

Chapter 2 Fickian Diffusion

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- 2.2 The Random Walk and Molecular Diffusion
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- 2.4 Solutions of the Diffusion Equation

Objectives

- present equations and concepts for molecular diffusion processes
- present two different rationalizations for the molecular diffusion equation
- discuss analytical solutions to the diffusion equations for different BCs

· molecular diffusion

fluids at rest → diffusion

moving fluids → diffusion + advection

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

· turbulent diffusion - large scale; analogous to molecular diffusion

2.1 Fick's Law of Diffusion

2.1.1 Diffusion Equation

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

Fick (1855) adopt Fourier's law of heat flow (1822) to diffusion

	Fourier	Fick
transport	heat	mass
gradient	temp.	conc.

1) Fick's law

→ 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.

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

Minus sign indicates transport is from high to low concentrations

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

(2.1)

q = solute mass flux (mass per unit area and per unit time)

C = mass concentration of dispersing solute

D = coefficient of proportionality

→ diffusion coefficient (m²/s), molecular diffusivity → distributed parameter

[Re] Two basic models for diffusion

1) Diffusion model (Fick's law)

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

q = mass flux per unit time and unit area

q_t = mass transfer per unit time

2) Mass transfer model

$$q = k\Delta C$$

k = mass transfer coefficient → lumped parameter

[Re] Fick's law in 3D

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

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

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

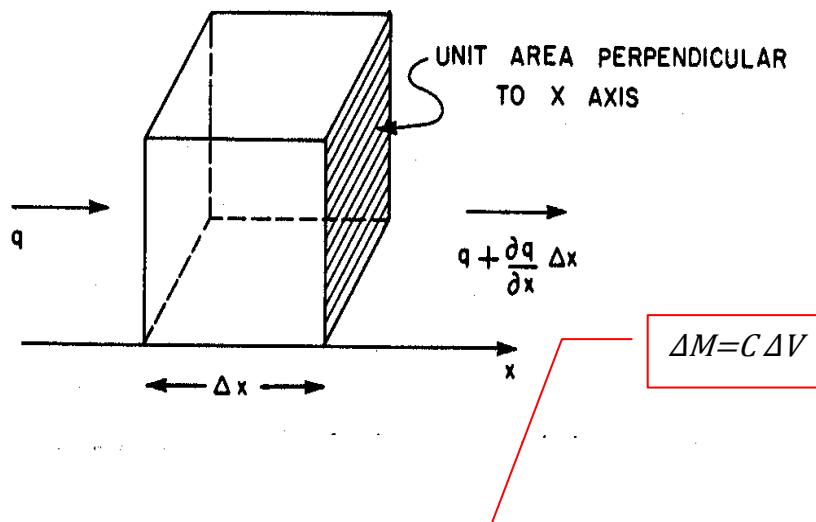
$$\nabla C = \left(\vec{i} \frac{\partial}{\partial x} + \vec{j} \frac{\partial}{\partial y} + \vec{k} \frac{\partial}{\partial z} \right) C$$

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

• gradient of scalar, C → vector, q

2) Conservation of Mass

Consider mass conservation for 1-D transport process



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

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

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

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

Now, combine (i) and (ii)

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

$$\frac{\partial C}{\partial t} = -\frac{\partial q}{\partial x} \tag{2.2}$$

3) Diffusion Equation

Combine Eq. (2.1) and (2.2)

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

$$\boxed{\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}} \quad \Rightarrow \text{Diffusion Equation (Heat Equation)}$$

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

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

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

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

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

[Re] Conservation of mass in 3D

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

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

Then consider \vec{q} by various transport mechanisms

- molecular diffusion (Fickian diffusion) $\rightarrow \vec{q} = -D\nabla C$

- advection by ambient current $\rightarrow \vec{q} = C\vec{u}$

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

Substitute (ii) into (i)

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

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

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

Continuity

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

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

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

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

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

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

Thus, (iii) becomes

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

write out fully in Cartesian coordinates

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

→ 3D advection-diffusion equation

For molecular diffusion only

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

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

→ linear, 2nd order PDE

[Re] Vector notation of conservation of mass

Consider a fixed volume V with surface area S

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

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

Consider conservation of mass

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

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

Green's theorem

$$\int_S \vec{q} \cdot \vec{n} dS = \int_V \nabla \cdot \vec{q} dV \quad (\text{b})$$

Substitute (b) into (a)

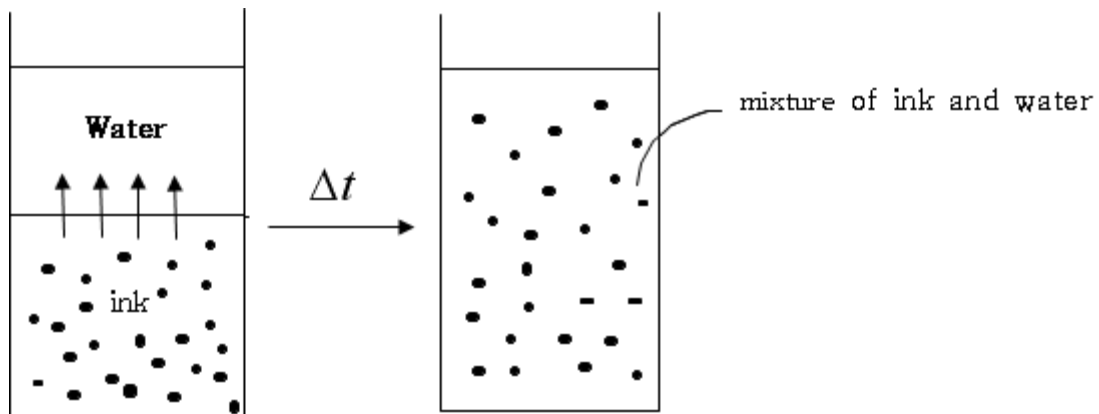
$$\int_V \left(\frac{\partial C}{\partial t} + \nabla \cdot \vec{q} \right) dV = 0$$

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

2.1.2 Diffusion Process

1. diffusion process

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



(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, it 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) 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.

(iii) 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.

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

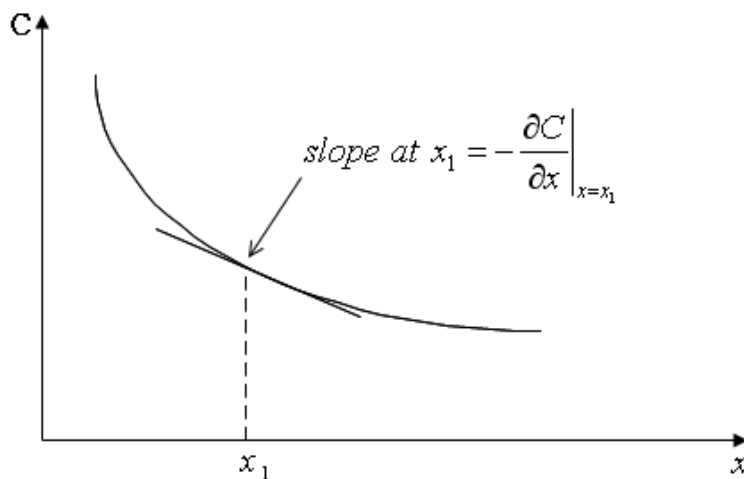
2. Molecular Diffusion

(i) Fick's 1st Law:

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

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

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



(ii) Fick's 2nd Law:

$$\text{Conservation of mass + Fick's 1st Law} \rightarrow \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

• Assumption for Fick's Law

→ Fick's 1st law is consistent only for an isotropic medium, whose structure and diffusion properties in the neighborhood of any point are the same relative to all directions.

