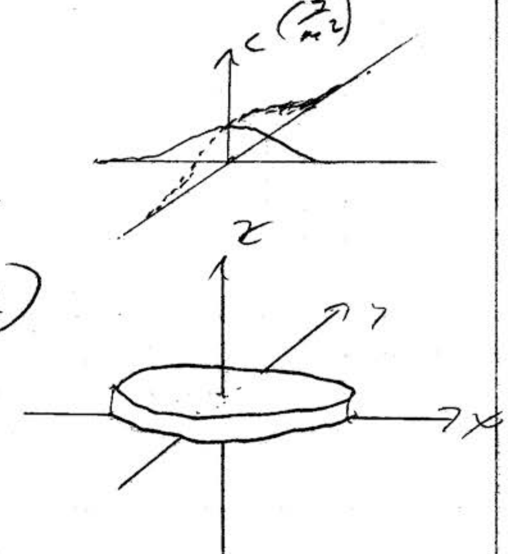


2-D disk



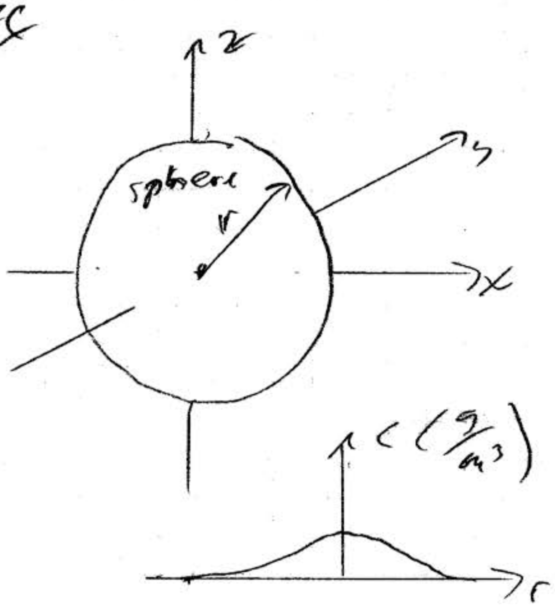
⇒ used for Gaussian plume ⇒ AERMOD

OR



⇒ used for hybrid puff/particle mode in Hysplit

3-D puff



Analogous to air parcel where all smoke has same mean advection as puff expands

⇒ used in puff mode of Hysplit