Chapter 2 Fickian Diffusion

◆ fluid at rest – diffusion

moving fluid – diffusion + advection

- molecular diffusion - only important in microscopic scale; not much important in environmental problems

◆ turbulent diffusion and dispersion process

- analogous to molecular diffusion

2.1 Fick's Law of Diffusion

2.1.1 Diffusion Equation

◆ Fourier's law of heat flow (1822)

- time rate of heat per unit area in a given direction is proportional to the temperature gradient in direction.

Fourier	Fick
heat	mass
temp.	conc.

1. Fick's law (1855)

- flux of solute mass, that is, the mass of a solute crossing a unit area per unit time in a given direction, is proportional to the gradient of solute concentration in that direction.

$$q \propto \frac{\partial C}{\partial x}$$

$$q = -D\frac{\partial C}{\partial x} \tag{2.1}$$

q = solute mass flux

C = mass concentration of dispersing solute

D = coefficient of proportionality

= diffusion coefficient (m^2/s), molecular diffusivity

- Minus sign indicates transport is from high to low concentrations

☞ Fick's law in 3D

C = concentration ⇒ scalar

$$\vec{q} = -D\nabla C \tag{2.1a}$$

$$\vec{q} = \vec{i}q_x + \vec{j}q_y + \vec{k}q_z \qquad \rightarrow \text{vector}$$

$$\nabla = \vec{i}\frac{\partial}{\partial x} + \vec{j}\frac{\partial}{\partial y} + \vec{k}\frac{\partial}{\partial z}$$

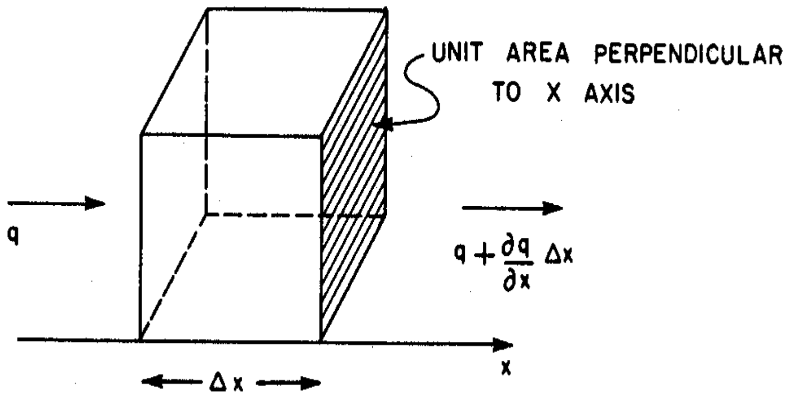
$$\nabla C = \left(\vec{i}\frac{\partial}{\partial x} + \vec{j}\frac{\partial}{\partial y} + \vec{k}\frac{\partial}{\partial z}\right)C$$

$$= \vec{i}\frac{\partial C}{\partial x} + \vec{j}\frac{\partial C}{\partial y} + \vec{k}\frac{\partial C}{\partial z} \qquad \rightarrow \text{vector}$$

● gradient of scalar → vector

2. Conservation of Mass

1-D transport process



i) time rate of change of mass in the volume $= \dfrac{\partial C}{\partial t}\,(\Delta x \cdot 1)$

ii) net change of mass in the volume $= \{(flux)_{in} - (flux)_{out}\} \times unit\ \ area$

$$= q - \left(q + \frac{\partial q}{\partial x}\Delta x \right)$$

$$= -\frac{\partial q}{\partial x}\Delta x$$

$$\therefore\ \frac{\partial C}{\partial t}\,\Delta x = -\frac{\partial q}{\partial x}\Delta x$$

$$\frac{\partial C}{\partial t} = -\frac{\partial q}{\partial x} \qquad (2.2)$$

3. Diffusion Equation

Combine Eq.(2.1) and (2.2)

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}\left(-D\frac{\partial C}{\partial x}\right)$$

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$ ⇒ Diffusion Equation (Heat Equation)

Diffusion Equation = Fick's law of diffusion + Conservation of mass

Differentiate Eq. (2.2) w.r.t. x

$$\frac{\partial}{\partial x}\left(\frac{\partial C}{\partial t}\right) = -\frac{\partial^2 q}{\partial x^2}$$

$$LHS = \frac{\partial}{\partial t}\left(\frac{\partial C}{\partial x}\right) = \frac{\partial}{\partial t}\left(-\frac{q}{D}\right) = -\frac{1}{D}\frac{\partial q}{\partial t}$$

$$\therefore \ -\frac{1}{D}\frac{\partial q}{\partial t} = -\frac{\partial^2 q}{\partial x^2}$$

☞ Conservation of mass in 3D

$$\frac{\partial C}{\partial t} = -\nabla \cdot \vec{q} = -\left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right)$$

$$\frac{\partial C}{\partial t} + \nabla \cdot \vec{q} = 0 \qquad \text{(i)}$$

Then consider $\vec{q}$ by various transport mechanisms

- molecular diffusion (Fickian diffusion) $\vec{q} = -D\nabla C$
- advection by ambient current $\vec{q} = C\vec{u}$

$$\therefore \ \vec{q} = C\vec{u} - D\nabla C \qquad \text{(ii)}$$

Substitute (ii) into (i)

$$\frac{\partial C}{\partial t} + \nabla\cdot\left(C\vec{u} - D\nabla C\right) = 0$$

$$\frac{\partial C}{\partial t} + \nabla\cdot\left(C\vec{u}\right) = D\nabla^2 C \qquad \text{(iii)}$$

$$\nabla\cdot\left(C\vec{u}\right) = \left(\nabla C\right)\vec{u} + C\left(\nabla\cdot\vec{u}\right)$$

$$\nabla\cdot\vec{u} = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} = 0 \quad \leftarrow \text{ Continuity}$$

$$\therefore\ \nabla(C\vec{u}) = \nabla C\vec{u}$$

$$= \left(\frac{\partial C}{\partial x}\vec{i} + \frac{\partial C}{\partial y}\vec{j} + \frac{\partial C}{\partial z}\vec{k}\right)\cdot\left(u_x\vec{i} + u_y\vec{j} + u_z\vec{k}\right)$$

$$= u_x\frac{\partial C}{\partial x} + u_y\frac{\partial C}{\partial y} + u_z\frac{\partial C}{\partial z}$$

$$(\because\ \vec{i}\cdot\vec{i} = \vec{j}\cdot\vec{j} = \vec{k}\cdot\vec{k} = |i||i|\cos 0° = 1$$

$$\vec{i}\cdot\vec{j} = \vec{j}\cdot\vec{k} = \vec{k}\cdot\vec{i} = 0)$$

Thus, (iii) becomes

$$\frac{\partial C}{\partial t} + \nabla C\cdot\vec{u} = D\nabla^2 C$$

$$\frac{\partial C}{\partial t} + u_x\frac{\partial C}{\partial x} + u_y\frac{\partial C}{\partial y} + u_z\frac{\partial C}{\partial z} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right)$$

$\rightarrow$ 3D advection-diffusion equation

For molecular diffusion only

$$\frac{\partial C}{\partial t} = DV^2 C$$

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right)$$

- linear, 2nd order PDE

◆ Vector notation of conservation of mass

fixed volume V with surface area S

total mass in the volume = $\int_V C(\vec{x},t)dV$

mass flux = $\vec{q}(\vec{x},t)$

Conservation of mass

$$\frac{\partial}{\partial t}\int_V C(\vec{x},t)dV + \int_s \vec{q}(\vec{x},t)\cdot\vec{n}dS = 0$$

$\vec{n}$ = unit vector normal to surface element dS

Green's theorem

$$\int_S \vec{q}\cdot\vec{n}dS = \int_v \nabla\cdot\vec{q}dV$$

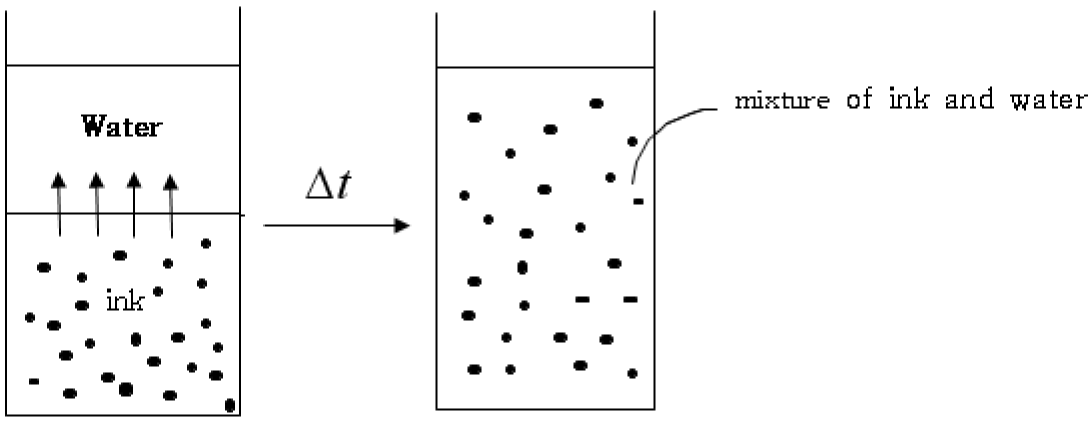
$$\int_V \left(\frac{\partial C}{\partial t} + \nabla\cdot\vec{q}\right)dV = 0$$

$$\frac{\partial C}{\partial t} + \nabla\cdot\vec{q} = 0$$

2.1.2 Diffusion Process

diffusion = process by which matter is transported from one part of a system to another as a result of random molecular motions

1. Random Walk Model



(i) Watch individual molecules of ink

→ Motion of each molecule is a random one.

→ Each molecule of ink behaves independently of the others.

→ Each molecule of ink is constantly undergoing collision with other.

→ As a result of collisions, if moves sometimes towards a region of higher, sometimes of lower concentrations, having no preferred direction of motion.

→ The motion of a single molecule is described in terms of random walk model

→ It is possible to calculate the mean-square distance travelled in given interval of time. It is not possible to say in what direction a given molecule will move in that time.

(ii) Transfer of ink molecules from the region of higher to that of lower concentration is observed.

(iii) On the average some fraction of the molecules in the lower element of volume will cross the interface from below, and the same fraction of molecule in the upper element will cross the interface from above in a given time.

(iv) Thus, simply because there are more ink molecules in the lower element than in the upper one, there is a net transfer from the lower to the upper side of the section as a result of random molecular motions.

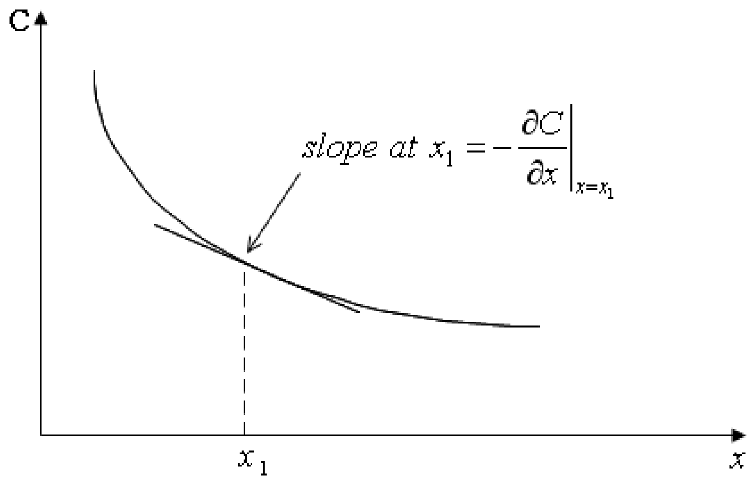
2. Molecular Diffusion

(i) Fick's First Law:

Rate of mass transport of material or flux through the liquid, by molecula diffusion is proportional to the concentration gradient of the material in the liquid.

Diffusive mass flux, $q = -D\dfrac{\partial C}{\partial x}$ (1)

(negative sign arises because diffusion occurs in the direct opposite to that of increasing concentration)



(ii) Fick's Second Law:

Conservation of mass + Fick's First Law $\rightarrow \dfrac{\partial C}{\partial t} = D\dfrac{\partial^2 C}{\partial x^2}$

●Assumption for Fick's Law

Fick's First Law is consistent only for an isotropic medium, whose structure and diffusion properties in the neighbourhood of any point are the same relative to all directions.

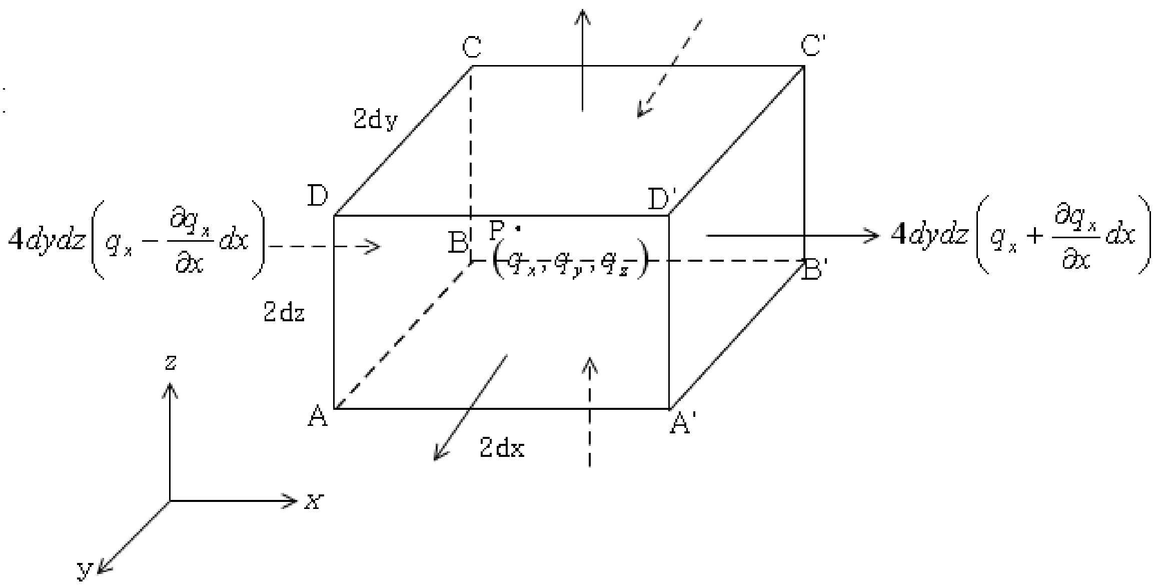
In molecular diffusion: $D_x = D_y = D_z = D$

In turbulent diffusion: $\varepsilon_x, \varepsilon_y, \varepsilon_z$

In shear flow dispersion: K_x, K_y, K_z

[Cf] anisotropic medium – diffusion properties depend on the direction in which they are measured

3.



(i) Rate at which diffusing substance enters the element through the face ABCD in the x direction

$$Influx = 4dydz\left(q_x - \frac{\partial q_x}{\partial x}dx\right)$$

In which $q_x =$ rate of transfer through unit area of the corresponding plane through P

(ii) Rate of loss of diffusing substance through the face A'B'C'D'

$$Outflux = 4dydz\left(q_x + \frac{\partial q_x}{\partial x}dx\right)$$

(iii) Contribution to the rate of increase of diffusing substance in the element from these two faces

$$Netflux = 4dydz\left(q_x - \frac{\partial q_x}{\partial x}dx\right) - 4dydz\left(q_x + \frac{\partial q_x}{\partial x}dx\right) = -8dxdydz\frac{\partial q_x}{\partial x}$$

(iv) Similarly from the other faces we obtain

$-8dxdydz\dfrac{\partial q_y}{\partial y}$ and

$-8dxdydz\dfrac{\partial q_z}{\partial z}$

(v) Rate at which the amount of diffusing substance in the element increases

$$\frac{\partial}{\partial t}(mass) = \frac{\partial}{\partial t}(volume \times conc.)$$

$$= 8dxdydz\frac{\partial c}{\partial t}$$

(vi) Combine (iii), (iv), and (v)

$$8dxdydz\frac{\partial c}{\partial t} = -8dxdydz\left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right)$$

$$\frac{\partial c}{\partial t} + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} = 0 \qquad (2)$$

(vii) Substitute Fick's law into Eq.(2)

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}\left(-D\frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial y}\left(-D\frac{\partial C}{\partial y}\right) - \frac{\partial}{\partial z}\left(-D\frac{\partial C}{\partial z}\right) = \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D\frac{\partial C}{\partial z}\right)$$

Remember D is isotropic for molecular diffusion.