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

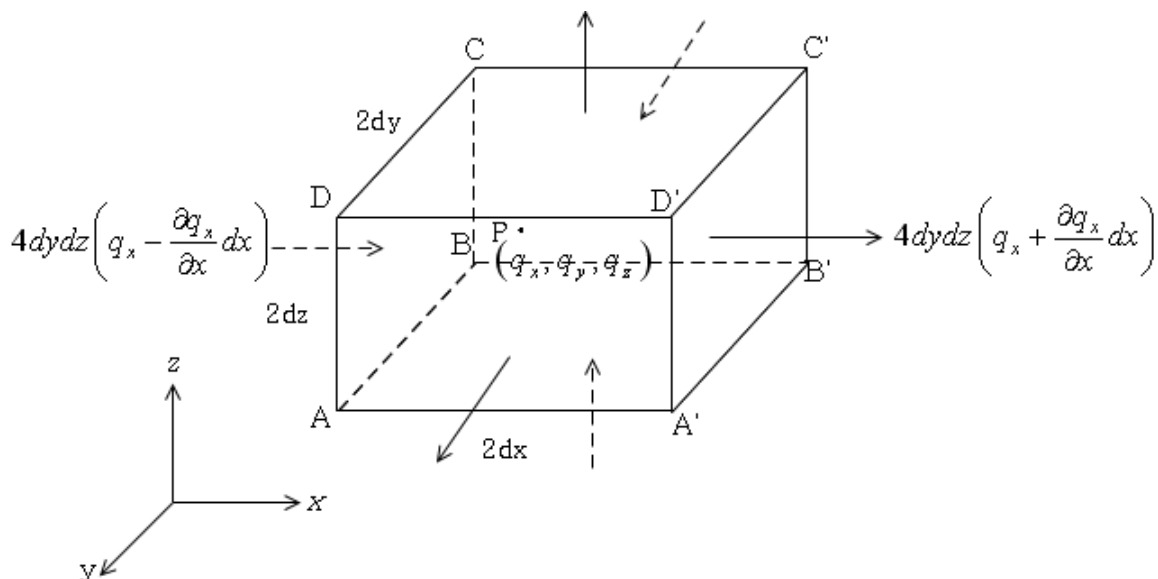
In turbulent diffusion: $\epsilon_x, \epsilon_y, \epsilon_z$

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. 3-D differential equation of diffusion



(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

$$-8dxdydz \frac{\partial q_y}{\partial y} \quad \text{and}$$

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

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

$$\begin{aligned}\frac{\partial}{\partial t}(\text{mass}) &= \frac{\partial}{\partial t}(\text{volume} \times \text{conc.}) \\ &= 8dx dy dz \frac{\partial c}{\partial t}\end{aligned}$$

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

$$\begin{aligned}8dx dy dz \frac{\partial c}{\partial t} &= -8dx dy dz \left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} \right) \\ \frac{\partial c}{\partial t} + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} &= 0\end{aligned}\tag{2}$$

(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

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \rightarrow \text{Fick's 2nd law of diffusion}$$

[Re] Vector Operations

Vectors = magnitude + direction

~ velocity, force

Scalar = magnitude

~ pressure, density, temperature, concentration

Vector \bar{F}

$$\bar{F} = F_x \bar{e}_x + F_y \bar{e}_y + F_z \bar{e}_z$$

$$\bar{e}_x, \bar{e}_y, \bar{e}_z = \text{unit vectors}$$

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

(1) Magnitude of \bar{F}

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

(2) Dot product = Scalar product

$$S = \bar{F} \cdot \bar{G} = |\bar{F}| |\bar{G}| \cos \phi$$

(3) Vector product = Cross product

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

$$\text{magnitude of } \bar{V} = |\bar{V}| = |\bar{F}| |\bar{G}| \sin \phi$$

direction of \bar{V} = perpendicular to the plane of \bar{F} and \bar{G}

→ right hand rule

(4) Derivatives of vectors

$$\frac{\partial \bar{F}}{\partial s} = \frac{\partial F_x}{\partial s} \bar{e}_x + \frac{\partial F_y}{\partial s} \bar{e}_y + \frac{\partial F_z}{\partial s} \bar{e}_z$$

(5) Gradient of F (scalar) → vector

$$\text{grad } F = \nabla F = \frac{\partial F}{\partial x} \bar{e}_x + \frac{\partial F}{\partial y} \bar{e}_y + \frac{\partial F}{\partial z} \bar{e}_z \quad \rightarrow \text{vector}$$

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

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

[Re] grad(scalar) → vector grad(F+G)=grad F+grad G

grad(vector) → tensor grad CF=c grad F

(6) Divergence of \bar{F} (vector) → scalar

$$\begin{aligned} \text{div} \bar{F} &= \nabla \cdot \bar{F} = \left(\frac{\partial}{\partial x} \bar{e}_x + \frac{\partial}{\partial y} \bar{e}_y + \frac{\partial}{\partial z} \bar{e}_z \right) \cdot \bar{F} \\ &= \left(\frac{\partial}{\partial x} \bar{e}_x + \frac{\partial}{\partial y} \bar{e}_y + \frac{\partial}{\partial z} \bar{e}_z \right) \cdot (F_x \bar{e}_x + F_y \bar{e}_y + F_z \bar{e}_z) \\ &= \left| \frac{\partial}{\partial x} \bar{e}_x \right| \left| F_x \bar{e}_x \right| \cos 0 + \frac{\partial F_y}{\partial x} \bar{e}_x \bar{e}_y \cos 90^\circ + \frac{\partial F_z}{\partial x} \bar{e}_x \bar{e}_z \cos 90^\circ \end{aligned}$$

$$\begin{aligned}
 & + \left| \frac{\partial F}{\partial y} \bar{e}_y \right| |F_y \bar{e}_y| \cos 0 + \left| \frac{\partial F}{\partial z} \bar{e}_z \right| |F_z \bar{e}_z| \cos 0 \\
 & = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} \quad \rightarrow \text{scalar}
 \end{aligned}$$

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

$$(8) \quad \text{div}(\text{grad } F) = \nabla \cdot \nabla F = \nabla^2 F \equiv \text{Laplacian of } F$$

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

$$\text{[Pf]} \quad \text{div}(\text{grad } F) = \text{div} \left(\frac{\partial F}{\partial x} \bar{e}_x + \frac{\partial F}{\partial y} \bar{e}_y + \frac{\partial F}{\partial z} \bar{e}_z \right)$$

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

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

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

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

2.1.3 Analytical Solution of Diffusion Equation

- Problem 1: Consider diffusion of an initial slug of mass M introduced instantaneously at time zero at the x origin

[Cf] Continuous input \rightarrow 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

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

Direct delta function=spike
function = $\frac{1}{\Delta x}$

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

Mass/area

iii) Solution by dimensional analysis

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

- dimensional analysis
- separation of variables
- Laplace transformation

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

Set $\eta = \frac{x}{\sqrt{4Dt}}$ (2.5)

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

Eq. (2.4):

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

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

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

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

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

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

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

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

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

Integrate once w.r.t. η

$$2\eta f + \frac{df}{d\eta} = 0 \quad (2.6)$$

Apply separation of variables to Eq. (2.6)

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

Integrate both sides

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

$$f = e^{-\eta^2 + C} = C_0 e^{-\eta^2} \quad (2.7)$$

Total mass, M

$$\int_{-\infty}^{\infty} C dx = M \quad (2.8)$$

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

Then, (2.4) becomes

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

C_p - peak

exponential decay

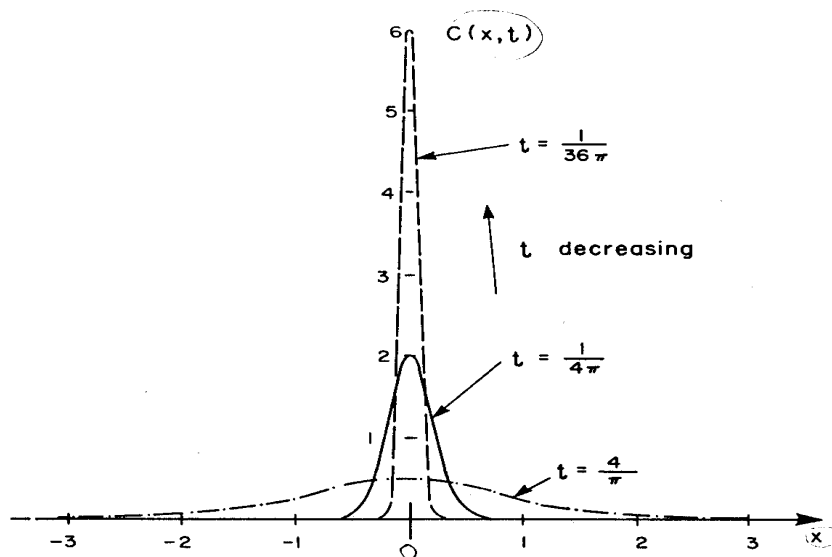
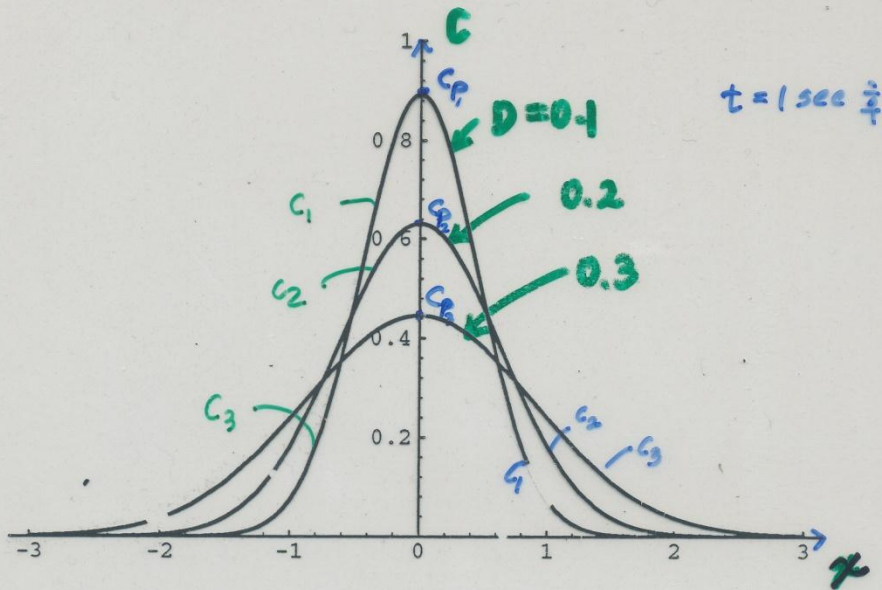