For homogeneous medium; $D \neq f_n(x, y, z)$

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right)$$

For 1-dimensional system

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$ → Fick's Second Law of Diffusion

◈ Vector Operations

Vectors = magnitude + direction

~ velocity, force

Scalar = magnitude

~ pressure, density, temperature, concentration

Vector $\overline{F}$

$$\overline{F} = F_x \overline{e_x} + F_y \overline{e_y} + F_z \overline{e_z}$$

$\overline{e_x}, \overline{e_y}, \overline{e_z} =$ unit vectors

$F_x, F_y, F_z =$ projections of the magnitude of $\overline{F}$ on the *x, y, z* axes

(1) Magnitude of $\overline{F}$

$$F = \left|\overline{F}\right| = \left(F_x^2 + F_y^2 + F_z^2\right)^{1/2}$$

(2) Dot product = Scalar product

$$S = \overline{F} \cdot \overline{G} = \left|\overline{F}\right|\left|\overline{G}\right| \cos\phi$$

(3) Vector product = Cross product

$$\overline{V} = \overline{F} \times \overline{G} \quad \rightarrow \text{ vector}$$

$$magnitude \;\; of \;\; \overline{V} = \left|\overline{V}\right| = \left|\overline{F}\right|\left|\overline{G}\right| \sin\phi$$

$direction \;\; of \;\; \overline{V} =$ perpendicular to the plane of $\overline{F}$ and $\overline{G}$

→ right hand rule

(4) Derivatives of vectors

$$\frac{\partial \overline{F}}{\partial s} = \frac{\partial F_x}{\partial s}\overline{e_x} + \frac{\partial F_y}{\partial s}\overline{e_y} + \frac{\partial F_z}{\partial s}\overline{e_z}$$

(5) Gradient of F (Scalar) $\rightarrow$ vector

$$grad\ \ F = \nabla F = \frac{\partial F}{\partial x}\overline{e_x} + \frac{\partial F}{\partial y}\overline{e_y} + \frac{\partial F}{\partial y}\overline{e_z} \qquad \rightarrow \text{ vector}$$

$[\nabla]=$ pronounced as ‘del’ or ‘nabla’

$$\nabla \equiv \overline{e}_i \frac{\partial}{\partial x_i}$$

[Re] grad(scalar) $\rightarrow$ vector grad(F+G)=gradF+grad G

grad(vector) $\rightarrow$ tensor grad CF=c grad F

(6) Divergence of $\overline{F}$ (vector) $\rightarrow$ scalar

$$div\overline{F} = \nabla \cdot \overline{F} = \left(\frac{\partial}{\partial x}\overline{e_x} + \frac{\partial}{\partial y}\overline{e_y} + \frac{\partial}{\partial z}\overline{e_z}\right)\cdot \overline{F}$$

$$= \left(\frac{\partial}{\partial x}\overline{e_x} + \frac{\partial}{\partial y}\overline{e_y} + \frac{\partial}{\partial z}\overline{e_z}\right)\cdot \left(F_x\overline{e_x} + F_y\overline{e_y} + F_z\overline{e_z}\right)$$

$$= \left|\frac{\partial}{\partial x}\overline{e_x}\right|\left|F_x\overline{e_x}\right|\cos 0 + \frac{\partial F_y}{\partial x}\overline{e_x e_y}\cos 90^\circ + \frac{\partial F_z}{\partial x}\overline{e_x e_z}\cos 90^\circ$$

$$+\left|\frac{\partial F}{\partial y}\overline{e_y}\right|\left|F_y e_y\right|\cos 0+\left|\frac{\partial}{\partial z}\overline{e_z}\right|\left|F_z e_z\right|\cos 0$$

$$=\frac{\partial F_x}{\partial x}+\frac{\partial F_y}{\partial y}+\frac{\partial F_z}{\partial z} \quad \rightarrow \text{ scalar}$$

(7) $$Curl\ \overline{V}=\nabla\times\overline{V}=\begin{vmatrix} \bar{i} & \bar{j} & \bar{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial x} & \frac{\partial}{\partial x} \\ v_1 & v_2 & v_3 \end{vmatrix}$$

(8) $$div\left(grad\ F\right)=\nabla\cdot\nabla F=\nabla^2 F\equiv Laplacian\ of\ F$$

$$=\frac{\partial^2 F_x}{\partial x^2}+\frac{\partial^2 F_y}{\partial y^2}+\frac{\partial^2 F_z}{\partial z^2}$$

[Pf]

$$div\left(grad\ F\right)=div\left(\frac{\partial F}{\partial x}\overline{e_x}+\frac{\partial F}{\partial y}\overline{e_y}+\frac{\partial F}{\partial z}\overline{e_z}\right)$$

$$=\frac{\partial}{\partial x}\left(\frac{\partial F}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{\partial F}{\partial y}\right)+\frac{\partial}{\partial z}\left(\frac{\partial F}{\partial z}\right)$$

$$=\frac{\partial^2 F_x}{\partial x^2}+\frac{\partial^2 F_y}{\partial y^2}+\frac{\partial^2 F_z}{\partial z^2}$$

$$\nabla\cdot\nabla=\left(\bar{i}\frac{\partial}{\partial x}+\bar{j}\frac{\partial}{\partial y}+\bar{k}\frac{\partial}{\partial z}\right)\left(\bar{i}\frac{\partial}{\partial x}+\bar{j}\frac{\partial}{\partial y}+\bar{k}\frac{\partial}{\partial z}\right)$$

$$=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}=\nabla^2$$

2.1.3 Analytical Solution of Diffusion Equation

● Consider diffusion of an initial slug of mass M introduced instantaneously at time zero at the x origin

[Cf] Continuous input → initial concentration specified as a function of time

i) Governing equation:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \tag{2.3}$$

ii) Initial & Boundary conditions:

-Spreading of an initial slug of mass M introduced instantaneously at time zero at the x origin

$$C(x=0, t=0) = M\delta(x)$$

$$C(x=\pm\infty, t) = 0$$

iii) Solution by dimensional analysis

$$C(x,t) = f(M, x, t, D)$$

$$C = \frac{M}{\sqrt{4\pi Dt}} f\left(\frac{x}{\sqrt{4Dt}}\right) \tag{2.4}$$

set $$\eta = \frac{x}{\sqrt{4Dt}} \tag{2.5}$$

Substitute Eq. (2.4) and Eq. (2.5) into Eq. (2.3)

Eq. (2.4):

$$C=\frac{M}{\sqrt{4\pi Dt}}f\left(\frac{x}{\sqrt{4Dt}}\right)=\frac{M}{\sqrt{4\pi Dt}}f\left(\eta\right)=C_p f\left(\eta\right)$$

$$\eta=\frac{x}{\sqrt{4Dt}}\rightarrow\frac{\partial\eta}{\partial t}=-\frac{\eta}{2t},\quad\frac{\partial\eta}{\partial x}=\frac{1}{\sqrt{4Dt}}$$

$$\frac{\partial C}{\partial t}=\frac{M}{\sqrt{4\pi Dt}}\frac{\partial f}{\partial t}+\left(\frac{M}{\sqrt{4\pi D}}\frac{1}{\sqrt{t}}\right)'f=C_p\frac{\partial f}{\partial\eta}\frac{\partial\eta}{\partial t}+C_p\left(-\frac{1}{2t}\right)f$$

$$=C_p\frac{\partial f}{\partial\eta}\left(-\frac{\eta}{2t}\right)+C_p\left(-\frac{1}{2t}\right)f \tag{a}$$

$$\frac{\partial C}{\partial x}=C_p\frac{\partial f}{\partial x}=C_p\frac{\partial f}{\partial\eta}\frac{\partial\eta}{\partial x}=C_p\frac{\partial f}{\partial\eta}\frac{1}{\sqrt{4Dt}}$$

$$\frac{\partial^2 C}{\partial x^2}=C_p\frac{\partial^2 f}{\partial\eta^2}\frac{1}{4Dt} \tag{b}$$

Substitute (a) and (b) into Eq. (2.3)

$$C_p\frac{\partial f}{\partial\eta}\left(-\frac{\eta}{2t}\right)+C_p\left(-\frac{1}{2t}\right)f=DC_p\frac{\partial^2 f}{\partial\eta^2}\frac{1}{4Dt}$$

$$2\eta\frac{\partial f}{\partial\eta}+2f+\frac{\partial^2 f}{\partial\eta^2}=0$$

$$\frac{\partial}{\partial\eta}\left(2\eta f\right)+\frac{\partial^2 f}{\partial\eta^2}=0$$

Integrate once w.r.t. η

$$2\eta f+\frac{df}{d\eta}=0 \tag{2.6}$$

Separation of variables

$$\frac{df}{f} = -2\eta d\eta$$

Integrate both sides

$$\ln f = -\eta^2 + C$$

$$f = e^{-\eta^2 + C} = C_0 \, e^{-\eta^2} \tag{2.7}$$

Total mass, M

$$\int_{-\infty}^{\infty} C dx = M \tag{2.8}$$

Substituting Eq.(2.4) and Eq.(2.7) into Eq.(2.8) yields $C_0 = 1$

Then, (2.4) becomes

$$C(x,t) = \frac{M}{\sqrt{4\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right) \tag{2.9}$$

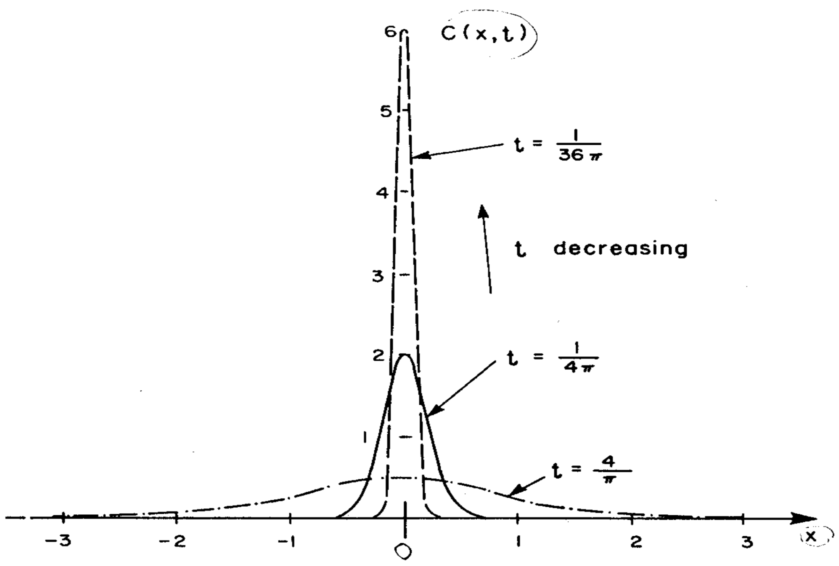


Figure 2.3 The reduction of the Gaussian distribution [Eq. (2.14)] to a "spike" as t decreases. The illustration uses the values $M = 1$, $D = \frac{1}{4}$.

[Re] Analytical Solution by Separation of Variables

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \tag{2.10}$$

$$C(x,t=0) = M\delta(x) \tag{2.11a}$$

$$C(x=\pm\infty, t) = 0 \tag{2.11b}$$

$$M = \lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon} f(x)dx \tag{2.11c}$$

Separation of Variables

$$C(x,t) = F(x)G(t) \tag{2.12}$$

Substitute Eq.(2.12) into Eq.(2.10)

$$F(x)\frac{\partial G}{\partial t} = DG(t)\frac{\partial^2 F}{\partial x^2}$$

$$FG' = DGF''$$

$$\frac{1}{D}\frac{G'}{G} = \frac{F''}{F} = k$$

where　k = const. $\neq f_n(x \;\; or \;\; t)$

$i)\;\; k > 0$

$$k = \omega^2$$

$$\frac{1}{D}\frac{G'}{G} = \frac{F''}{F} = \omega^2$$

$$\rightarrow F'' - \omega^2 F = 0 \tag{2.13a}$$

$$G' - D\omega^2 G = 0 \qquad (2.13b)$$

Solution of (2.13a) is $F = C_1 e^{wx} + C_2 e^{-wx}$ (a)

Substituting (2.11b) into (a) yields $C_1 = 0$

Then

$$F = C_2 e^{-wx}$$

Solution of (2.13b) is $G = C_3 e^{\sqrt{D\omega t}}$

Substituting B.C. (2.11b) gives $C_3 = 0$

This means that C = F·G = 0 at all points, which is not true.

$\rightarrow$ $k \le 0$

ii) $k = 0$

$$F'' = 0 \rightarrow F = ax + b \rightarrow a = 0 \quad \therefore F = b$$

$$G' = 0 \rightarrow G = k$$

$$\therefore C = FG = bk = \text{ const.} \rightarrow \text{ not true}$$

$\rightarrow$ $k < 0$

iii) $k < 0$

$$k = -p^2$$

$$\frac{1}{D}\frac{G'}{G} = \frac{F''}{F} = -p^2$$

$$F' + p^2 F = 0 \qquad (2.13c)$$

$$G' + Dp^2 G = 0 \qquad (2.13d)$$

Assume solution of Eq. (2.13c) as $F = e^{\lambda x}$

Substitute this into Eq. (2.13c) and derive characteristic equation (2.14)

$$\lambda^2 + p^2 = 0$$

$$\therefore\ \lambda = \pm pi$$

$$\therefore\ F = C_1 e^{pxi} + C_2 e^{-pxi}$$

$$= C_1(\cos px + i\sin px) + C_2(\cos px - i\sin px)$$

$$= A\cos px + B\sin px$$

(2.14)

Assume solution of Eq. (2.13d) as and $G = e^{\lambda t}$

Substitute this into Eq. (2.13d) and derive characteristic equation

$$\lambda + Dp^2 = 0$$

$$\therefore \lambda = -Dp^2$$

$$\therefore G = C_1 e^{-Dp^2 t} \tag{2.15}$$

Substitute Eq. (2.14) and (2.15) into Eq. (2.12)

$$C(x,t) = F(x)G(t) = (A\cos px + B\sin px)e^{-Dp^2 t} \tag{2.16}$$

Use Fourier integral for nonperiodic function.

Assume $A, B = f_n(p)$

$$C(x,t;p) = \{A(p)\cos px + B(p)\sin px\}\left(-Dp^2t\right) \tag{2.17}$$

$$C(x,t) = \int_0^\infty C(x,t;p)\,dp$$

$$= \int_0^\infty \left\{A(p)\cos px + B(p)\sin px\right\}\exp\left(-Dp^2t\right)dp \tag{2.18}$$

Since Eq. (2.10) is linear and homogeneous, integral of Eq. (2.18) exists

I.C. Eq. (2.11a) and Eq. (2.11c)

$$C(x,t=0) = \int_0^\infty \left\{A(p)\cos px + B(p)\sin px\right\}dp = f(x)$$

f(x)= Fourier integral

$$\equiv \frac{1}{\pi}\int_0^\infty \left\{\cos px \int_0^\infty f(v)\cos(pv)\,dv + \sin px \int_{-\infty}^\infty f(v)\sin(pv)\,dv\right\}dp$$

$$A(p) = \frac{1}{\pi}\int_{-\infty}^\infty f(v)\cos(pv)\,dv$$

$$B(p) = \frac{1}{\pi}\int_{-\infty}^\infty f(v)\sin(pv)\,dv$$

Use Trigonometric rule

$$C(x,0) = \frac{1}{\pi}\int_0^\infty \left\{\int_{-\infty}^\infty f(v)\cos px \sin pv dv + \int_{-\infty}^\infty f(v)\sin px \sin pv dv\right\}dp$$

$$= \frac{1}{\pi}\int_0^\infty \left\{\int_{-\infty}^\infty f(v)\cos(px - pv)\,dv\right\}dp \tag{2.19}$$

Substitute Eq. (2.19) into Eq. (2.18)

$$C(x,t) = \frac{1}{\pi}\int_0^\infty \left\{\int_{-\infty}^\infty f(v)\cos(px - pv)\exp(-Dp^2t)\,dv\right\}dp$$

Switch order of integral

$$C(x,t) = \frac{1}{\pi}\int_0^\infty f(v)\underbrace{\left\{\int_{-\infty}^\infty \exp(-Dp^2t)\cos(px-pv)dv\right\}}_{(e)}dp \qquad (2.20)$$

Let (e) = $\int_0^\infty \exp(-Dp^2t)\cos(px-pv)dp$

Use residue theorem to get integral of (e)

$$\int_0^\infty e^{-s^2}\cos 2bsds = \frac{\sqrt{\pi y}}{2}e^{-b^2} \qquad (2.21)$$

Set $\quad s = p\sqrt{Dt},\ b = \dfrac{x-v}{2\sqrt{Dt}}$

Then $\ 2bs = (x-v)p,\ ds = \sqrt{Dt}dp$

$\therefore$ (e) becomes

$$\int_0^\infty \exp(-Dp^2t)\cos(px-pv)dp = \frac{\sqrt{\pi}}{2\sqrt{Dt}}\exp\left\{-\frac{(x-v)^2}{4Dt}\right\} \qquad (2.22)$$

Substitute Eq. (2.22) into Eq. (2.20)

$$C(x,t) = \frac{1}{\sqrt{4\pi Dt}}\int_{-\infty}^\infty f(v)\exp\left\{-\frac{(x-v)^2}{4Dt}\right\}dv$$

$$= \frac{1}{\sqrt{4\pi Dt}}\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon} f(v)\exp\left\{-\frac{(x-v)^2}{4Dt}\right\}dv$$

$$= \frac{M}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right) \qquad (2.23)$$

2.2 The Random Walk and Molecular Diffusion

2.2.1 The Random Walk

i) Think motion of a tracer molecule consists of a series of random steps

→ whether the step is forward or backward is entirely random

● Central limit theorem: in the limit of many steps probability of the particle being $m\Delta x$ between and $(m+1)\Delta x$ → normal distribution

mean: zero

variance : $\sigma^2 = \dfrac{t(\Delta x)^2}{\Delta t}$

normal distribution: $P(x,t)dx = \dfrac{1}{\sigma\sqrt{2\pi}} \exp\left(-\dfrac{x^2}{2\sigma^2}\right)$

$$= \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) dx \tag{2.15}$$

where $\sigma^2 = \dfrac{t(\Delta x)^2}{\Delta t} = 2Dt$

ii)Now think whole group of particles

$$C(x,t) = \iint p(x,t)dxdn$$

$$C(x,t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$$

→ same as Eq. (2.14)

→ random walk process leads to the same result that an slug of tracer diffuses according to the diffusion equation, Eq. (2.4)

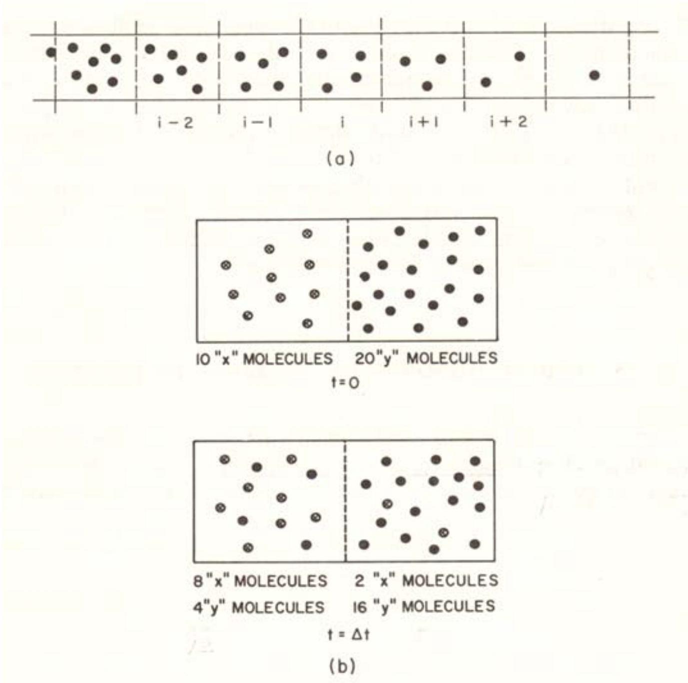
2.2.2 The Gradient-Flux Relationship

- Think random motion of large number of molecules at the same time.

→ probability of a molecule passing through the surface is proportional to the average number of molecule near the surface

- differences in mean concentration are, on the average, always reduced, never increased.

◆ flux of material across the bounding surface



$q_l = kM_l$ - flux of material from left to right

$q_r = kM_r$ - flux of material from right to left

where k = transfer probability [1/t]

M_l = mass of the tracer in the left-hand box

M_r = mass of the tracer in the right-hand box

○ q = net flux = net rate at which tracer mass is exchange per unit time and per unit area

$$q = k(M_l - M_r) \qquad \text{(a)}$$

Define

$$C_l = \frac{\bar{M}_l}{\Delta x} \qquad \text{(b)}$$

$$C_r = \frac{\bar{M}_r}{\Delta x} \qquad \text{(c)}$$

$\bar{M}_l$ = average masses in the left-hand box

$\bar{M}_r$ = average masses in the right-hand box

Combine (b) and (c)

$$\bar{M}_l - \bar{M}_r = \Delta x (C_l - C_r)$$

$$= (\Delta x)^2 \left[-\frac{C_r - C_l}{\Delta x} \right]$$

$$\approx (\Delta x)^2 \left[-\frac{\partial C}{\partial x} \right] if \quad \Delta x \quad \text{is small} \qquad \text{(d)}$$

Substitute (d) into (a)

$$q = -k(\Delta x)^2 \frac{\partial C}{\partial x}$$

$$= -D \frac{\partial C}{\partial x}$$

$D = k(\Delta x)^2 \Rightarrow$ diffusion coefficient (constant)

2.3 Some Mathematics of the Diffusion Equation

2.3.1 Concentration Distribution

i) G.E.

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

ii) Initial condition for instantaneous point source

$$C(x,0) = M\delta(x) \qquad (2.18)$$

M = initial slugs of mass introduced at time zero at the origin

δ = Dirac delta function (=$\frac{1}{\Delta x}$)

- representing a unit mass of tracer concentrated into an infinitely small space with an infinitely large conc.

→ spike distribution

[Ex] bucket of concentrated dye dumped into a large river

iii) Solution

$$C\left(x,t\right) = \frac{M}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right) \qquad (2.14)$$

→ Gaussian distribution (Normal if M = 1)

[Re] Normal distribution ~ $N(\mu, \sigma^2)$

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}}\exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}, \; -\infty < x < \infty$$

$E(x) = \mu$

$Var(x) = \sigma^2$

$\rightarrow \quad \mu = 0, \ \sigma = \sqrt{2Dt}$

2.3.2 Moments of Concentration Distribution

1. Moments

Zeroth moment = $M_0 = \int_{-\infty}^{\infty} C(x,t)\,dx$

First moment = $M_1 = \int_{-\infty}^{\infty} C(x,t)\,x\,dx$

2nd moment = $M_2 = \int_{-\infty}^{\infty} C(x,t)\,x^2\,dx$

Pth moment = $M_p = \int_{-\infty}^{\infty} C(x,t)\,x^p\,dx$

i) Mass $M = M_0$

ii) Mean $\mu = M_1 / M_0$

iii) Variance $\sigma^2 = \dfrac{\int_{-\infty}^{\infty} (x-\mu)^2 C(x,t)\,dx}{M_0} = \dfrac{M_2}{M_0} - \mu^2$

iv) Skewness $S_t = \dfrac{\dfrac{M_3}{M_0} - 3\mu\dfrac{M_2}{M_0} + 2\mu^3}{\left(\sigma^2\right)^{3/2}}$

- measure of skew
- for normal dist. $S_t = 0$

◆ For a normal distribution M = 1

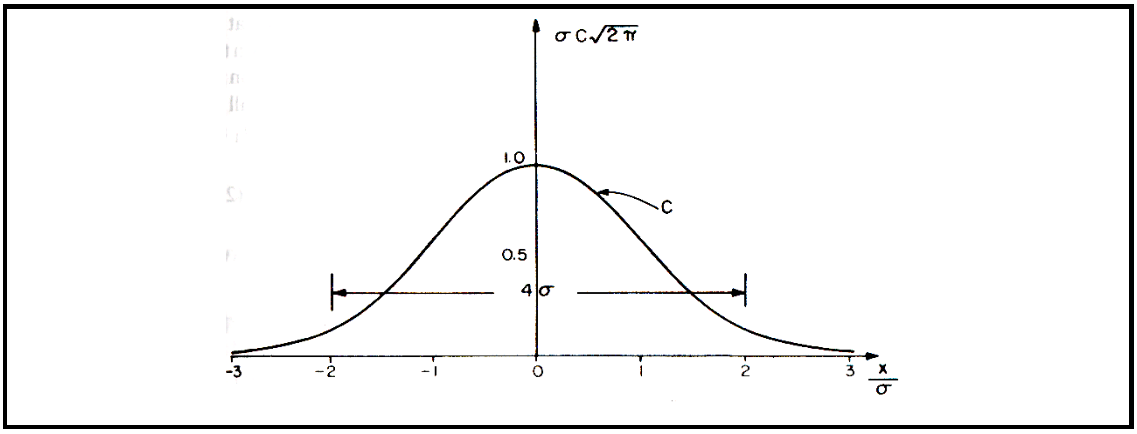
$$C(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$$

$M_0 = 1$

$\mu = 0 \rightarrow$ location of centroid of concentration distribution

$\sigma^2 = 2Dt \rightarrow$ measure of the spread of the distribution

2. Diffusion coefficient



The normal distribution

◆ Measure of spread of dispersing tracer

$\sigma = \sqrt{2Dt}$ ⇒ standard deviation (see Table 2.1)

$4\sigma = 4\sqrt{2Dt}$ ⇒ estimate of the width of a dispersing cloud

⇒ include 95% of the total mass

[Cf] $6\sigma = 6\sqrt{2Dt}$ ⇒ include 99.5% of the total mass

◆ Calculation of diffusion coefficient

$$D = \frac{1}{2}\frac{d\sigma^2}{dt} \tag{2.22}$$

→ Change of moment method

i)Normal distribution: it is obvious

ii)Eq. (2.22) can be also true for any distribution, provided that it is dispersing in accord with the Fickian diffusion equation.

[Pf]

Start with Fickian diffusion equation

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \tag{a}$$

Multiply each side by x^2

$$x^2 \frac{\partial C}{\partial t} = Dx^2 \frac{\partial^2 C}{\partial x^2}$$

Integrate from to $-\infty$ and $+\infty$ w.r.t x

$$\int_{-\infty}^{\infty} \frac{\partial C}{\partial t} x^2 dx = \int_{-\infty}^{\infty} Dx^2 \frac{\partial^2 C}{\partial x^2} dx$$

Apply <u>integration by parts</u> into right hand side

$$\frac{\partial}{\partial t}\int_{-\infty}^{\infty} Cx^2 dx = D\left\{\left[x^2 \frac{\partial C}{\partial x}\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} 2x\frac{\partial C}{\partial x}dx\right\}$$

$$= -2D\int_{-\infty}^{\infty} x\frac{\partial C}{\partial x}dx \qquad \left(\because \left.\frac{\partial C}{\partial x}\right]_{\pm\infty} \approx 0\right)$$

$$= -2D\left\{\left[xC\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} Cdx\right\}$$

$$= 2D\int_{-\infty}^{\infty} Cdx \qquad (\because C]_{-\infty}^{\infty} \approx 0)$$

$$2D = \frac{\frac{\partial}{\partial t}\int_{-\infty}^{\infty} Cx^2 dx}{\int_{-\infty}^{\infty} Cdx} = \frac{\frac{\partial}{\partial t}M_2}{M_0} = \frac{\partial}{\partial t}\left(\frac{M_2}{M_0}\right)$$

$$D = \frac{1}{2}\frac{\partial}{\partial t}\left(\frac{M_2}{M_0}\right) \qquad \text{(b)}$$

By the way, multiply each side of Eq. (a) by x

$$\int_{-\infty}^{\infty} x\frac{\partial C}{\partial t}dx = \int_{-\infty}^{\infty} Dx\frac{\partial^2 C}{\partial x^2}dx = D\left\{\left. x\frac{\partial C}{\partial x}\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{\partial C}{\partial x}dx\right\}$$

$$= -D\int_{-\infty}^{\infty}\frac{\partial C}{\partial x}dx = -D[C]_{-\infty}^{\infty} = 0$$

$$\therefore \frac{\partial}{\partial t}\int_{-\infty}^{\infty} Cxdx = 0$$

$$\therefore \frac{\partial}{\partial t}M_1 = 0$$

$$\frac{\partial}{\partial t}(M_1 / M_0) = \frac{\partial}{\partial t}(\mu) = 0$$

→ μ is independent of time.

By the way,

$$\sigma^2 = \frac{M_2}{M_0} - \mu^2$$

$$\frac{\partial}{\partial t}(\sigma^2) = \frac{\partial}{\partial t}\left(\frac{M_2}{M_0}\right) - \frac{\partial}{\partial t}\left(\mu^2\right) = \frac{\partial}{\partial t}\left(\frac{M_2}{M_0}\right) \quad \text{(c)}$$

Combine Eq.(a) and Eq.(c)

$$D = \frac{1}{2}\frac{\partial \sigma^2}{\partial t} \quad (2.25)$$

→ Variance of a finite distribution increases at the rate 2D no matter what its shape.

→ Property of the Fickian diffusion equation

→ Any finite initial distribution eventually decays into Gaussian distribution.

◆ Change of moment method

- Calculate diffusion coefficient from concentration curves

From Eq.(2.25)

$$\sigma^2 = 2Dt + C$$

$$\sigma_2^{\ 2} = 2Dt_2 + C \quad (1)$$

$$\sigma_1^{\ 2} = 2Dt_1 + C \quad (2)$$

Subtract (1) from (2)

$$\sigma_2^{\,2} - \sigma_1^{\,2} = 2D(t_2 - t_1)$$

$$D = \frac{1}{2}\frac{\sigma_2^{\,2} - \sigma_1^{\,2}}{t_2 - t_1} \qquad (2.26)$$

$\sigma_1^{\,2}$ = variance of conc. distr. at $t = t_1$

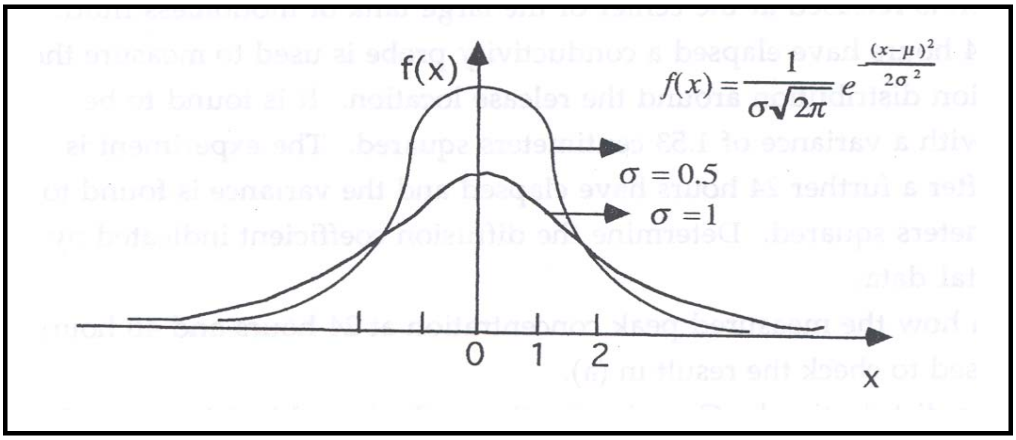
$\sigma_2^{\,2}$ = variance of conc. distr. at $t = t_2$

- Concentration curves - more than 2 curves

$\rightarrow$ $D = \frac{1}{2}\left(slope\ of\ \sigma^2\ vs\ t\ curve\right)$

[Re] Normal Gaussian distribution

- often obtained in practice
- bell-formed distribution occur around a mean value



Distribution function: $\int_{-\infty}^{x} \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{(t-\mu)^2}{2\sigma^2}} dt$

Homework #2-1

Due: 1 week from Today

Taking care to create as little disturbance as possible, a small sample of salt solution is released at the center of the large tank of motionless fluid.