Figure 2.3 The reduction of the Gaussian distribution [Eq. (2.14)] to a “spike” as t decreases. The illustration uses the values $M = 1$, $D = \frac{1}{4}$.

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

In[141]:=

```
M=1;
t=1;
f[x_,Dx_]:= M/(Sqrt[4 Pi Dx t])*Exp[-(x^2/(4*Dx*t))]
Plot[{f[x,0.1],f[x,0.2],f[x,0.4]},{x,-3,3}, PlotRange->{0,1}]
```



Out[141]=

-Graphics-

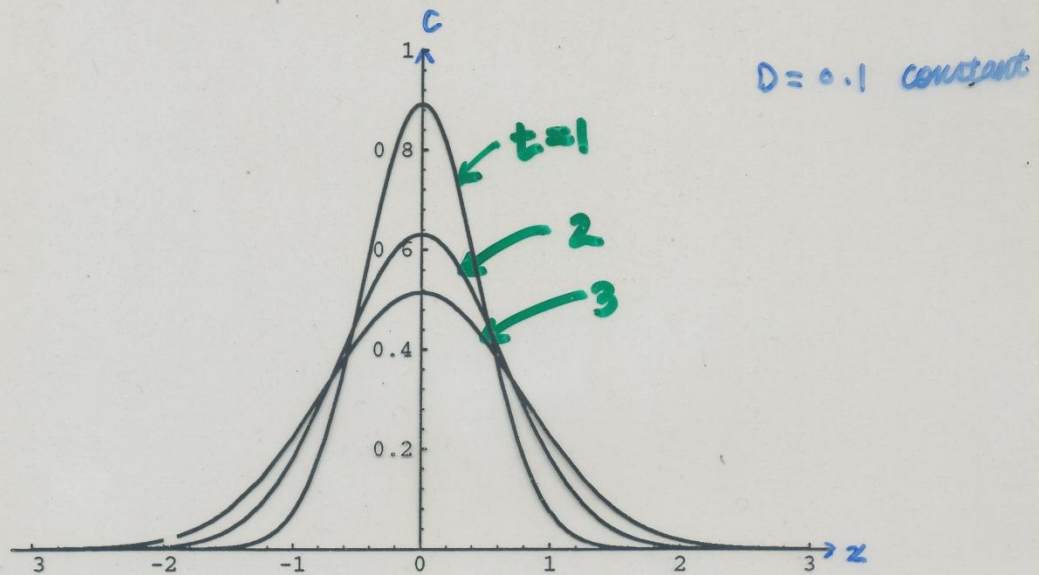
$$C = \underbrace{\frac{M}{\sqrt{4\pi Dt}}}_{c_p(t)} \exp\left\{-\frac{x^2}{4Dt}\right\}$$

decay (exponential)

- Peak concentration occurs at $x=0$ (When advection does not exist)
- Gaussian distribution ... symmetrical shape (normal)

$$\int_{-\infty}^{\infty} c_1 dx = \int_{-\infty}^{\infty} c_2 dx = \int_{-\infty}^{\infty} c_3 dx = M \text{ (for conservative substance)}$$

```
In[88]:=  
Dx=0.1;  
M=1;  
f[x_,t_]:= M/(Sqrt[4 Pi Dx t])*Exp[-(x^2/(4*Dx*t,))]  
g=Plot[{f[x,1],f[x,2],f[x,3]},{x,-3,3}, PlotRange->{0,1}]
```



```
Out[88]=  
-Graphics-
```

[Re] Boundary conditions

For the 1-D models, three boundary conditions are commonly encountered;

$$C(x = 0)$$

$$C(x = -\infty)$$

$$C(x = +\infty)$$

• Types of boundary conditions:

1) Constant concentration

$$C(x = 0, t) = C_0$$

2) Constant mass flux

a) Finite flux: $J_0 = -D \frac{\partial C}{\partial x} \Big|_{x=0}$

b) No flux: $\frac{\partial C}{\partial x} \Big|_{x=0} = 0$

3) Advective mass flux

$$J_0 = -D \frac{\partial C}{\partial x} \Big|_{x=0} = k_m [C(0, t) - C_\infty]$$

where k_m = mass transfer coefficient

[Re] Analytical solution by separation of variables

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (2.10)$$

$$C(x, t = 0) = M \delta(x) \quad (2.11a)$$

$$C(x = \pm\infty, t) = 0 \quad (2.11b)$$

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

Separation of variables

$$C(x, t) = F(x)G(t) \quad (2.12)$$

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

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

$$FG' = DGF''$$

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

where $k = \text{const.} \neq f_n(x \text{ or } t)$

i) $k > 0$

$$k = \omega^2$$

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

$$\rightarrow \begin{cases} F'' - \omega^2 F = 0 & (2.13a) \\ G' - D\omega^2 G = 0 & (2.13b) \end{cases}$$

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

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

Then

$$F = C_2 e^{-\omega x}$$

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 $C = F \cdot G = 0$ at all points, which is not true.

Therefore, $k \leq 0$

ii) $k = 0$

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

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

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

Therefore, $k < 0$

iii) $k < 0$

$$k = -p^2$$

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

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

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

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

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

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

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

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

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

$$= A \cos px + B \sin px \quad (2.14)$$

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

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

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

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

$$\therefore G = C_1 e^{-Dp^2 t} \quad (2.15)$$

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

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

Use Fourier integral for non-periodic function.

Assume $A, B = f_n(p)$

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

$$\begin{aligned} C(x,t) &= \int_0^\infty C(x,t;p) dp \\ &= \int_0^\infty \{A(p)\cos px + B(p)\sin px\} \exp(-Dp^2t) dp \end{aligned} \quad (2.18)$$

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

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

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

where $f(x)$ = 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

$$\begin{aligned}
 C(x, 0) &= \frac{1}{\pi} \int_0^{\infty} \left\{ \int_{-\infty}^{\infty} f(v) \cos px \sin pv dv + \int_{-\infty}^{\infty} f(v) \sin px \sin pv dv \right\} dp \\
 &= \frac{1}{\pi} \int_0^{\infty} \left\{ \int_{-\infty}^{\infty} f(v) \cos(px - pv) dv \right\} dp
 \end{aligned} \tag{2.19}$$

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

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

Switch order of integral

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

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

Use residue theorem to get integral of (e)

$$\int_0^{\infty} e^{-s^2} \cos 2bs ds = \frac{\sqrt{\pi y}}{2} e^{-b^2} \tag{2.21}$$

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

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

(e) becomes

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

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

$$\begin{aligned} C(x,t) &= \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} f(v) \exp\left\{-\frac{(x-v)^2}{4Dt}\right\} dv \\ &= \frac{1}{\sqrt{4\pi Dt}} \lim_{\varepsilon \rightarrow 0} \int_{-\varepsilon}^{\varepsilon} f(v) \exp\left\{-\frac{(x-v)^2}{4Dt}\right\} dv \\ &= \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) \end{aligned} \quad (2.23)$$