(a) After 24 hours have elapsed a conductivity probe is used to measure the concentration distribution around the release location. It is found to be Gaussian with a variance of 1.53 centimeters squared. The experiment is repeated after a further 24 hours have elapsed and the variance is found to be 3.25 centimeters squared. Determine the diffusion coefficient indicated by the experimental data.

(b) Explain how the measured peak concentration at 24 hours and 48 hours could be used to check the result in (a).

(c) Must the distribution be Gaussian for the method used in (a) to apply?

2.4 Solutions of the Diffusion Equation

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \tag{2.31}$$

2.4.1 An Initial Spatial Distribution C(x, 0)

(1) Mass M released at time t=0 at the point x $= \xi$

$$I.C. \quad C(x,0) = M\delta(x-\xi)$$

$$B.C. \quad C(\pm\infty,t) = 0$$

Set $X = x - \xi$

Then, I.C. becomes

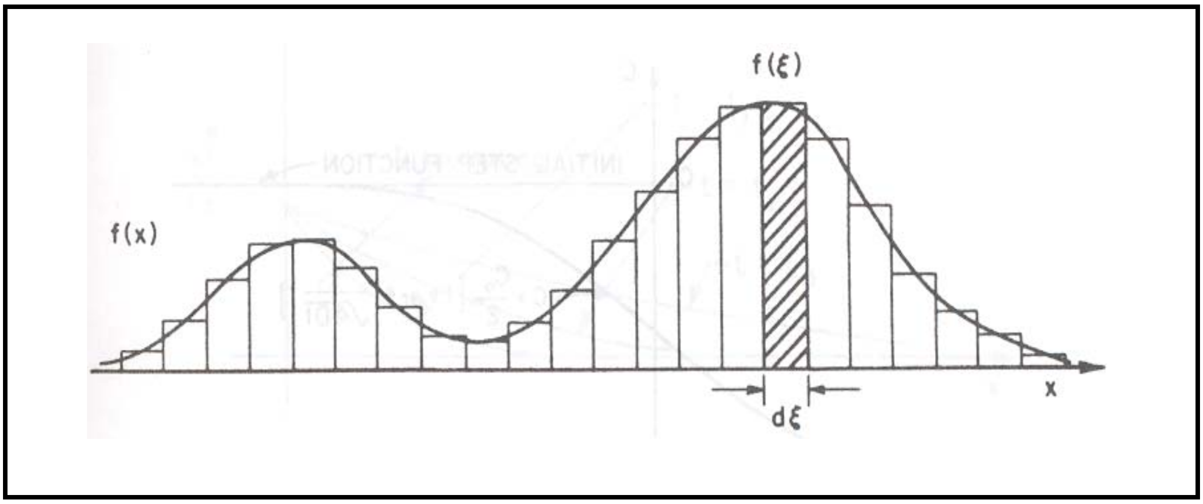
$$C(X,0) = M\delta(X)$$

Solution is

$$C(X,t) = \frac{M}{\sqrt{4\pi Dt}}\exp\left[\frac{-X^2}{4Dt}\right]$$

$$C(x,t) = \frac{M}{\sqrt{4\pi Dt}}\exp\left[\frac{-(x-\xi)^2}{4Dt}\right] \tag{2.28}$$

(2) Distributed source at time t=0



$$I.C.: \; C(x,0) = f(x), \quad -\infty < x < \infty$$

f(x) = arbitrary function

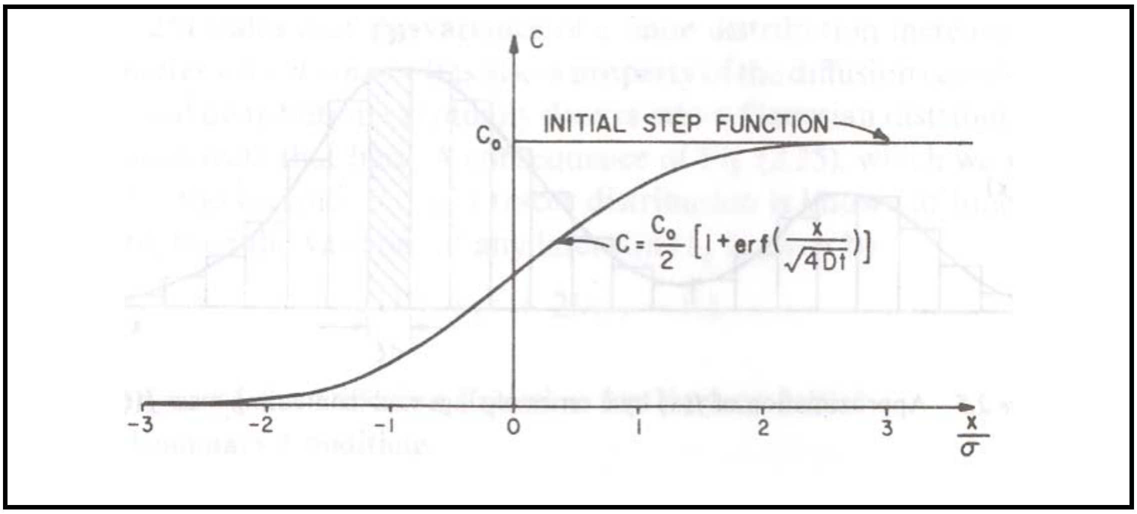
- is composed from a distributed series of separate slugs, which all diffuse independently
- motion of individual particles is independent of the concentration of other particles

$$dC(x,t) = \frac{f(\xi)d\xi}{\sqrt{4\pi Dt}} \exp\left[\frac{-(x-\xi)^2}{4Dt}\right]$$

$$C(x,t) = \int_{-\infty}^{\infty} \frac{f(\xi)}{\sqrt{4\pi Dt}} \exp\left[\frac{-(x-\xi)^2}{4Dt}\right] d\xi \qquad (2.30)$$

→ superposition integral

(3) Distributed source with step function



$$I.C.\quad C(x,0)=\begin{cases}0 & x<0\\ C_0 & x>0\end{cases}$$

According to (2.30)

$$C(x,t)=\int_0^\infty \frac{C_0}{\sqrt{4\pi Dt}}\exp\left[\frac{-(x-\xi)^2}{4Dt}\right]d\xi \qquad \text{(a)}$$

Set $\quad u=\dfrac{(x-\xi)}{\sqrt{4Dt}}$

$$\xi=0:\quad u=\frac{x}{\sqrt{4Dt}}$$

$$\xi=\infty:\quad u=-\infty$$

$$du=\frac{-d\xi}{\sqrt{4Dt}}\rightarrow d\xi=-\sqrt{4Dt}\,du \qquad \text{(b)}$$

Substitute (b) into (a)

$$C(x,t) = \frac{C_0}{\sqrt{\pi}} \int_{-\infty}^{\frac{x}{\sqrt{4Dt}}} e^{-u^2} du$$

$$= \frac{C_0}{2} \left[\frac{2}{\sqrt{\pi}} \int_{-\infty}^{0} e^{-u^2} du + \frac{2}{\sqrt{\pi}} \int_{0}^{\frac{x}{\sqrt{4Dt}}} e^{-u^2} du \right]$$

$$= \frac{C_0}{2} \left[1 + \frac{2}{\sqrt{\pi}} \int_{0}^{\frac{x}{\sqrt{4Dt}}} e^{-u^2} du \right]$$

$$= \frac{C_0}{2} \left[1 + erf\left(\frac{x}{\sqrt{4Dt}} \right) \right] \qquad (2.33)$$

[Re] $\quad \dfrac{2}{\sqrt{\pi}} \int_{-\infty}^{0} e^{-u^2} du = erf\,(-\infty) = 1$

■ Error function

$$erf\ z = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-\xi^2) d\xi \quad \rightarrow \text{Table 2.1}$$

$$erf\ z = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-\xi^2) d\xi = \frac{2}{\sqrt{\pi}} \sqrt{\pi} \int_0^z \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{w^2}{2} \right) dw$$

$$= 2 \int_0^z \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{w^2}{2} \right) dw$$

$$= 2 \left[\int_{-\infty}^{z} \frac{1}{\sqrt{2\pi}} \exp\left(\frac{w^2}{2} \right) dw - \int_{-\infty}^{0} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{w^2}{2} \right) dw \right]$$

$$= 2\Phi(z) - 1$$

■ Normal distribution

- Most important distribution in statistical application since many measurements have approximate Normal distributions.
- The random variable X has a Normal distribution if its p.d.f. is defined by

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-\mu^2)}{2\sigma^2} \right], \; -\infty < x < \infty$$

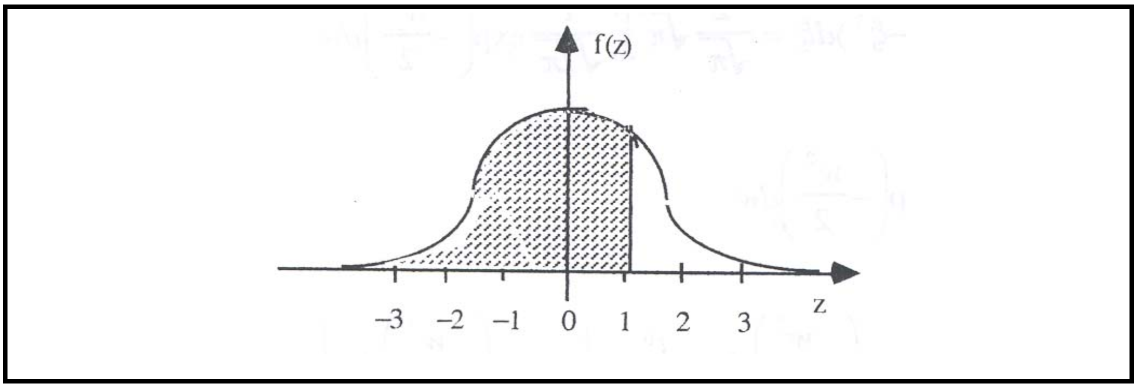
• Integral of Normal distribution

$$I = \int_{-\infty}^{\infty} \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2} \right] dx$$

Let $z = \dfrac{x-\mu}{\sigma} \quad \left(dz = \dfrac{1}{\sigma} dx \right)$

$$I = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{z^2}{2} \right] dz$$

$$\Phi(z) = P(-\infty < z \le Z) = \int_{-\infty}^{z} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{w^2}{2} \right) dw$$



$$\Phi(\infty) = 1$$

$$\Phi(-z) = 1 - \Phi(z)$$

(4) Distributed source with step function C_0 *for* $x<0$

I.C. $$C(x,0)=\begin{Bmatrix} C_0, & x<0 \\ 0, & x>0 \end{Bmatrix}$$

By line source of $C_0\delta\xi$

$$dC=\frac{C_0\delta\xi}{\sqrt{4\pi Dt}}\exp\left[-\frac{(x-\xi)^2}{4Dt}\right]$$

$$C(x,t)=\frac{C_0}{\sqrt{4\pi Dt}}\int_{-\infty}^{0}\exp\left[-\frac{(x-\xi)^2}{4Dt}\right]d\xi$$

Set $\eta=\dfrac{x-\xi}{\sqrt{4Dt}}$

Then $d\eta=-\dfrac{d\xi}{\sqrt{4Dt}}$ and $\begin{pmatrix} \xi=-\infty & \to\eta=\infty \\ \xi=0 & \to\eta=\dfrac{x}{\sqrt{4Dt}} \end{pmatrix}$

$$C(x,t)=\frac{C_0}{\sqrt{\pi}}\int_{\infty}^{x/\sqrt{4Dt}}\exp\left(-\eta^2\right)\left(-d\eta\right)=\frac{C_0}{\sqrt{\pi}}\int_{x/\sqrt{4Dt}}^{\infty}\exp\left(-\eta^2\right)d\eta$$

$$=\frac{C_0}{2}\left(\frac{2}{\sqrt{\pi}}\int_{x/\sqrt{4Dt}}^{\infty}\exp\left(-\eta^2\right)d\eta\right)$$

$$=\frac{C_0}{2}\left[\frac{2}{\sqrt{\pi}}\int_0^{\infty}\exp\left(-\eta^2\right)d\eta-\frac{2}{\sqrt{\pi}}\int_0^{x/\sqrt{4Dt}}\exp\left(-\eta^2\right)d\eta\right]$$

$$=\frac{C_0}{2}\left[1-erf\left(\frac{x}{\sqrt{4Dt}}\right)\right]$$

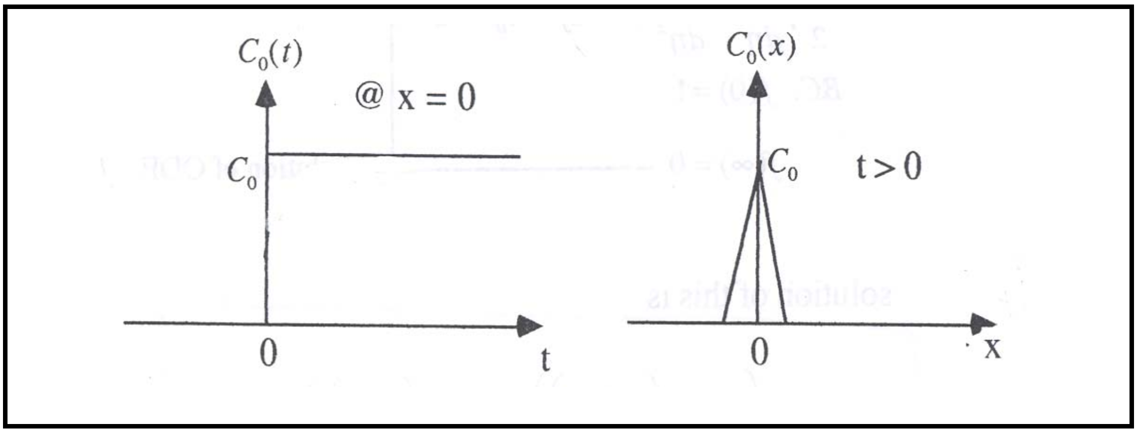
$$=\frac{C_0}{2}erfc\left(\frac{x}{\sqrt{4Dt}}\right)$$ complementary error function

→ summing the effect of a series of line sources,

each yielding an exponential of distribution

2.4.2 Concentration Specified as a Function of Time C(0, t)

(1) Continuous input with step function $C_0 = C_0(t)$



Continuous step input at x = 0

$$I.C.\quad C(x, t=0) = 0$$

$$B.C.\quad C(x=0, t>0) = C_0$$

◆ Solution by dimensional analysis

$$C = C_0 f\left(\frac{x}{\sqrt{Dt}}\right)$$

Set $\eta = \dfrac{x}{\sqrt{Dt}}$

$$\rightarrow \frac{\partial \eta}{\partial t} = \frac{x}{\sqrt{D}} - \frac{1}{2} t^{-\frac{3}{2}} = -\frac{1}{2t}\frac{x}{\sqrt{Dt}} = -\frac{1}{2t}\eta$$

$$\rightarrow \frac{\partial \eta}{\partial x} = \frac{1}{\sqrt{Dt}}$$

Then $\frac{\partial C}{\partial t} = \frac{dC}{d\eta}\frac{\partial \eta}{\partial t} = -\frac{1}{2t}\eta\frac{dC}{d\eta}$

$$\frac{\partial^2 C}{\partial x^2} = \frac{1}{tD}\frac{d^2 C}{d\eta^2} \quad \left(\because \frac{\partial^2 C}{\partial x^2} = \frac{d^2 C}{d\eta^2}\frac{\partial^2 \eta}{\partial x^2}\right)$$

Substitute these into Eq. (2.31) to obtain O.D.E.

$$-\frac{1}{2}\eta\frac{df}{d\eta} = \frac{d^2 f}{d\eta^2}$$

$$\rightarrow 2f'' + \eta f' = 0 \qquad \text{(a)}$$

B.C. $f(0) = 1$

$f(\infty) = 0$

Solution of this is

$$C = C_0\left[1 - erf\left(\frac{x}{\sqrt{4Dt}}\right)\right] = C_0 erfc\left(\frac{x}{\sqrt{4Dt}}\right) \quad x > 0$$

[Re] Laplace transformation

(1) For ODE

- transform ODE into algebraic problem

(2) For PDE

- transform PDE into ODE

i) inverse transform

$$C(x,t) = L^{-1}(F)$$

ii) linearity of Laplace transformation

$$L\{af(t) + bg(t)\} = aL\{f(t) + bL\{g(t)\}$$

iii) integration of f(t)

$$L\left\{\int_0^t f(\tau)d\tau\right\} = \frac{1}{s}L\{f(t)\}$$

iv) use Laplace transformation("operational calculus")

$$F_n(x,s) = L(C) = \int_0^\infty e^{-st}C(x,t)dt = \overline{C}$$

$$L(C') = sL(C) - C(x,0) = s\overline{C} - C(x,0)$$

$$L(C'') = s^2L(C) - sC(x,0) - C'(x,0)$$

[Re] Analytical Solution

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2}$$ Advection-Diffusion Equation

B.C. & I.C.

$$C(x = 0,\, t > 0) = C_0 \qquad \text{(a)}$$

$$C(x \geq 0,\, t = 0) = 0 \qquad \text{(b)}$$

$$C(x = \pm\infty,\, t \geq 0) = 0 \qquad \text{(c)}$$

$$D\frac{\partial^2 C}{\partial x^2} - U\frac{\partial C}{\partial x} - \frac{\partial C}{\partial t} = 0$$

Apply Laplace transformation

$$D\frac{\partial^2 \overline{C}}{\partial x^2} - U\frac{\partial \overline{C}}{\partial x} - s\overline{C} - C(t=0) = 0$$

$C(t=0) = 0$ from I.C.

$$D\frac{\partial^2 \overline{C}}{\partial x^2} - U\frac{\partial \overline{C}}{\partial x} - s\overline{C} = 0$$

Set $\overline{C}' = \frac{\partial \overline{C}}{\partial x}$, $\overline{C}'' = \frac{\partial^2 \overline{C}}{\partial x^2}$

Then

$$\overline{C}'' - \frac{U}{D}\overline{C}' - \frac{s}{D}\overline{C} = 0$$

Assume $\overline{C} = e^{\lambda x}$

Derive characteristic equation as

$$\lambda^2 - \frac{U}{D}\lambda - \frac{s}{D} = 0$$

Solution is

$$\lambda = \frac{\frac{U}{D} \pm \sqrt{\left(\frac{U}{D}\right)^2 + 4\left(\frac{s}{D}\right)}}{2} = \frac{U \pm \sqrt{U^2 + 4sD}}{2D}$$

$$\overline{C} = C_1 e^{-\lambda_1 x} + C_2 e^{-\lambda_2 x}$$

$$= C_1(s)\exp\left\{\frac{U+\sqrt{U^2+4sD}}{2D}x\right\} + C_2(s)\exp\left\{\frac{U-\sqrt{U^2+4sD}}{2D}\right\}(1)$$

Laplace transformation of B.C. Eq. (c)

$$\lim_{x\to\infty}\bar{C}(x,s) = \lim_{x\to\infty}\int_0^\infty e^{-st}C(x,t)dt$$

$$= \int_0^\infty \left\{e^{-st}\lim_{x\to\infty}C(x,t)dt\right\} = 0$$

If we apply this to Eq. (1)

$$\lim_{x\to\infty}\bar{C}(x,s) = \lim_{x\to\infty}\left[C_1(s)\exp\left\{\frac{U+\sqrt{U^2 4sD}}{2D}x\right\}\right]$$

$$+\lim_{x\to\infty}\left[C_2(s)\exp\left\{\frac{U+\sqrt{U^2 4sD}}{2D}x\right\}\right] = 0$$

$\therefore\ C_1(s)$ should be zero

$$\therefore\therefore\ \bar{C} = C_2(s)\exp\left\{\frac{U-\sqrt{U^2+4sD}}{2D}x\right\}$$

Apply B.C.Eq. (a)

Laplace transformation

$$\bar{C}(0,s) = \frac{1}{s}C_0$$

$$\therefore C_2(s) = C_0 / s$$

$$\therefore\therefore \bar{C} = \frac{C_0}{s}\exp\left\{\frac{U-\sqrt{U^2+4sD}}{2D}x\right\}$$

$$= C_0 \exp\left(\frac{Ux}{2D}\right)\frac{1}{s}\exp\left(-\frac{x}{\sqrt{D}}\sqrt{\frac{U^2}{4D}+s}\right)$$

Get inverse Laplace transformation using Laplace transform table

$$\frac{2}{s}\exp\left\{-a(s+b^2)^{\frac{1}{2}}\right\} \Leftrightarrow e^{-ab}erfc\left(\frac{a}{2\sqrt{t}}-b\sqrt{t}\right)+e^{ab}erfc\left(\frac{a}{2\sqrt{t}}+b\sqrt{t}\right)$$

Set $a=\frac{x}{\sqrt{D}}, b=\frac{U}{2\sqrt{D}}$

$$e^{-ab} = \exp\left\{-\left(\frac{x}{\sqrt{D}}\frac{U}{2\sqrt{D}}\right)\right\} = \exp\left\{-\frac{xU}{2D}\right\}$$

$$e^{ab} = \exp\left\{\frac{x}{\sqrt{D}}\frac{U}{2\sqrt{D}}\right\} = \exp\left(\frac{xU}{2D}\right)$$

$$\frac{a}{2\sqrt{t}}-b\sqrt{t} = \frac{x/\sqrt{D}}{2\sqrt{t}}-\frac{U}{2\sqrt{D}}\sqrt{t} = \frac{x-Ut}{\sqrt{4Dt}}$$

$$\frac{a}{2\sqrt{t}}+b\sqrt{t} = \frac{x/\sqrt{D}}{2\sqrt{t}}+\frac{U}{2\sqrt{D}}\sqrt{t} = \frac{x+Ut}{\sqrt{4Dt}}$$

$$\therefore C = \frac{C_0}{2}\exp\left(\frac{Ux}{2D}\right)\left\{\exp\left(\frac{-Ux}{2D}\right)erfc\left(\frac{x-Ut}{\sqrt{4Dt}}\right)+\exp\left(\frac{Ux}{2D}\right)erfc\left(\frac{x+Ut}{\sqrt{4Dt}}\right)\right\}$$

$$= \frac{C_0}{2}\left\{erfc\left(\frac{x-Ut}{\sqrt{4Dt}}\right)+\exp\left(\frac{Ux}{D}\right)erfc\left(\frac{x+Ut}{\sqrt{4Dt}}\right)\right\}$$

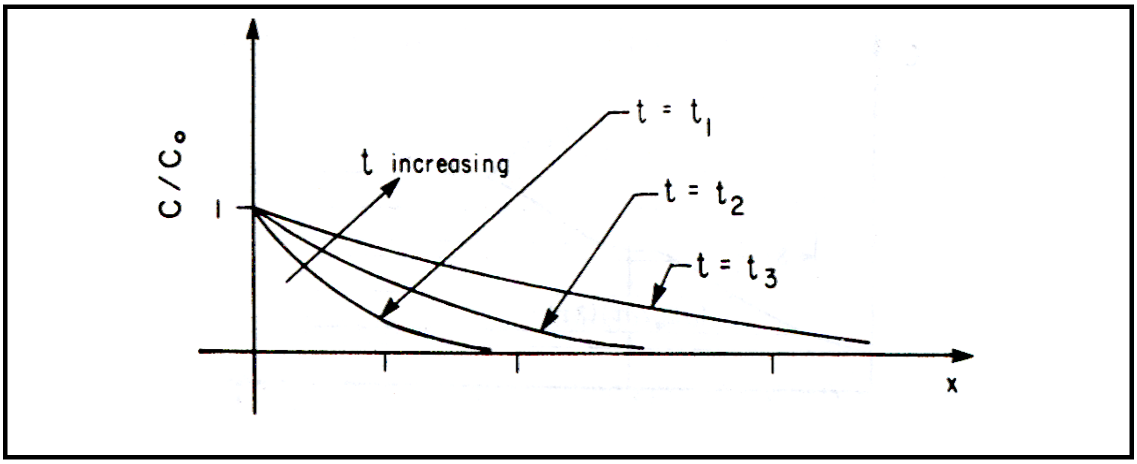
In case U=0

$$C = \frac{C_0}{2}\left\{erfc\left(\frac{x}{\sqrt{4Dt}}\right)+erfc\left(\frac{x}{\sqrt{4Dt}}\right)\right\}$$

$$= C_0 erfc\left(\frac{x}{\sqrt{4Dt}}\right) \qquad (2.37)$$

where erfc = complementary error function

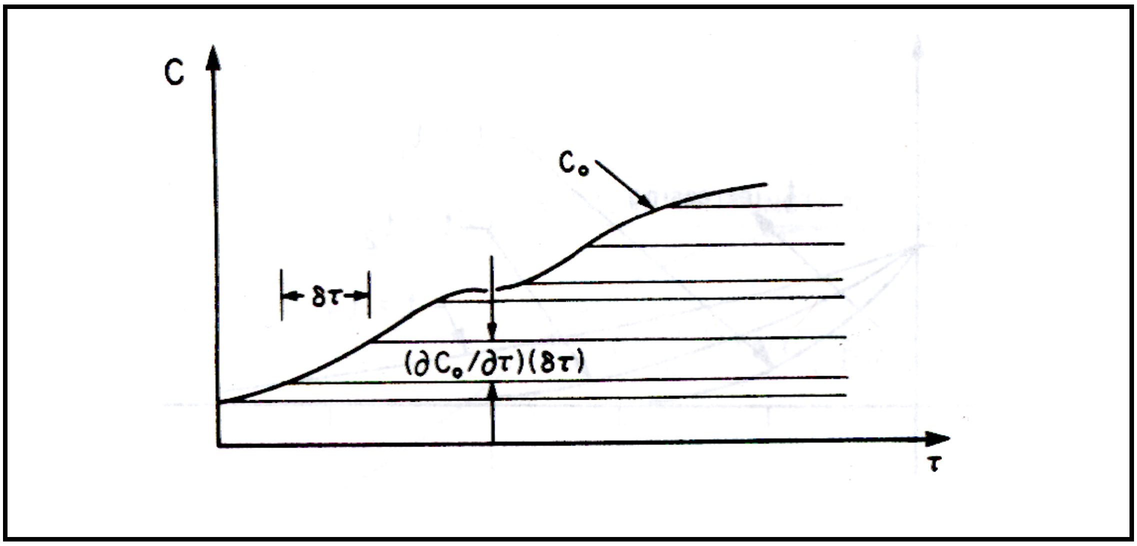
$$erfc(z) = 1 - erf(z)$$



(2) Concentration specified as a function of time at fixed point

$$C(x,t=0)=0$$

$$C(x=0,t>0)=C_0\left(\tau\right)$$ → time variable concentration



$$\delta C=\frac{\partial C_0}{\partial \tau}\delta\tau\, erfc\left(\frac{x}{\sqrt{4D(t-\tau)}}\right) \qquad t>\tau$$

$$C=\int_{-\infty}^{t}\frac{\partial C_0}{\partial \tau}erfc\left(\frac{x}{\sqrt{4D(t-\tau)}}\right)d\tau$$

2.4.3 Input of mass specified as a function of time

(1) Continuous injection of mass at the rate $\dot{M}$, $-\infty < t < \infty$

$$C = \int_{-\infty}^{t} \frac{\dot{M}(\tau)}{\sqrt{4\pi D(t-\tau)}} \exp\left[-\frac{x^2}{4D(t-\tau)}\right] d\tau$$

where $\dot{M}(\tau)$ = rate of input mass at time τ and may vary with time

= [$ML^{-2}t^{-1}$]

(2) Continuous injection of mass of constant strength $\dot{M}$ at t > 0

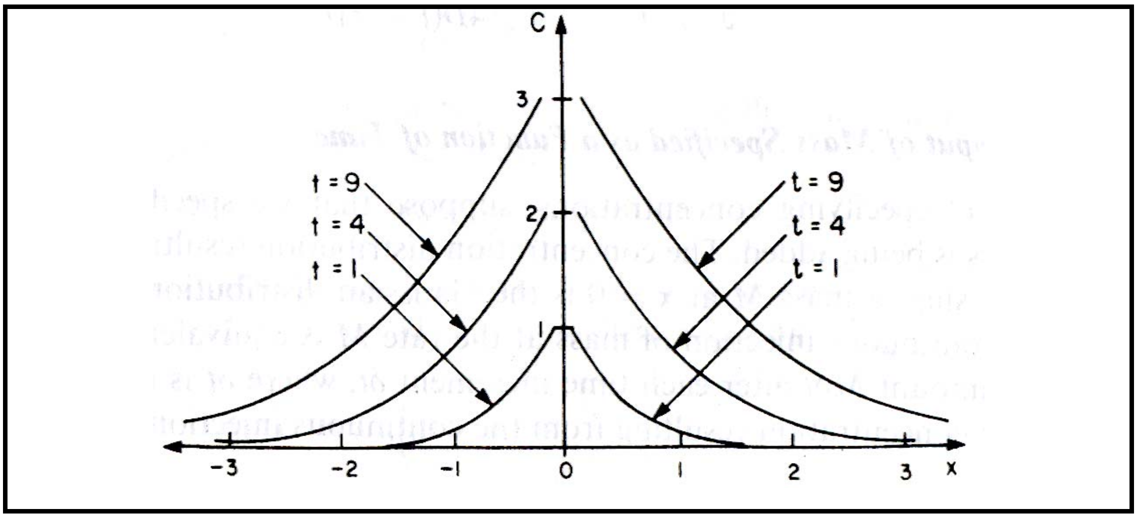
$$C(x,t) = \frac{\dot{M}}{\sqrt{4\pi D}} \int_{0}^{t} \frac{1}{\sqrt{t-\tau}} \exp\left[-\frac{x^2}{4D(t-\tau)}\right] d\tau$$

Set $u = \dfrac{4D(t-\tau)}{x^2}$

→ $du = -\dfrac{4D}{x^2} d\tau$

$d\tau = -\dfrac{x^2}{4D} du$

Then $C(x,t) = \dfrac{\dot{M}x}{4D\sqrt{\pi}} \displaystyle\int_{0}^{\frac{4Dt}{x^2}} u^{-\frac{1}{2}} \exp(-\frac{1}{u}) du$



(3) Distributed source of mass m(x,t)

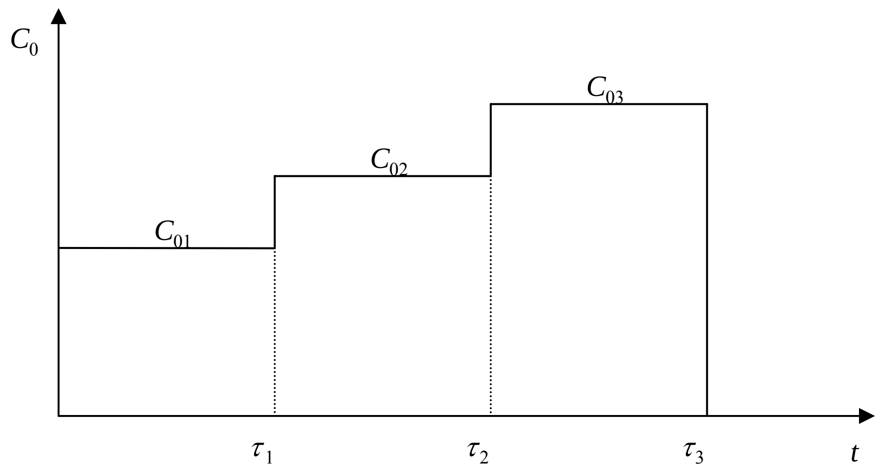
m = mass per unit length per unit time= [$ML^{-3}t^{-1}$]

$$C(x,t) = \int_{-\infty}^{t}\int_{-\infty}^{\infty} \frac{m(\xi,\tau)}{\sqrt{4\pi D(t-\tau)}} \exp\left[-\frac{(x-\xi)^2}{4D(t-\tau)}\right] d\xi d\tau$$

→ superposition in space and then in time

Homework #2-2

Due: 1 week from today



a) Derive analytical solution

G. E.: $\dfrac{\partial C}{\partial t} = D\dfrac{\partial^2 C}{\partial x^2}$

I. C.: $\mathrm{C}(x,\ t=0)=0$

B. C.: $\mathrm{C}(x=0,\ 0<t\le\tau_1)=C_{01}$

$\mathrm{C}(x=0,\ \tau_1<t\le\tau_2)=C_{02}$

$\mathrm{C}(x=0,\ \tau_2<t\le\tau_3)=C_{03}$

$\mathrm{C}(x=0,\ \tau_3<t)=0$

b) Plot *C* vs *x* for various time *t* with assumed C_0s, for example $C_{01}=C_0/2$;

$C_{02}=C_0$; $C_{03}=\dfrac{3}{2}C_0$.

c) Plot *C* vs *t* for various distance *x*.