2.2 The Random Walk and Molecular Diffusion

• Two different ways for the molecular diffusion

- 1) study the statistics of motion of single molecule or particle and generalizing
→ random walk model
- 2) study the integrated effect of random motion of a large number of particles
simultaneously → gradient-flux equation

2.2.1 The Random Walk

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

→ whether the step is forward or backward is entirely random

Use central limit theorem → in the limit of many steps probability of the particle being

$m\Delta x$ between and $(m+1)\Delta x$ is the normal distribution

mean: $\mu = 0$

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

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

Designate $\sigma^2 = \frac{t(\Delta x)^2}{\Delta t} = 2Dt$

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

Now think whole group of particles

$$C(x,t) = \iint p(x,t) dx dn$$

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

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

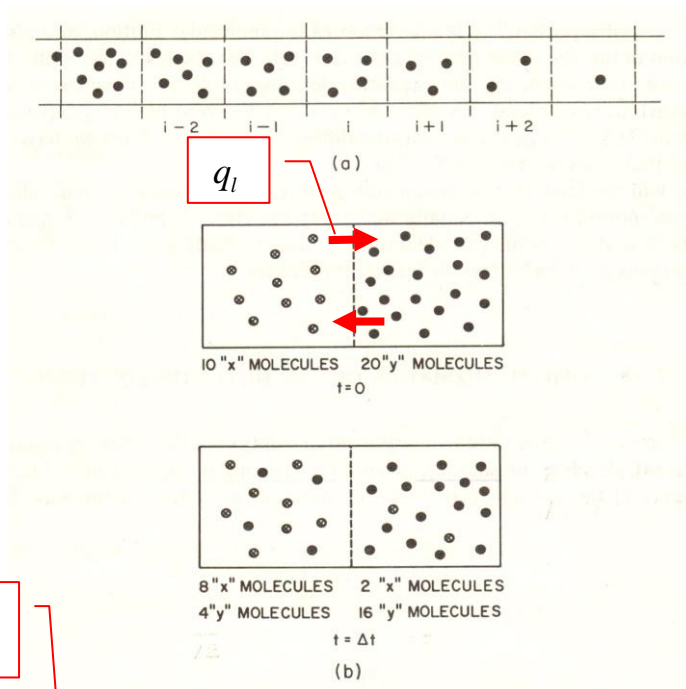
2.2.2 The Gradient-Flux Relationship

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.

Consider flux of material across the bounding surface



Mass transfer per unit time

$$q_l = kM_l - \text{flux of material from left to right}$$

$$q_r = kM_r - \text{flux of material from right to left}$$

where $k =$ transfer probability $[1/t] \rightarrow$ mass transfer coefficient

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

$$q = k(M_l - M_r) \quad (a)$$

Define

$$\bar{M}_l = C_l \text{Vol} = C_l \Delta x$$

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

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

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

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

Combine (b) and (c)

$$\begin{aligned} \bar{M}_l - \bar{M}_r &= \Delta x(C_l - C_r) \\ &= (\Delta x)^2 \left[-\frac{C_r - C_l}{\Delta x} \right] \\ &\approx (\Delta x)^2 \left[-\frac{\partial C}{\partial x} \right] \text{if } \Delta x \text{ is small} \quad (d) \end{aligned}$$

Substitute (d) into (a)

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

$$= -D \frac{\partial C}{\partial x} \Rightarrow \text{Fick's law}$$

$$D = k(\Delta x)^2 \Rightarrow \text{Diffusion coefficient (constant)}$$

→ Convert mass transfer model to diffusion model

[Re] Two basic models for diffusion

- 1) Diffusion model (Fick's law)

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

q = mass flux per unit time and unit area

D = diffusion coefficient [L^2/t] → distributed parameter

- 2) Mass transfer model

$$q_t = k\Delta C$$

q_t = mass transfer per unit time

k = mass transfer coefficient [$1/t$] → lumped parameter

2.3 Some Mathematics of the Diffusion Equation

2.3.1 Concentration Distribution

G.E. and BCs for instantaneous point source

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

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

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

The solution is

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

→ Gaussian distribution (Normal distribution if $M = 1$)

[Re] M

For 1D model, $M = \text{total mass} / \text{area}$ → plane source

For 2D model, $M = \text{total mass} / \text{length}$ → line source

For 3D model, $M = \text{total mass}$ → point source

2.3.2 Moments of Concentration Distribution

1. Moments

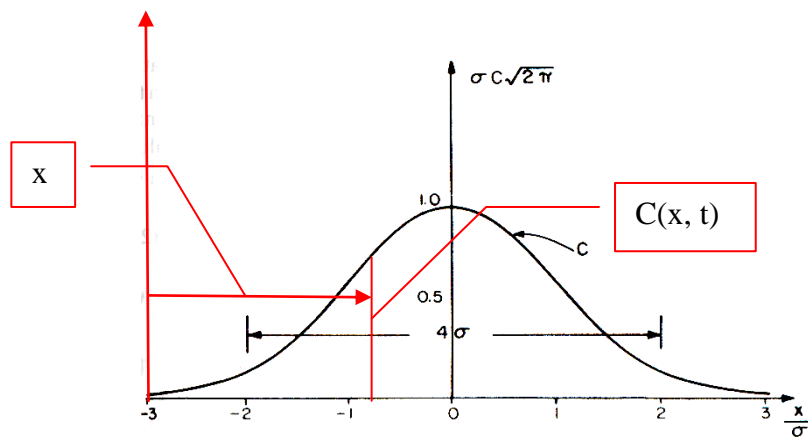
Moments of concentration distributions are defined as

$$0\text{th moment} = M_0 = \int_{-\infty}^{\infty} C(x,t) dx$$

$$1\text{st moment} = M_1 = \int_{-\infty}^{\infty} C(x,t) x dx$$

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

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



i) Mass: $M = M_0$

ii) Mean: $\mu = M_1 / M_0$

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

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

- measure of skew

- For normal dist., $S_t = 0$

Normal distribution is given as

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

$$E(x) = \mu; \quad \text{Var}(x) = \sigma^2$$

For concentration distribution, substitute $\mu = 0, \sigma = \sqrt{2Dt}$

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

Then, $M_0 = 1$

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

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

2. Diffusion coefficient

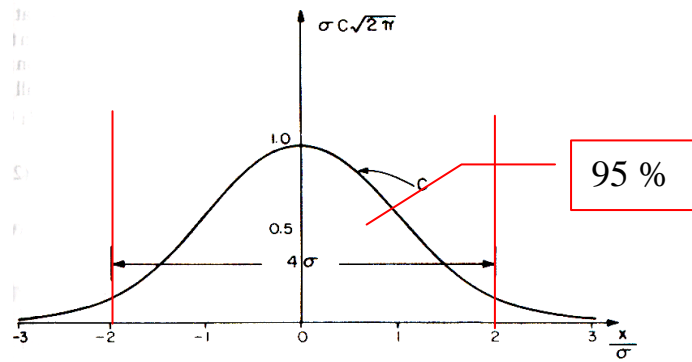
Measure of spread of dispersing tracer

$$\sigma = \sqrt{2Dt} \Rightarrow \text{standard deviation (see Table 2.1)} \quad (a)$$

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

\Rightarrow include 95% of the total mass

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



• Calculation of diffusion coefficient

\rightarrow change of moment method

Start from (a)

$$Dt = \frac{1}{2} \sigma^2$$

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

(2.22)

i) For 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

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

$\int uv' = uv - \int u'v$

Apply integration by parts into right hand side

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

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

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

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

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

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

Now, multiply each side of Eq. (a) by x

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

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

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

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

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

$\rightarrow \mu$ is independent of time.

By the way,

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

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

Combine Eq.(b) 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

a) Calculate diffusion coefficient from 2 concentration curves

Start 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)

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

Rearrange

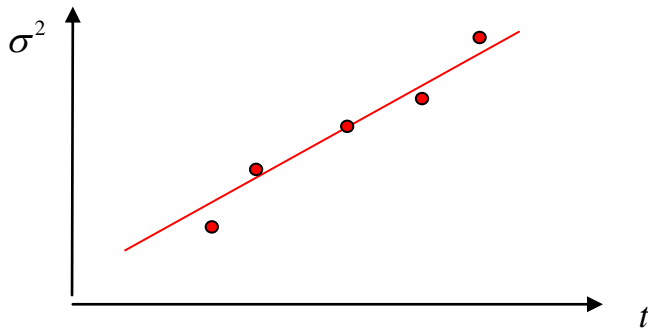
$$D = \frac{1}{2} \frac{\sigma_2^2 - \sigma_1^2}{t_2 - t_1} \quad (2.26)$$

σ_1^2 = variance of concentration distribution at $t = t_1$

σ_2^2 = variance of concentration distribution at $t = t_2$

b) Calculate diffusion coefficient from more than 2 curves

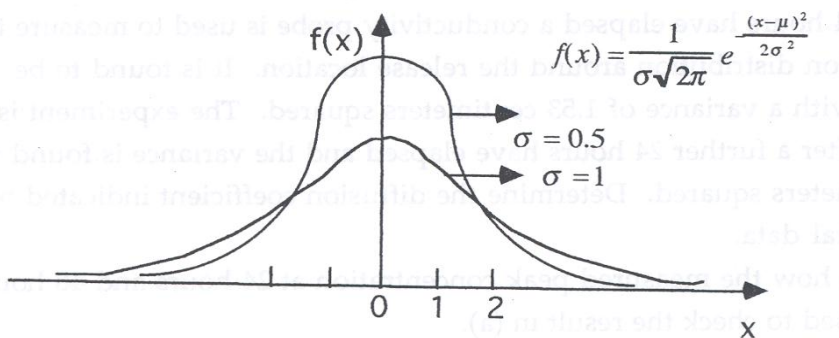
$$\rightarrow D = \frac{1}{2} (\text{slope of } \sigma^2 \text{ vs } t \text{ curve})$$



[Re] Normal (Gaussian) distribution

- bell-formed distribution occur around a mean value

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



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

G.E.:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (2.31)$$

B.C.:

Series 1: instantaneous inputs

Series 2: continuous inputs

Series 3: instantaneous inputs with boundary walls

Series 4: instantaneous inputs in 2D & 3D fluids

Series 5: advective diffusion

Series 6: maintained point discharges in 2D & 3D flows

Problem 1-1: initial slug of mass M introduced instantaneously at time zero at the x origin

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

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

Solution:

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

2.4.1 An Initial Spatial Distribution $C(x, 0)$

(1) Mass M released at time $t = 0$ at the point $x = \xi$ → **Problem 1-2**

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

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

Set $X = x - \xi$

Then, I.C. becomes

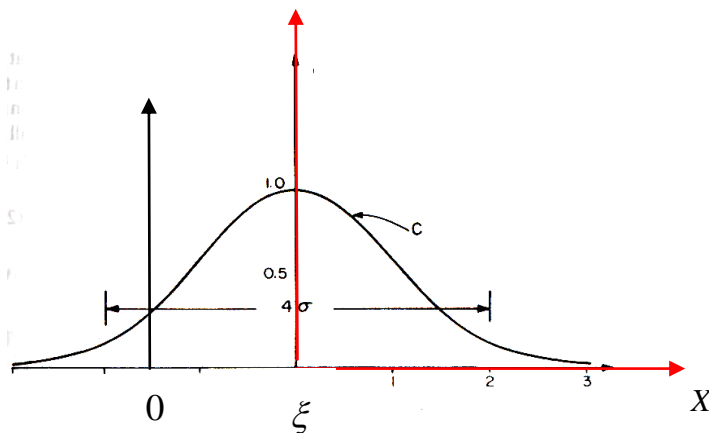
$$C(X, 0) = M \delta(X)$$

Solution is

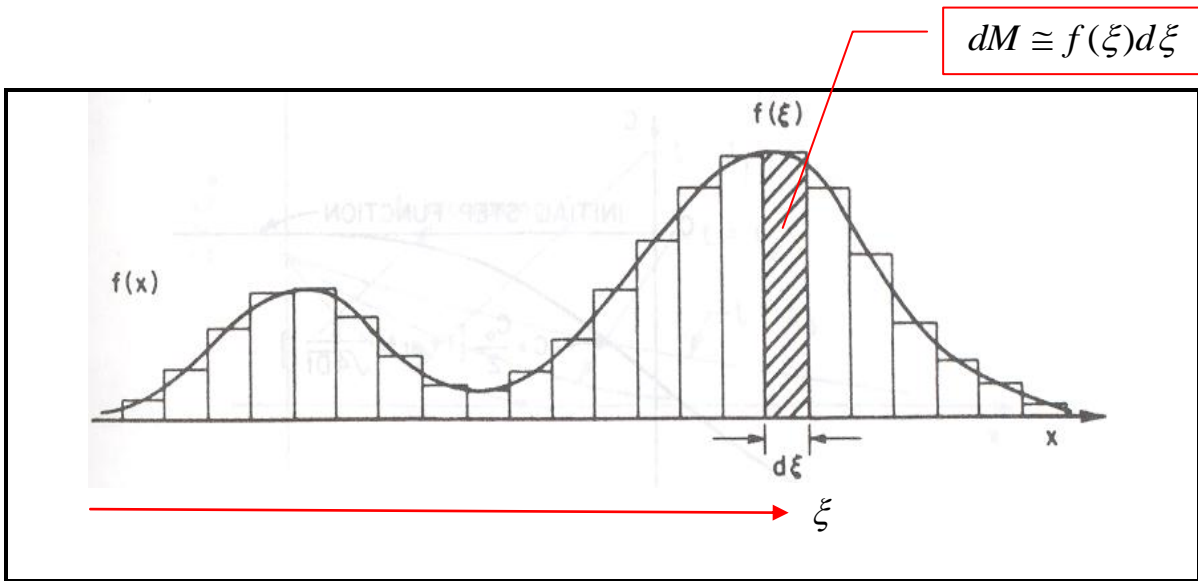
$$C(X, t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left[\frac{-X^2}{4Dt}\right]$$

Convert X into x

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



(2) Distributed source at time $t = 0 \rightarrow$ **Problem 1-3**



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

$f(x) \sim$ arbitrary function

Assume that

- the initial input 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

Approximate $f(x)$ by a series of slugs each containing mass $f(\xi)d\xi$

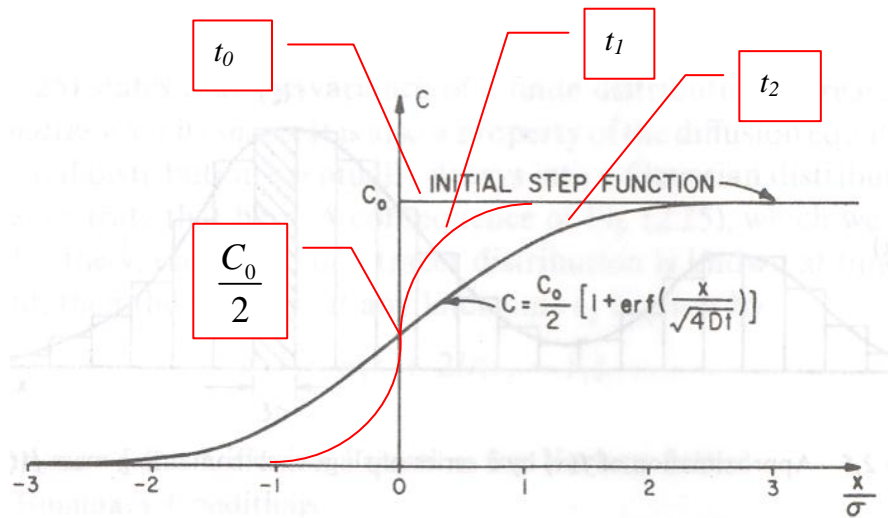
$$dC(x,t) = \frac{f(\xi)d\xi}{\sqrt{4\pi Dt}} \exp\left[\frac{-(x-\xi)^2}{4Dt}\right]$$

Then, total contribution from all slugs is the integral sum of all the individual contributions

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

\rightarrow superposition integral

(3) Distributed source with step function, C_0 for $x > 0 \rightarrow$ **Problem 1-4**



Consider a particular case where $f(x)$ is given by a step function

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

According to (2.30), solution is given as

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

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

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

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

$$du = \frac{-d\xi}{\sqrt{4Dt}} \rightarrow d\xi = -\sqrt{4Dt} du$$

(b)

Substitute (b) into (a)

$$\begin{aligned}
 C(x,t) &= \frac{C_0}{\sqrt{\pi}} \int_{-\infty}^{\frac{x}{\sqrt{4Dt}}} e^{-u^2} du \\
 &= \frac{C_0}{2} \left[\frac{2}{\sqrt{\pi}} \int_{-\infty}^0 e^{-u^2} du + \frac{2}{\sqrt{\pi}} \int_0^{\frac{x}{\sqrt{4Dt}}} e^{-u^2} du \right] \\
 &= \frac{C_0}{2} \left[1 + \frac{2}{\sqrt{\pi}} \int_0^{\frac{x}{\sqrt{4Dt}}} e^{-u^2} du \right] \\
 &= \frac{C_0}{2} \left[1 + \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right] \\
 \boxed{C(x,t) = \frac{C_0}{2} \left[1 + \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right]} & \qquad (2.33)
 \end{aligned}$$

$$\operatorname{erf} z = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-\xi^2) d\xi$$

[Re] Error function

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

$$\operatorname{erf}(\infty) = \frac{2}{\sqrt{\pi}} \int_0^\infty \exp(-\xi^2) d\xi = 1$$

[Re] Normal distribution

- Most important distribution in statistical application since many measurements have approximately normal distributions.