2.4.4 Solution Accounting for Boundaries

- Spreading restricted by the presence of boundaries

• Principle of superposition

→ If the equation and boundary conditions are linear it is possible to superimpose any number of individual solutions of the equation to obtain a new solution.

The method of superposition for matching the boundary condition of zero transport through the walls (single boundary)

(1) Mass input at x = 0 with nondiffusive boundary at x = -L

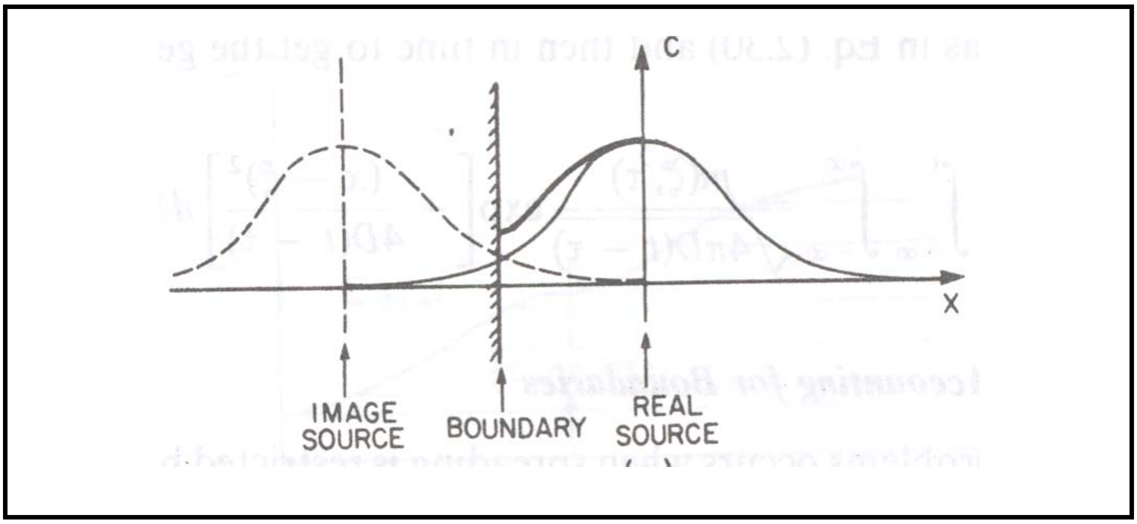
I.C. : unit mass of solute at x=0 at t=0

B.C.: wall through which concentration cannot diffuse located at x = -L

$$q\big|_{x=-L} = -D\frac{\partial C}{\partial x}\Big|_{x=-L} = 0 \qquad \rightarrow \text{Neumann type B.C.}$$

→ Concentration gradient must be zero at the wall.

→ zero transport through the wall



• This condition would be met if an <u>additional unit mass of solute</u> (image source) was concentrated at the point x = -2L

• Solution with the real boundary = sum of the solutions for real plus the image source w/o the boundary

$$C = \frac{1}{\sqrt{4\pi Dt}} \left\{ \exp\left(-\frac{x^2}{4Dt} \right) + \exp\left(-\frac{(x+2L)^2}{4Dt} \right) \right\}$$

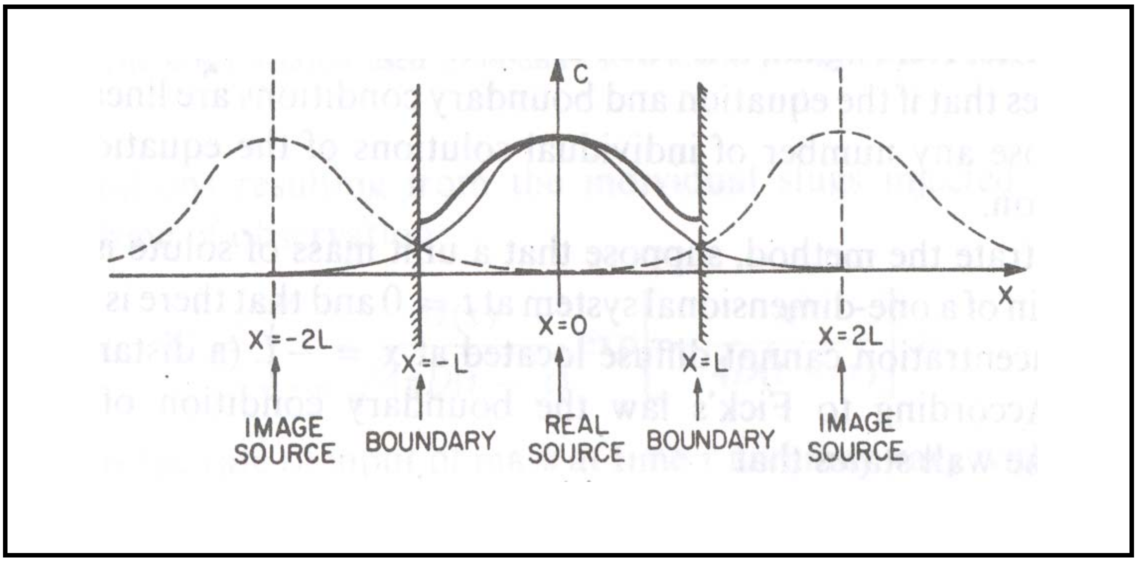
(2) Mass input x = 0 with nondiffusive boundaries at x = - L and at x = + L

→ put image slugs at   -2L, +2L, 4L, -6L, 8L, ……

(∵ slug at x = -2L causes a positive gradient at the boundary at +L , which must be counteracted by another slug located at x = +4L, and so on)

$$C(x,t) = \sum_{n=-\infty}^{\infty} \frac{1}{\sqrt{4\pi Dt}} \exp\left[\frac{-(x + +2nL)^2}{4Dt} \right]$$

→ n = -2, -1, 0, +1, =2



(3) Zero concentration at x= $\pm L$

$\rightarrow$ $C(x = \pm L, \quad t) = 0$ $\rightarrow$ Dirichlet type B.C.

$\rightarrow$ negative image slugs at $x = \pm 2L$

positive image slugs at $x = \pm 4L$ etc.

$$C(x,t) = \frac{1}{\sqrt{4\pi Dt}} \sum_{n=-\infty}^{\infty} \left\{ \exp\left[\frac{-(x+4nL)^2}{4Dt} \right] - \exp\left[\frac{-\left[x+(4n-2)L\right]^2}{4Dt} \right] \right\}$$

(4) Mass input x = 0 with nondiffusive boundaries at x = 0

$\rightarrow$ Solution for negative x is reflected in the plane x=0 and superposed on the original distribution in the region x>0.

$\rightarrow$ reflection at a boundary x=0 means the adding of two solutions of the diffusion equation

$$C = \frac{1}{\sqrt{4\pi Dt}} \left\{ \exp\left(-\frac{x^2}{4Dt} \right) + \exp\left(-\frac{(x+0)^2}{4Dt} \right) \right\}$$

$$= \frac{1}{\sqrt{\pi Dt}} \exp\left(-\frac{x^2}{4Dt} \right)$$

2.4.5 Solutions in Two and Three Dimensions

(1) 2-D Fluid

- A mass M [M/L] deposited at t=0 at x=0, y=0

G. E.: $\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2}$ (a)

molecular diffusion $D_x = D_y = D$

I.C.: $C(x, y, 0) = M\delta(x)\delta(y)$

• Product rule

$$C(x, y, t) = C_1(x, t)C_2(y, t)$$

where $C_1 \neq f(y), C_2 \neq f(x)$

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial t}(C_1 C_2) = C_1 \frac{\partial C_2}{\partial t} + C_2 \frac{\partial C_1}{\partial t}$$

$$\frac{\partial^2 C}{\partial x^2} = \frac{\partial^2}{\partial x^2}(C_1 C_2) = C_2 \frac{\partial^2 C_1}{\partial x^2}$$

$$\frac{\partial^2 C}{\partial y^2} = \frac{\partial^2}{\partial y^2}(C_1 C_2) = C_1 \frac{\partial^2 C_2}{\partial y^2}$$

(a) becomes

$$C_1 \frac{\partial C_2}{\partial t} + C_2 \frac{\partial C_1}{\partial t} = D_x C_2 \frac{\partial^2 C_1}{\partial x^2} + D_y C_1 \frac{\partial^2 C_2}{\partial y^2}$$

Rearrange

$$C_2 \left[\frac{\partial C_1}{\partial t} - D_x \frac{\partial^2 C_1}{\partial x^2} \right] + C_1 \left[\frac{\partial C_2}{\partial t} - D_y \frac{\partial^2 C_2}{\partial y^2} \right] = 0$$

Whole equation = 0 if

$$\left.\begin{aligned}\frac{\partial C_1}{\partial t} &= D_x \frac{\partial^2 C_1}{\partial x^2} \\ \frac{\partial C_2}{\partial t} &= D_y \frac{\partial^2 C_2}{\partial y^2}\end{aligned}\right] \quad \rightarrow \text{ 1-D diffusion equation}$$

$$\therefore\ C_1 = \frac{\int_{-\infty}^{\infty} C dx}{\sqrt{4\pi D_x t}} \exp\left(-\frac{x^2}{4D_x t}\right)$$

$$C_2 = \frac{\int_{-\infty}^{\infty} C dy}{\sqrt{4\pi D_y t}} \exp\left(-\frac{y^2}{4D_y t}\right)$$

$$\therefore\therefore\ C = C_1 C_2 = \frac{M}{4\pi t\sqrt{D_x D_y}} \exp\left(-\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t}\right) \qquad (2.53)$$

where $M = \iint_{-\infty}^{\infty} C\ dxdy$

→ lines of constant concentration = set of concentric ellipses

= Isoconcentration lines

$$C = \frac{M}{4\pi t\sqrt{D_x D_y}} e^{\left(-\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t}\right)}$$

$$e^{\left(-\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t}\right)} = \frac{4\pi t\sqrt{D_x D_y} C}{M}$$

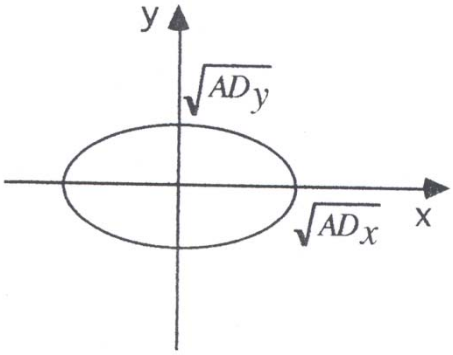
$$\frac{x^2}{4D_x t} + \frac{y^2}{4D_x t} = -ln\left(\frac{4\pi t\sqrt{D_x D_y} C}{M}\right) = ln\left(\frac{M}{4\pi t\sqrt{D_x D_y} C}\right)$$

$$\therefore\ \frac{x^2}{\left(\sqrt{D_x}\right)^2} + \frac{y^2}{\left(\sqrt{D_y}\right)^2} = 4t ln\left(\frac{M}{4\pi t\sqrt{D_x D_y} C}\right)$$

$$\frac{x^2}{\left(\sqrt{D_x}\right)^2}+\frac{y^2}{\left(\sqrt{D_y}\right)^2}=A$$

$$\frac{x^2}{\left(\sqrt{AD_x}\right)^2}+\frac{y^2}{\left(\sqrt{AD_y}\right)^2}=1$$

If $D_x = D_y$ Then $x^2 + y^2 = R^2$



(2) 3-D fluid

- A mass M [M] deposited at t=0 at x=0, y=0, z=0

G. E.: $\frac{\partial C_2}{\partial t}=D_x\frac{\partial^2 C_2}{\partial x^2}+D_y\frac{\partial^2 C_2}{\partial y^2}+D_z\frac{\partial^2 C_2}{\partial z^2}$ (b)

I.C.: $C\left(x,y,z,0\right)=M\delta\left(x\right)\delta\left(y\right)\delta\left(z\right)$ $\rightarrow$ point source

• Product rule

$$C(x,y,z,t)=C_1(x,t)C_2(y,t)C_3(z,t)$$

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial t}(C_1C_2C_3)=C_1\frac{\partial(C_2C_3)}{\partial t}+C_2C_3\frac{\partial C_1}{\partial t}$$

$$= C_1 C_2 \frac{\partial C_3}{\partial t} + C_1 C_3 \frac{\partial C_2}{\partial t} + C_2 C_3 \frac{\partial C_1}{\partial t}$$

$$\frac{\partial^2 C}{\partial x^2} = \frac{\partial^2}{\partial x^2}(C_1 C_2 C_3) = C_2 C_3 \frac{\partial^2 C_1}{\partial x^2}$$

$$\frac{\partial^2 C}{\partial y^2} = \frac{\partial^2}{\partial y^2}(C_1 C_2 C_3) = C_1 C_3 \frac{\partial^2 C_1}{\partial y^2}$$

$$\frac{\partial^2 C}{\partial z^2} = \frac{\partial^2}{\partial z^2}(C_1 C_2 C_3) = C_1 C_2 \frac{\partial^2 C_3}{\partial z^2}$$

Substituting these relations into (b) yields

$$C_1 C_2 \frac{\partial C_3}{\partial t} + C_1 C_3 \frac{\partial C_2}{\partial t} + C_2 C_3 \frac{\partial C_1}{\partial t} = D_x C_2 C_3 \frac{\partial^2 C_1}{\partial x^2} + D_y C_1 C_3 \frac{\partial^2 C_1}{\partial y^2} + D_z C_1 C_2 \frac{\partial^2 C_3}{\partial z^2}$$

$$C_1 C_2 \left[\frac{\partial C_3}{\partial t} - D_z \frac{\partial^2 C_3}{\partial z^2} \right] + C_1 C_3 \left[\frac{\partial C_2}{\partial t} - D_y \frac{\partial^2 C_1}{\partial y^2} \right] + C_2 C_3 \left[\frac{\partial C_1}{\partial t} - D_x \frac{\partial^2 C_1}{\partial x^2} \right] = 0$$

$$C_1 = \frac{\int C dx}{\sqrt{4\pi D_x t}} \exp\left(-\frac{x^2}{4 D_x t} \right)$$

$$C_2 = \frac{\int C dy}{\sqrt{4\pi D_y t}} \exp\left(-\frac{y^2}{4 D_y t} \right)$$

$$C_3 = \frac{\int C dz}{\sqrt{4\pi D_z t}} \exp\left(-\frac{z^2}{4 D_z t} \right)$$

$$\therefore C = C_1 C_2 C_3 = \frac{M}{(4\pi t)^{\frac{3}{2}} \left(D_x D_y D_z \right)^{\frac{1}{2}}} \exp\left(-\frac{x^2}{4 D_x t} - \frac{y^2}{4 D_y t} - \frac{z^2}{4 D_z t} \right)$$

$$M = \iiint C dx dy dz$$

2.4.6 Advective Diffusion

(1) Governing Equation

Fluid moving with velocity $\vec{u}$

$$\vec{u} = u\vec{i} + v\vec{j} + w\vec{k}$$

• Advection = transport by the mean motion of the fluid

• Assumption

- transports by advection and by diffusion are separate and additive processes

→ rate of mass transport through unit area (yz plane) by x the component of velocity, q_u

$$q_u = uC$$

[Re] advective flux

mass = volume · concentration

mass rate = volume rate · conc.