- The random variable X has a normal distribution if its p.d.f. is defined by

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

- Integral of normal distribution

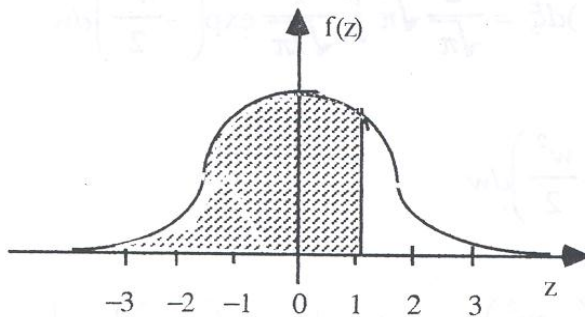
$$I = \int_{-\infty}^{\infty} \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] dx$$

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

Then,

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

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



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

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

(4) Distributed source with step function C_0 for $x < 0 \rightarrow$ **Problem 1-5**

Consider instantaneous input of step function

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

Solution by line source of $C_0\delta\xi$ is given as

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

Then, total contribution is

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

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

$$\text{Then } d\eta = -\frac{d\xi}{\sqrt{4Dt}}$$

$$\xi = -\infty \rightarrow \eta = \infty$$

$$\xi = 0 \rightarrow \eta = \frac{x}{\sqrt{4Dt}}$$

Substituting this relation yields

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

$$\begin{aligned}
&= \frac{C_0}{2} \left[\frac{2}{\sqrt{\pi}} \int_0^{\infty} \exp(-\eta^2) d\eta - \frac{2}{\sqrt{\pi}} \int_0^{x/\sqrt{4Dt}} \exp(-\eta^2) d\eta \right] \\
&= \frac{C_0}{2} \left[1 - \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right] \\
&= \frac{C_0}{2} \operatorname{erfc} \left(\frac{x}{\sqrt{4Dt}} \right)
\end{aligned}$$

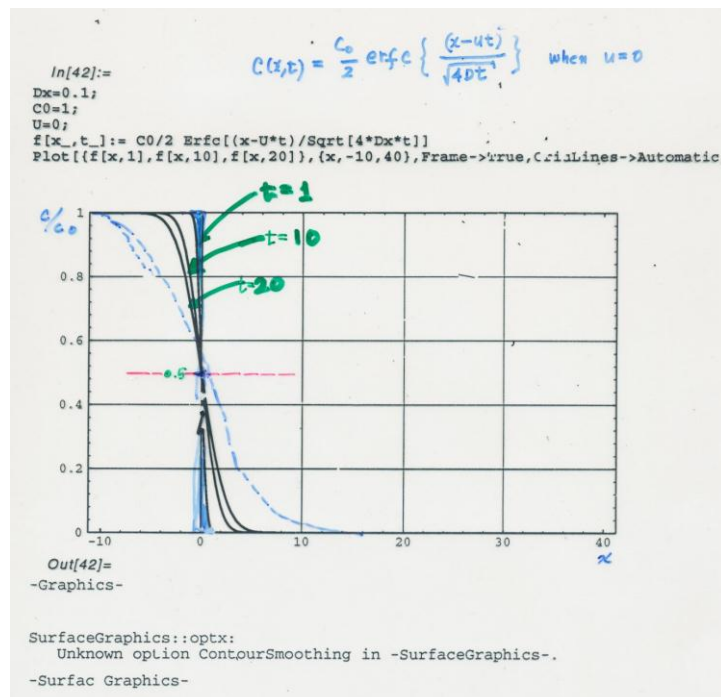
$$C(x,t) = \frac{C_0}{2} \left[1 - \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right] = \frac{C_0}{2} \operatorname{erfc} \left(\frac{x}{\sqrt{4Dt}} \right)$$

→ complementary error function

→ summing the effect of a series of line sources, each yielding an exponential of distribution

[Re] complementary error function

$$\operatorname{erfc}(z) = 1 - \operatorname{erf}(z)$$

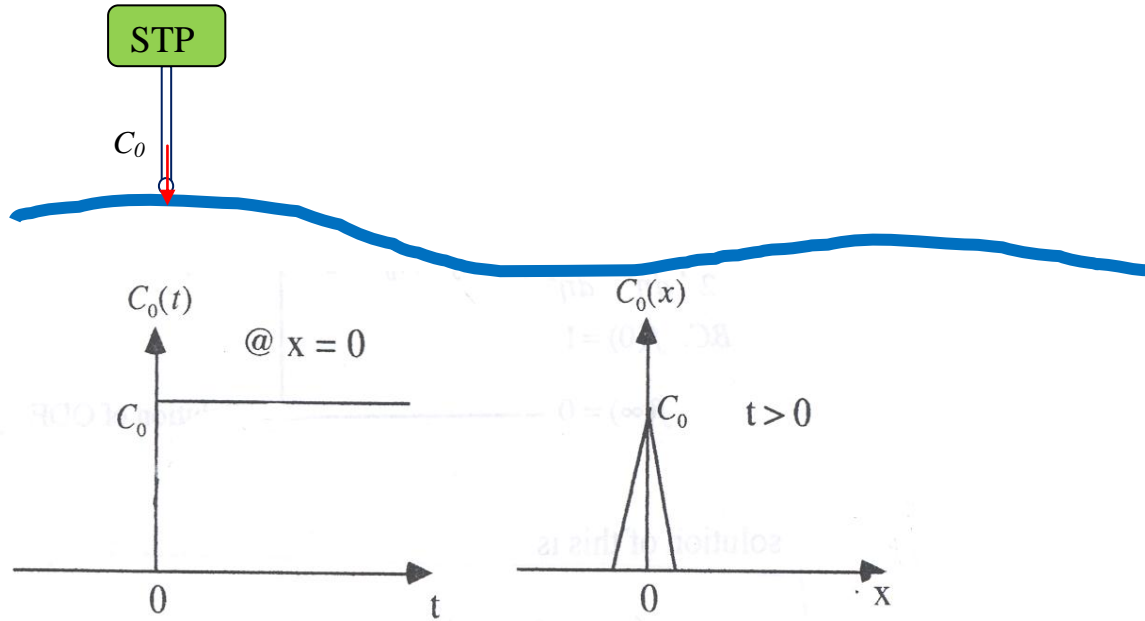


• Summary of solutions for instantaneous inputs (Series 1)

Case	Initial and boundary conditions	Solution
1-1	M introduced instantaneously at time zero at the x origin	$C(X,t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left[\frac{-x^2}{4Dt}\right]$
1-2	M released at time $t = 0$ at the point $x = \xi$	$C(x,t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left[\frac{-(x-\xi)^2}{4Dt}\right]$
1-3	Distributed source at time $t = 0$ $C(x,0) = f(x)$ for $-\infty < x < \infty$	$C(x,t) = \int_{-\infty}^{\infty} \frac{f(\xi)}{\sqrt{4\pi Dt}} \exp\left[\frac{-(x-\xi)^2}{4Dt}\right] d\xi$
1-4	Distributed source with step function $C(x,0) = C_0$ for $x > 0$	$C(x,t) = \frac{C_0}{2} \left[1 + \operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right) \right]$
1-5	Distributed source with step function $C(x,0) = C_0$ for $x < 0$	$C(x,t) = \frac{C_0}{2} \left[1 - \operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right) \right]$

2.4.2 Concentration Specified as a Function of Time

(1) **Continuous** input with step function $C_0 = C_0(t) \rightarrow$ **Problem 2-1**



Consider continuous input with 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

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

$$\text{Set } \eta = \frac{x}{\sqrt{Dt}}$$

$$\frac{\partial \eta}{\partial t} = \frac{x}{\sqrt{D}} \left(-\frac{1}{2}\right) t^{-\frac{3}{2}} = -\frac{1}{2t} \frac{x}{\sqrt{Dt}} = -\frac{1}{2t} \eta$$

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

Then

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

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

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

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

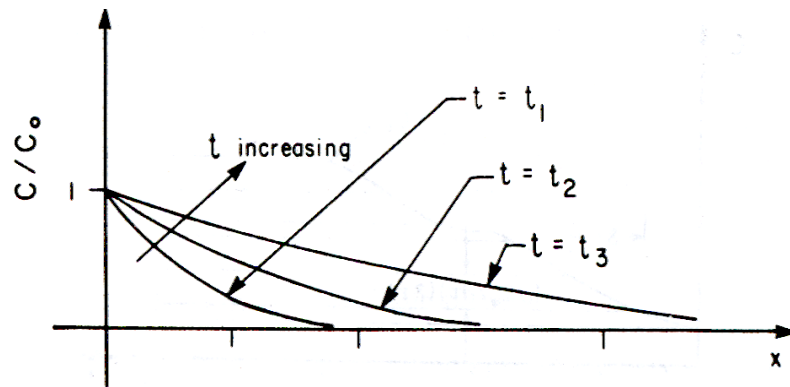
$$2f'' + \eta f' = 0 \tag{a}$$

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

$$f(\infty) = 0$$

Solution of this is

$$C = C_0 \left[1 - \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right] = C_0 \operatorname{erfc} \left(\frac{x}{\sqrt{4Dt}} \right) \quad x > 0 \tag{2.37}$$



[Re] Laplace transformation

For ODE, it transforms ODE into algebraic problem.

For PDE, it transforms 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")

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

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

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

[Re] Analytical solution by Laplace transformation

Consider advection-diffusion equation as G.E.

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

B.C. & I.C. for continuous input are given as

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

$$C(x \geq 0, t = 0) = 0 \quad (b)$$

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

Rewrite G.E.

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

Apply Laplace transformation

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

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

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

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

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

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

Derive characteristic equation as

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

Solution is

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

Then, \bar{C} is

$$\begin{aligned} \bar{C} &= C_1 e^{-\lambda_1 x} + C_2 e^{-\lambda_2 x} \\ &= C_1(s) \exp\left\{\frac{U + \sqrt{U^2 + 4sD}}{2D} x\right\} + C_2(s) \exp\left\{\frac{U - \sqrt{U^2 + 4sD}}{2D} x\right\} \quad (1) \end{aligned}$$

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

$$\begin{aligned} \lim_{x \rightarrow \infty} \bar{C}(x, s) &= \lim_{x \rightarrow \infty} \int_0^{\infty} e^{-st} C(x, t) dt \\ &= \int_0^{\infty} \left\{ e^{-st} \lim_{x \rightarrow \infty} C(x, t) dt \right\} = 0 \end{aligned}$$

If we apply this to Eq. (1)

$$\begin{aligned} \lim_{x \rightarrow \infty} \bar{C}(x, s) &= \lim_{x \rightarrow \infty} \left[C_1(s) \exp\left\{\frac{U + \sqrt{U^2 + 4sD}}{2D} x\right\} \right] \\ &\quad + \lim_{x \rightarrow \infty} \left[C_2(s) \exp\left\{\frac{U - \sqrt{U^2 + 4sD}}{2D} x\right\} \right] = 0 \end{aligned}$$

$\therefore C_1(s)$ should be zero

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

Apply B.C., Eq. (a)

Laplace transformation

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

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

$$\begin{aligned} \therefore \bar{C} &= \frac{C_0}{s} \exp\left\{\frac{U - \sqrt{U^2 + 4sD}}{2D} x\right\} \\ &= C_0 \exp\left(\frac{Ux}{2D}\right) \frac{1}{s} \exp\left(-\frac{x}{\sqrt{D}} \sqrt{\frac{U^2}{4D} + s}\right) \end{aligned}$$

Get inverse Laplace transformation using Laplace transform table

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

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

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

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

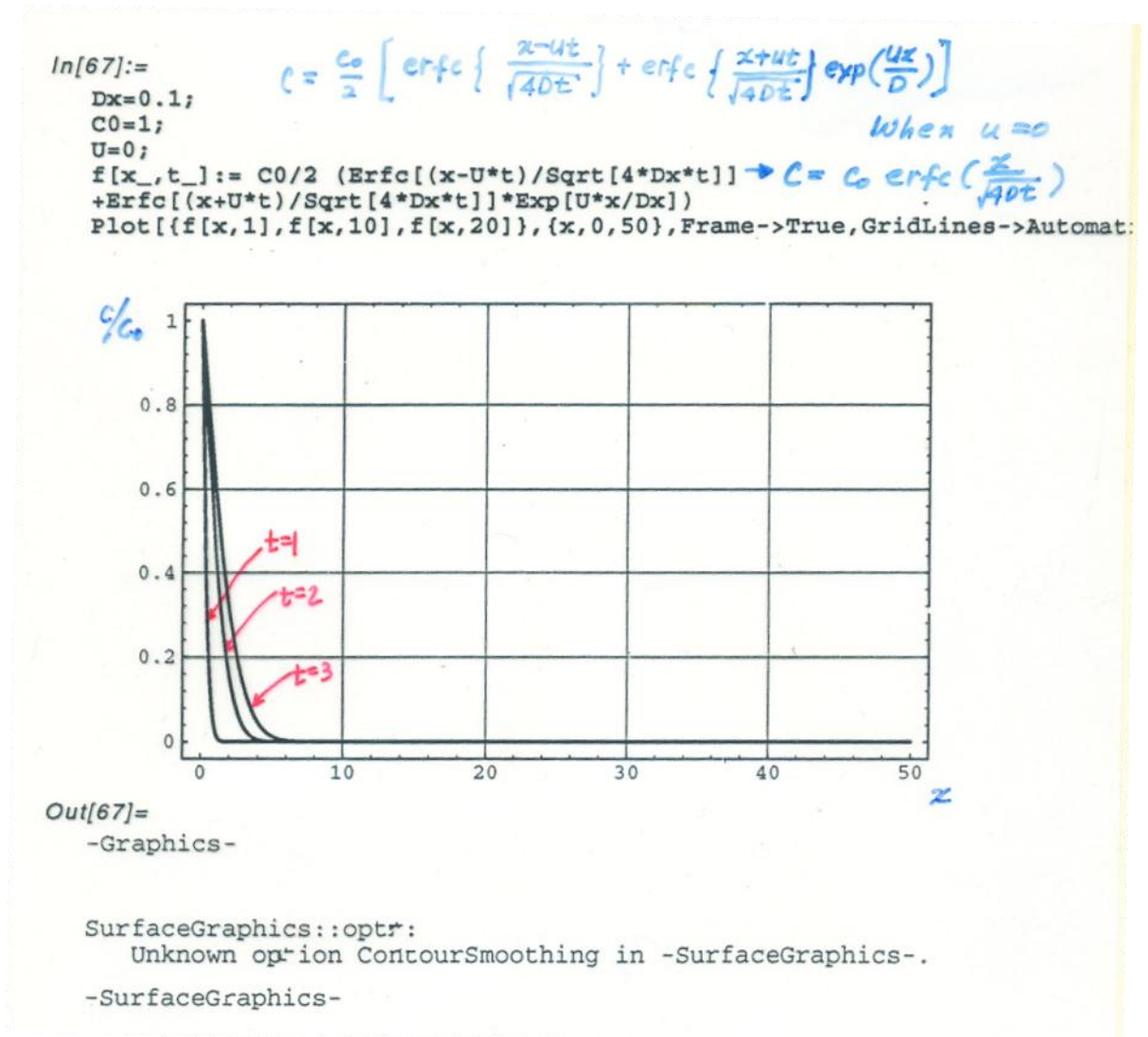
$$\frac{a}{2\sqrt{t}} - b\sqrt{t} = \frac{x/\sqrt{D}}{2\sqrt{t}} - \frac{U}{2\sqrt{D}} \sqrt{t} = \frac{x - Ut}{\sqrt{4Dt}}$$