= discharge · conc.

= velocity · area · conc.

∴ Advective flux = mass rate /area = velocity · conc.

Total rate of mass transport

$$q = uC + \left(-D\frac{\partial C}{\partial x} \right) \tag{2.55}$$

= advective flux + diffusive flux

Substitute (2.55) into mass conservation equation, (2.3)

$$\frac{\partial C}{\partial t} + \frac{\partial q}{\partial x} = 0$$

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}\left(uC - D\frac{\partial C}{\partial x} \right) = 0$$

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(uC) = D\frac{\partial^2 C}{\partial x^2}$$ 1-D Advection-Diffusion Equation

• In 3-D

i) Mass conservation equation

$$\frac{\partial C}{\partial t} = -\nabla \cdot \vec{q}$$ (a) (divergence $\rightarrow \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}$)

ii) Rate of mass transport

$$\vec{q} = C\vec{u} - D\nabla C$$ (b) (gradient $\rightarrow \frac{\partial C}{\partial x}\vec{i} + \frac{\partial C}{\partial y}\vec{j} + \frac{\partial C}{\partial z}\vec{k}$)

Substitute (b) into (a)

$$\frac{\partial C}{\partial t} + \nabla \cdot \left(C\vec{u} - D\nabla C \right) = 0$$

$$\frac{\partial C}{\partial t} + \nabla \cdot \left(C\vec{u} \right) = D\nabla^2 C \qquad (2.57)$$

2nd term of LHS

$$\nabla \cdot \left(C\vec{u} \right) = \nabla C \cdot \vec{u} + C\nabla \cdot \vec{u}$$

By the way

$$\nabla \cdot \vec{u} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$ (continuity)

$$\therefore \nabla \cdot (C\vec{u}) = \nabla C \cdot \vec{u}$$

$$= \left(\frac{\partial C}{\partial x}\vec{i} + \frac{\partial C}{\partial y}\vec{j} + \frac{\partial C}{\partial z}\vec{k} \right)\left(u\vec{i} + v\vec{j} + w\vec{k} \right)$$

$$= u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z}$$

(2.57) becomes

$$\frac{\partial C}{\partial t} + \nabla C \cdot \vec{u} = D\nabla^2 C \qquad (2.58)$$

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = D\left[\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right] \qquad (2.59)$$

(2) Analytical Solutions

1) Instantaneous mass input

Assume that u is constant and gradient in y-direction is small

G.E.: $\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2}$

I.C.: $C(x,0) = M\delta(x)$

B.C.: $C(\pm\infty, t) = 0$

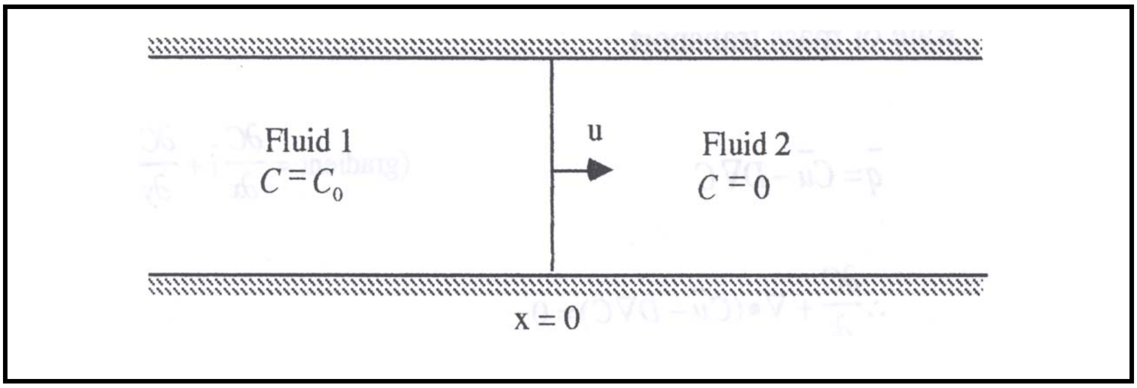
$$C(x,t) = \frac{M}{\sqrt{4\pi Dt}}\exp\left(-\frac{(x-ut)^2}{4Dt} \right)$$

2) Instantaneous concentration input over x<0

• Problem of pipe filled with one fluid being displaced at a mean velocity *u* by another fluid with a tracer in concentration C_0

I.C.: $C(x,0) = 0, \quad x > 0$

$C(x,0) = C_0, \quad x < 0$



• Transform coordinate system whose origin moves at velocity u

Let $x' = x - ut,\ t = t$

$$\rightarrow \frac{\partial x'}{\partial x} = 1, \frac{\partial x'}{\partial t} = -u$$

use chain rule

$$\frac{\partial}{\partial x} = \frac{\partial x'}{\partial x}\frac{\partial}{\partial x'} + \frac{\partial t}{\partial x}\frac{\partial}{\partial t} = \frac{\partial}{\partial x'}$$

$$\frac{\partial}{\partial t} = \frac{\partial x'}{\partial t}\frac{\partial}{\partial x'} + \frac{\partial t}{\partial t}\frac{\partial}{\partial x'} = -u\frac{\partial}{\partial x'} + \frac{\partial}{\partial t}$$

$$\therefore \frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x'} + \frac{\partial C}{\partial t}$$

$$u\frac{\partial C}{\partial x} = u\frac{\partial C}{\partial x'}$$

$$D\frac{\partial^2 C}{\partial x^2} = D\frac{\partial^2 C}{\partial x'^2}$$

Then G.E. becomes

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x'^2} \qquad \text{(a)}$$

→ Now, this problem is identical to distributed source with step function $C_0 \;\; for \;\; x < 0$ (p.2-40)

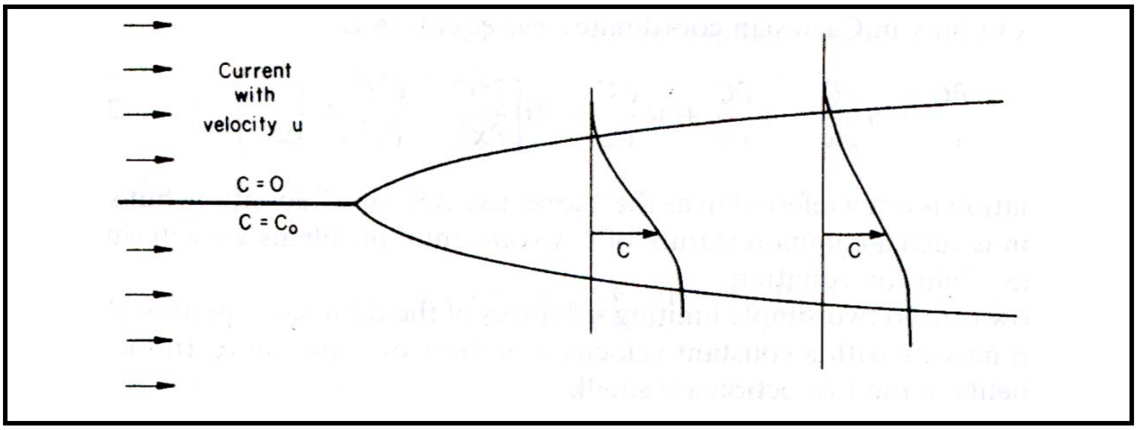
There, solution is

$$C\left(x',t\right) = \frac{C_0}{2}\left[1 - erf\left(\frac{x'}{\sqrt{4Dt}}\right)\right]$$

$$C(x,t) = \frac{C_0}{2}\left[1 - erf\left(\frac{x - ut}{\sqrt{4Dt}}\right)\right] \tag{2.63}$$

3) Lateral (Transverse) Diffusion Problem

- transverse mixing of two streams of different uniform concentrations flowing side by side



Start with 2-D advection-diffusion equation

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = D\left[\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right]$$

Assumptions:

i) continous input $\rightarrow \frac{\partial C}{\partial t} \rightarrow 0$

ii) velocity in transverse direction is small $\rightarrow v\dfrac{\partial C}{\partial y} \rightarrow 0$

iii) advection in x-direction is bigger than diffusion $\rightarrow D\dfrac{\partial^2 C}{\partial x^2} \rightarrow 0$

Then, G.E. becomes

$$u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial y^2}$$

B. C.: $C(0, y) = 0 \quad y > 0$

$C(0, y) = C_0, \quad y < 0$

→ Now, this problem is similar to Case 2) with t = x/u; x′ = y

There, solution is

$$\therefore C = \frac{C_0}{2}\left[1 - erf\left(\frac{y}{\sqrt{4Dx/u}}\right)\right] \tag{2.64}$$

4) Continuous plane source

G.E.: $\dfrac{\partial C}{\partial t} + u\dfrac{\partial C}{\partial x} = D\dfrac{\partial^2 C}{\partial x^2}$

B.C.: $C(0, t) = C_0$ $\quad 0 < t < \infty$ → steady continuous input

$C(x, 0) = 0$ $\quad 0 < x < \infty$

→ This problem is identical to continuous input with step function $C_0 = C_0(t)$ (p. 2-41)

The solution is

$$C(x,t) = \frac{C_0}{2}\left[erfc\left(\frac{x - ut}{\sqrt{4Dt}}\right) + erfc\left(\frac{x + ut}{\sqrt{4Dt}}\right)\exp\left(\frac{ux}{D}\right)\right] \tag{2.65}$$

$$\frac{C(x,t)}{C_0} = \frac{1}{2} erfc\left[\left(\frac{P_e}{4t_R}\right)^{\frac{1}{2}}(1-t_R)\right] + \frac{1}{2} erfc\left[\left(\frac{P_e}{4t_R}\right)^{\frac{1}{2}}(1+t_R)\right]\exp(P_e)$$

where

P_e = Peclet number $= \dfrac{ux}{D}$

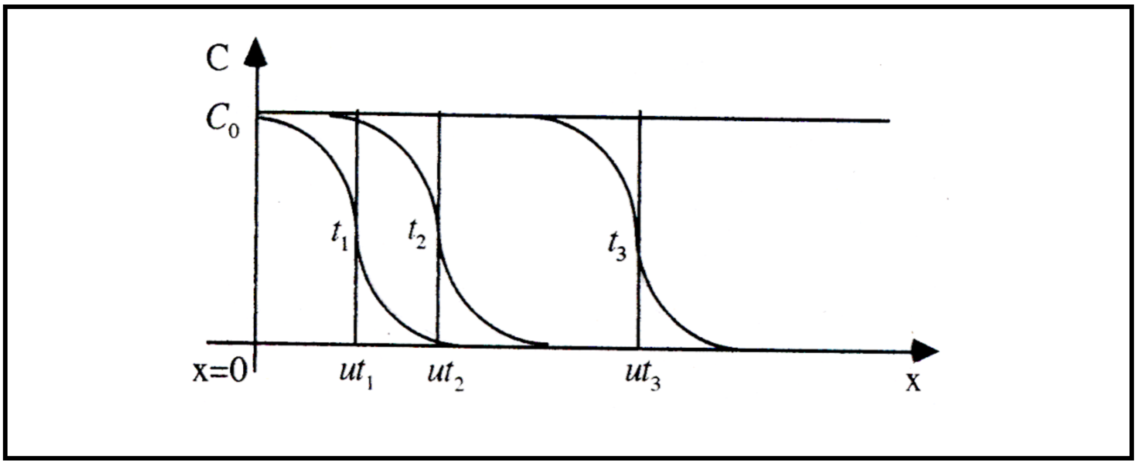
$t_R = \dfrac{ut}{x} = \dfrac{t}{x/u}$

• Advection-dominated case

For large u; $P_e > 500$; $\dfrac{C}{C_0} \approx \dfrac{1}{2} erfc\left(\dfrac{x-ut}{\sqrt{4Dt}}\right)$

• Diffusion problem

u = 0; $\dfrac{C}{C_0} = erfc\left(\dfrac{x}{\sqrt{4Dt}}\right)$



Homework Assignment #2-3

Due: Two Weeks from Today

a) Derive analytical solution for 1-D dispersion equation with continuous plane source condition which is given as

$$C(0,t) = C_0, \qquad 0 < t < \infty$$

$$C(x,t=0) = 0, \qquad 0 < x < \infty$$

$$C(x=\pm\infty,t) = 0, \qquad 0 < t < \infty$$

$$C(x,t) = \frac{C_0}{2}\left[erfc\left(\frac{x-ut}{\sqrt{4Dt}}\right) + erfc\left(\frac{x+ut}{\sqrt{4Dt}}\right)\exp\left(\frac{ux}{D}\right)\right]$$

b) Plot C vs. x for various values Pe of and t.

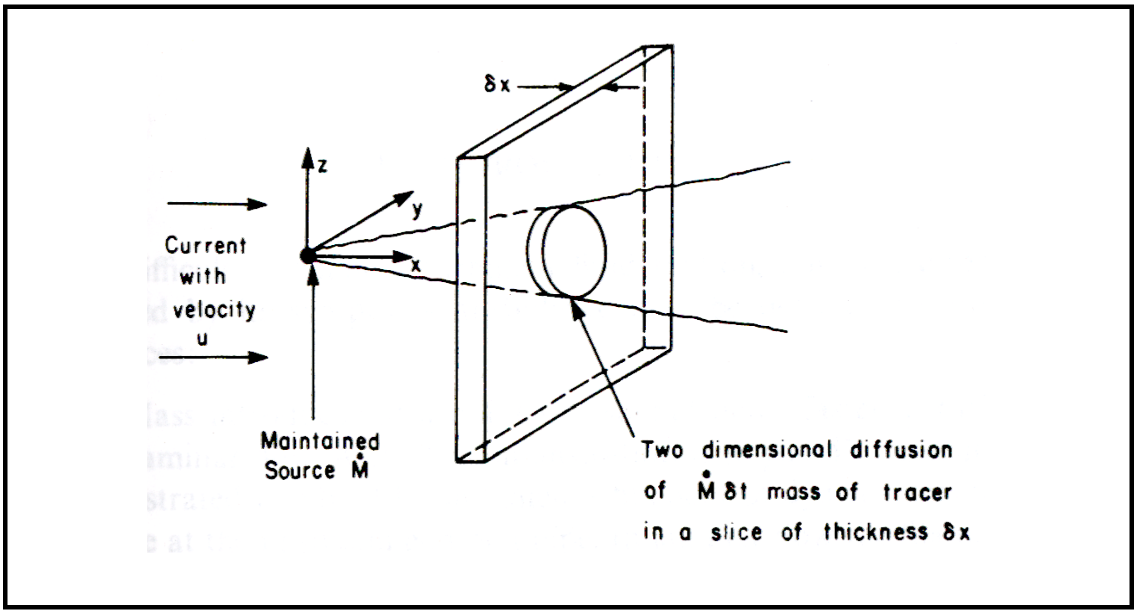
2.4.7 Maintained point source

(1) Constant point source in 3D

- mass input at the rate $\dot{M}$ at the origin (x, y, z,) in three-dimensional flow

G.E.: $\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right)$

I.C.: $C(x, y, z, 0) = M\delta(x)\delta(y)\delta(z)$



• Reduction of a three-dimensional problem to two dimensions by considering diffusion in a moving slice

→ visualize the flow as consisting of a series of parallel slices of thickness δx

→ slices are being advected past the source, and during the passage each one receives a slug of mass of amount $\dot{M}\delta t$

- time taken for slice to pass source; $\delta t = \frac{\delta x}{u}$

mass collected by slice at it passes source $= \dot{M}\,\delta t = \dot{M}\,\dfrac{\delta x}{u}$

2-D solution $\leftarrow$ (2.53)

$$C = \frac{M}{4\pi t\sqrt{D_x D_y}} \exp\left(-\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t} \right)$$

$$C = \frac{\dot{M}\,\dfrac{\delta x}{u}}{4\pi D t} \exp\left(-\frac{\left(x^2 + y^2\right)}{4Dt} \right)$$

Substitute $t = \dfrac{x}{u}$ and $\dot{M} = \dfrac{\dot{M}}{\delta x}$

$$C(x, y, z) = \frac{\dot{M}}{4\pi D x} \exp\left(-\frac{\left(x^2 + y^2\right)u}{4Dx} \right) \tag{2.67}$$

In case $ut >> \sqrt{2Dt}$ *or* $t >> 2D/u^2$

$\rightarrow$ neglect diffusion in the direction of flow

(2) Maintained point source in 2D

$$C_1 = \frac{\dot{M}\,\delta x/u}{\sqrt{4\pi D t}} \exp\left(-\frac{y^2}{4Dt} \right)$$

Substitute $t = \dfrac{x}{u}$ and $\dot{M} = \dfrac{\dot{M}}{\delta x}$

$$C(x, y) = \frac{\dot{M}}{u\sqrt{4\pi D x/u}} \exp\left(-\frac{y^2 u}{4Dx} \right) \tag{2.68}$$

$\dot{M}$ = strength of a line source in units of mass per unit length per unit time

2.4.8 Solutions for Mixing in Rivers

(1) 2-D Instantaneous Input

Assume rapid vertical mixing

G.E.: $$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}=D_x\frac{\partial^2 C}{\partial x^2}+D_y\frac{\partial^2 C}{\partial y^2}$$

B.C.: $$\left.\frac{\partial C}{\partial y}\right|_{y=0,\ w}=0$$ → impermeable, non-diffusion boundary

I.C.: $$C(x,y,0)=M\delta(x)\delta(y)$$

i) Case A: Right-bank input

Use product rule $C=C_1(x,t)C_2(y,t)$

$$C_2\left[\frac{\partial C_1}{\partial t}+u\frac{\partial C}{\partial x}-D_x\frac{\partial^2 C_1}{\partial x^2}\right]+C_1\left[\frac{\partial C_2}{\partial t}-D_y\frac{\partial^2 C_2}{\partial y^2}\right]=0$$

$$C_1=\frac{M_1}{\sqrt{4\pi D_x t}}\exp\left(-\frac{(x-ut)^2}{4D_x t}\right)$$

$$C_2=\sum_{n=-\infty}^{\infty}\frac{M_2}{\sqrt{4\pi D_y t}}\left[\exp\left\{-\frac{(y+2nW)^2}{4D_y t}\right\}\right]$$

$$C=\frac{M}{4\pi t\sqrt{D_x D_y}}\exp\left(-\frac{(x-ut)^2}{4D_x t}\right)\sum_{n=-\infty}^{\infty}\left[\exp\left\{-\frac{(y+2nW)^2}{4D_y t}\right\}\right]$$

ii) Case B: Centerline input

a) For axis at right bank

$$C_1 = \frac{M_1}{\sqrt{4\pi D_x t}} \exp\left(-\frac{(x-ut)^2}{4D_x t} \right)$$

$$C_2 = \sum_{n=-\infty}^{\infty} \frac{M_2}{\sqrt{4\pi D_y t}} \exp\left[-\frac{\left\{ y + (2n-1)\frac{W}{2} \right\}^2}{4D_y t} \right]$$

$$C = \frac{M}{4\pi t \sqrt{D_x D_y}} \exp\left(-\frac{(x-ut)^2}{4D_x t} \right) \sum_{n=-\infty}^{\infty} \exp\left[-\frac{\left\{ y + (2n-1)\frac{W}{2} \right\}^2}{4D_y t} \right]$$

b) For axis at centerline

$$C_1 = \frac{M_1}{\sqrt{4\pi D_x t}} \exp\left(-\frac{(x-ut)^2}{4D_x t} \right)$$

$$C_2 = \sum_{n=-\infty}^{\infty} \frac{M_2}{\sqrt{4\pi D_y t}} \left[\exp\left\{ -\frac{(y+nW)^2}{4D_y t} \right\} \right]$$

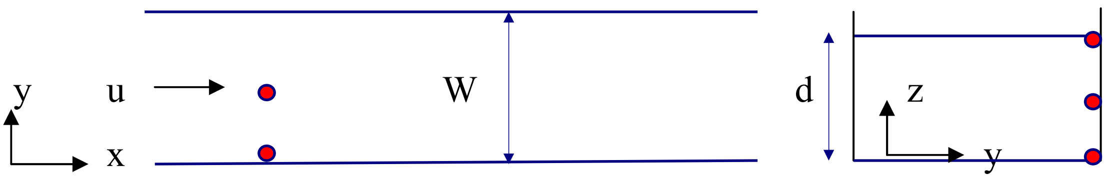
$$C = \frac{M}{4\pi t \sqrt{D_x D_y}} \exp\left(-\frac{(x-ut)^2}{4D_x t} \right) \sum_{n=-\infty}^{\infty} \left[\exp\left\{ -\frac{(y+nW)^2}{4D_y t} \right\} \right]$$

[Re] Decaying substance

G.E.: $\dfrac{\partial C}{\partial t} + u\dfrac{\partial C}{\partial x} = D_x \dfrac{\partial^2 C}{\partial x^2} + D_y \dfrac{\partial^2 C}{\partial y^2} - kC$

$C(x, y, t) = C(k = 0)\exp(-kt)$

(2) 3-D Instantaneous Input



G.E.: $$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2}$$

B.C.:

i) water surface $\left.\frac{\partial C}{\partial z}\right|_{z=d} = 0$ impermeable, non-diffusive

ii) solid boundary $\left.\frac{\partial C}{\partial y}\right|_{y=0,W} = 0$

$$\left.\frac{\partial C}{\partial z}\right|_{z=0} = 0$$

I.C.: $C(x, y, z, 0) = M\delta(x)\delta(y)\delta(z)$

i) Case A:　Right-bank input – surface input

Use product rule $C = C_1(x,t)C_2(y,t)C_3(z,t)$

$$C_1 = \frac{M_1}{\sqrt{4\pi D_x t}} \exp\left(-\frac{(x-ut)^2}{4D_x t}\right)$$

$$C_2 = \sum_{n=-\infty}^{\infty} \frac{M_2}{\sqrt{4\pi D_y t}} \left[\exp\left\{-\frac{(y+2nW)^2}{4D_y t}\right\}\right]$$

$$C_3 = \sum_{n=-\infty}^{n} \frac{M_3}{\sqrt{4\pi D_z t}} \left[\exp\left\{-\frac{(z+(2n-1)d)^2}{4D_y t}\right\}\right]$$

$$C = \frac{M}{(4\pi t)^{3/2}\sqrt{D_x D_y D_z}} \exp\left(-\frac{(x-ut)^2}{4D_z t}\right)$$

$$\cdot \sum_{n=-\infty}^{\infty}\left[\exp\left\{-\frac{(y+2nW)^2}{4D_y t}\right\}\exp\left\{-\frac{(z+(2n-1)d)^2}{4D_y t}\right\}\right]$$

ii) Case B: Right-bank input – mid-depth input

$$C_3 = \sum_{n=-\infty}^{n} \frac{M_3}{\sqrt{4\pi D_y t}}\left[\exp\left\{-\frac{(z+(2n-1)\frac{d}{2})^2}{4D_z t}\right\}\right]$$

$$C = \frac{M}{(4\pi t)^{3/2}\sqrt{D_x D_y D_z}} \exp\left(-\frac{(x-ut)^2}{4D_x t}\right)$$

$$\cdot \sum_{n=-\infty}^{\infty}\left[\exp\left\{-\frac{(y+2nW)^2}{4D_y t}\right\}\exp\left\{-\frac{(z+(2n-1)\frac{d}{2})^2}{4D_z t}\right\}\right]$$

iii) Case C: Right-bank input – bottom input

$$C_3 = \sum_{n=-\infty}^{n} \frac{M_3}{\sqrt{4\pi D_z t}}\left[\exp\left\{-\frac{(z+2nd)^2}{4D_z t}\right\}\right]$$

$$C = \frac{M}{(4\pi t)^{3/2}\sqrt{D_x D_y D_z}} \exp\left(-\frac{(x-ut)^2}{4D_x t}\right)$$

$$\cdot \sum_{n=-\infty}^{\infty}\left[\exp\left\{-\frac{(y+2nW)^2}{4D_y t}\right\}\exp\left\{-\frac{(z+2nd)^2}{4D_z t}\right\}\right]$$

iv) Case D: Centerline input – bottom input

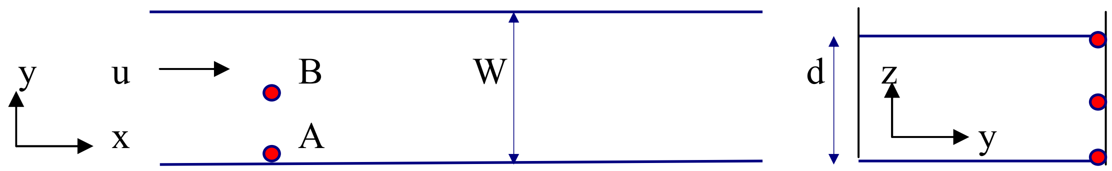
$$C_2 = \sum_{n=-\infty}^{\infty} \frac{M_2}{\sqrt{4\pi D_y t}} \left[\exp\left\{ -\frac{(y+(2n-1)\frac{W}{2})^2}{4D_y t} \right\} \right]$$

$$C_3 = \sum_{n=-\infty}^{n} \frac{M_3}{\sqrt{4\pi D_z t}} \left[\exp\left\{ -\frac{(z+2nd)^2}{4D_z t} \right\} \right]$$

$$C = \frac{M}{(4\pi t)^{3/2}\sqrt{D_x D_y D_z}} \exp\left(-\frac{(x-ut)^2}{4D_x t} \right)$$

$$\cdot \sum_{n=-\infty}^{\infty} \left[\exp\left\{ -\frac{(y+(2n-1)\frac{W}{2})^2}{4D_y t} \right\} \exp\left\{ -\frac{(z+2nd)^2}{4D_z t} \right\} \right]$$

(3) 2-D Analytical Solutions for continuous point injection



* Governing Equation

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial c}=D_x\frac{\partial^2 C}{\partial x^2}+D_y\frac{\partial^2 C}{\partial y^2}$$

Case I: side injection

$$\left.\frac{\partial C}{\partial y}\right|_{y=0,w}=0, \qquad C(0,0,t)=C_0$$

$$C(x,y,0)=0$$

Case II: centerline injection

$$\left.\frac{\partial C}{\partial y}\right|_{y=0,w}=0, \qquad C(0,w/2,t)=C_0$$

$$C(x,y,0)=0$$

* Product Rule

$$C=C_1(x,t)C_2(y,t)$$

Then, the governing equation will be modified as

$$C_2 \frac{\partial C_1}{\partial t} + C_1 \frac{\partial C_2}{\partial t} + uC_2 \frac{\partial C_1}{\partial x} = D_x C_2 \frac{\partial^2 C_1}{\partial x^2} + D_y C_1 \frac{\partial^2 C_2}{\partial y^2}$$

$$\rightarrow C_2 \left[\frac{\partial C_1}{\partial t} + u \frac{\partial C_1}{\partial x} - D \frac{\partial^2 C_1}{\partial x^2} \right] + C_1 \left[\frac{\partial C_2}{\partial t} - D_y \frac{\partial^2 C_2}{\partial y^2} \right] = 0$$

After that, we must to solve two equations

$$\frac{\partial C_1}{\partial t} + u \frac{\partial C_1}{\partial x} - D \frac{\partial^2 C_1}{\partial x^2} = 0 \qquad \text{(A)}$$

and

$$\frac{\partial C_2}{\partial t} - D_y \frac{\partial^2 C_2}{\partial y^2} = 0 \qquad \text{(B)}$$

i) Case I:

(A) $$C_1 = \frac{C_{1o}}{2} \left\{ erfc\left(\frac{x-ut}{\sqrt{4D_x t}} \right) + \exp\left(\frac{ux}{D_x} \right) erfc\left(\frac{x+ut}{\sqrt{4D_x t}} \right) \right\}$$

(B) $$C_2 = C_{2o} \left\{ erfc\left(\frac{y}{\sqrt{4D_y t}} \right) + \sum_{n=1}^{\infty} erfc\left(\frac{y+2nw}{\sqrt{4D_y t}} \right) + \sum_{n=1}^{\infty} erfc\left(\frac{-(y-2nw)}{\sqrt{4D_y t}} \right) \right\}$$

$$\therefore C = \left[\frac{C_{1o}}{2} \left\{ erfc\left(\frac{x-ut}{\sqrt{4D_x t}} \right) + \exp\left(\frac{ux}{D_x} \right) erfc\left(\frac{x+ut}{\sqrt{4D_x t}} \right) \right\} \right]$$

$$\left[C_{2o}\left\{erfc\left(\frac{y}{\sqrt{4D_y t}}\right)+\sum_{n=1}^{\infty}erfc\left(\frac{y+2nw}{\sqrt{4D_y t}}\right)+\sum_{n=1}^{\infty}erfc\left(\frac{-(y-2nw)}{\sqrt{4D_y t}}\right)\right\}\right]$$

$$=\frac{C_o}{2}\left[erfc\left(\frac{x-ut}{\sqrt{4D_x t}}\right)+\exp\left(\frac{ux}{D_x}\right)erfc\left(\frac{x+ut}{\sqrt{4D_x t}}\right)\right]$$

$$\left[erfc\left(\frac{y}{\sqrt{4D_y t}}\right)+\sum_{n=1}^{\infty}erfc\left(\frac{y+2nw}{\sqrt{4D_y t}}\right)+\sum_{n=1}^{\infty}erfc\left(\frac{-(y-2nw)}{\sqrt{4D_y t}}\right)\right]$$

ii) Case II:

(A) $$C_1=\frac{C_{1o}}{2}\left\{erfc\left(\frac{x-ut}{\sqrt{4D_x t}}\right)+\exp\left(\frac{ux}{D_x}\right)erfc\left(\frac{x+ut}{\sqrt{4D_x t}}\right)\right\}$$

(B) $$C_2=\sum_{n=-\infty}^{\infty}C_{2o}erfc\left(\frac{y+2nw}{\sqrt{4D_y t}}\right)$$

$$\therefore C=\left[\frac{C_{1o}}{2}\left\{erfc\left(\frac{x-ut}{\sqrt{4D_x t}}\right)+\exp\left(\frac{ux}{D_x}\right)erfc\left(\frac{x+ut}{\sqrt{4D_x t}}\right)\right\}\right]\left[\sum_{n=-\infty}^{\infty}C_{2o}\left(\frac{y+2nw}{\sqrt{4D_y t}}\right)\right]$$

$$=\frac{C_o}{2}\left[erfc\left(\frac{x-ut}{\sqrt{4D_x t}}\right)+\exp\left(\frac{ux}{D_x}\right)erfc\left(\frac{x+ut}{\sqrt{4D_x t}}\right)\right]\left[\sum_{n=-\infty}^{\infty}erfc\left(\frac{y+2nw}{\sqrt{4D_y t}}\right)\right]$$