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

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

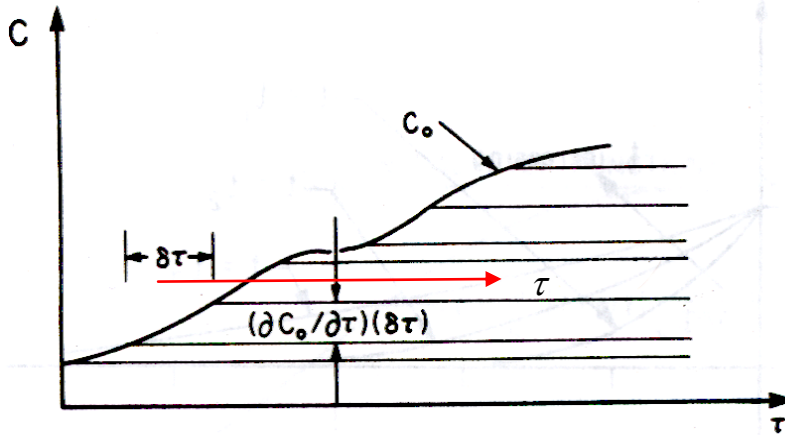
In case $U=0$

$$C = \frac{C_0}{2} \left\{ \operatorname{erfc}\left(\frac{x}{\sqrt{4Dt}}\right) + \operatorname{erfc}\left(\frac{x}{\sqrt{4Dt}}\right) \right\} = C_0 \operatorname{erfc}\left(\frac{x}{\sqrt{4Dt}}\right) \quad (2.37)$$



(2) Concentration specified as a function of time at fixed point → **Problem 2-2**

Consider the case where $C_0(\tau)$ is a time variable concentration at $x = 0$



I.C. and B.C. are

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

$$C(x = 0, t > 0) = C_0(\tau)$$

The solution is obtained by a superposition of solution, (2.37).

In each time increment $\delta\tau$ the concentration at $x = 0$ changes by an amount $\frac{\partial C}{\partial \tau} \delta\tau$.

Thus, for a change occurring at time τ the result for all future times, due to the incremental changes, is given as

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

Then, total contribution is

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

2.4.3 Input of mass specified as a function of time

(1) Continuous injection of mass at the rate \dot{M} , $-\infty < t < \infty \rightarrow$ **Problem 2-3**

We can assume that a continuous injection of mass at the rate \dot{M} (M/t) is equivalent to injecting a slug of amount $\dot{M} \delta\tau$ after each time increment $\delta\tau$.

Then, the concentration resulting from the continuous injection is the sum of the concentrations resulting from the individual slugs injected at all time prior to the time of observation.

Thus, concentration resulting from the individual slug is

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

Total contribution is

$$C = \int_{-\infty}^t \frac{\dot{M}(\tau)}{\sqrt{4\pi D(t-\tau)}} \exp\left[-\frac{x^2}{4D(t-\tau)}\right] d\tau \tag{2.41}$$

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} , $t > 0 \rightarrow$ **Problem 2-4**

Eq. (2.41) gives

$$C(x,t) = \frac{\dot{M}}{\sqrt{4\pi D}} \int_0^t \frac{1}{\sqrt{t-\tau}} \exp\left[-\frac{x^2}{4D(t-\tau)}\right] d\tau \tag{1}$$

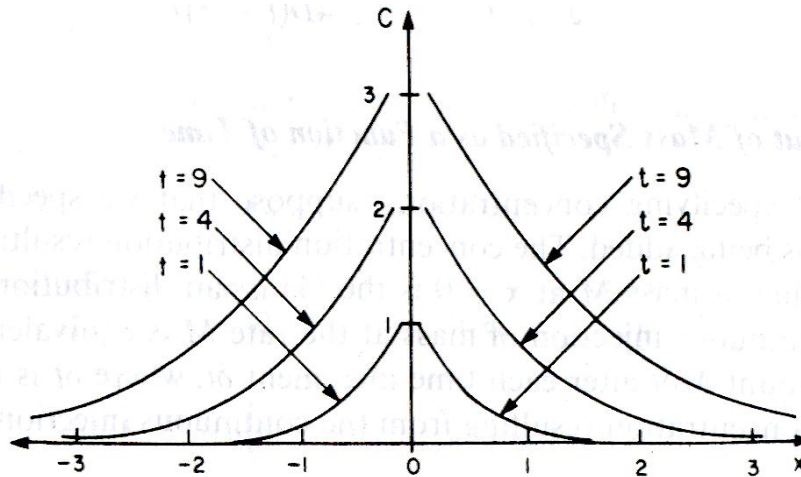
Set $u = \frac{4D(t-\tau)}{x^2}$

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

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

Then, substituting this into (1) yields

$$C(x,t) = \frac{\dot{M}x}{4D\sqrt{\pi}} \int_0^{\frac{4Dt}{x^2}} u^{-\frac{1}{2}} \exp\left(-\frac{1}{u}\right) du \quad (2.42)$$



(3) Continuous injection of distributed source of mass $m(x, t) \rightarrow$ **Problem 2-5**

\rightarrow superposition in space and then in time to get solution

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

$$C(x,t) = \int_{-\infty}^t \int_{-\infty}^{\infty} \frac{m(\xi, \tau)}{\sqrt{4\pi D(t-\tau)}} \exp\left[-\frac{(x-\xi)^2}{4D(t-\tau)}\right] d\xi d\tau \quad (2.43)$$

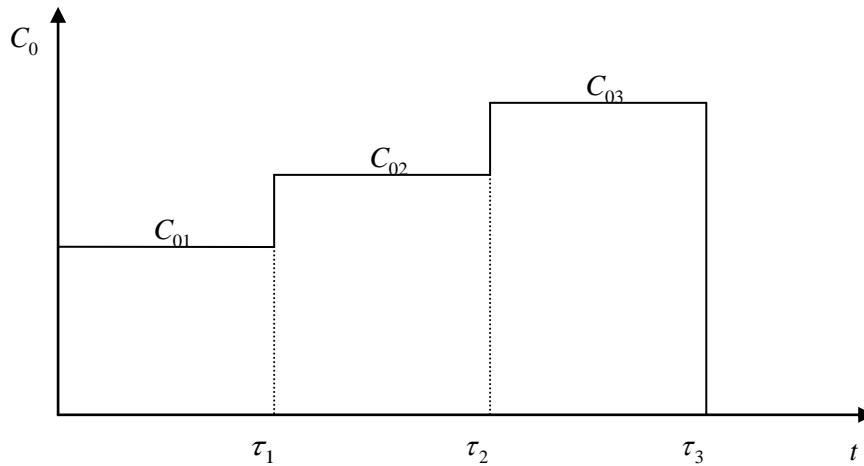
• Summary of solutions for continuous inputs (Series 2)

Cas e	Initial and boundary conditions	Solution
2-1	Continuous input with step function $C_0 = C_0(t)$	$C(x,t) = C_0 \left[1 - \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right] = C_0 \operatorname{erfc} \left(\frac{x}{\sqrt{4Dt}} \right)$
2-2	$C_0(\tau)$ as a time variable concentration at $x = 0$	$C(x,t) = \int_{-\infty}^t \frac{\partial C_0}{\partial \tau} \operatorname{erfc} \left(\frac{x}{\sqrt{4D(t-\tau)}} \right) d\tau$
2-3	Continuous injection of mass at the rate \dot{M} , $-\infty < t < \infty$	$C(x,t) = \int_{-\infty}^t \frac{\dot{M}(\tau)}{\sqrt{4\pi D(t-\tau)}} \exp \left[-\frac{x^2}{4D(t-\tau)} \right] d\tau$
2-4	Continuous injection of mass of constant strength \dot{M} , $t > 0$	$C(x,t) = \frac{\dot{M}x}{4D\sqrt{\pi}} \int_0^{\frac{4Dt}{x^2}} u^{-\frac{1}{2}} \exp(-\frac{1}{u}) du$
2-5	Continuous injection of distributed source of mass $m(x, t)$	$C(x,t) = \int_{-\infty}^t \int_{-\infty}^{\infty} \frac{m(\xi, \tau)}{\sqrt{4\pi D(t-\tau)}} \exp \left[-\frac{(x-\xi)^2}{4D(t-\tau)} \right] d\xi d\tau$

Homework #2-2

Due: 1 week from today

Consider pulse input of concentration specified as a step function



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

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

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

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

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

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

a) Derive analytical solution using Laplace transformation.

b) Plot C vs x for various time t with assumed C_0 s, for example, $C_{01} = C_0/2$; $C_{02} = C_0$;

$$C_{03} = \frac{3}{2}C_0.$$

c) Plot C vs t for various distance x .

2.4.4 Solution Accounting for Boundaries

- Consider 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 non-diffusive boundary at $x = -L$ → **Problem 3-1**

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

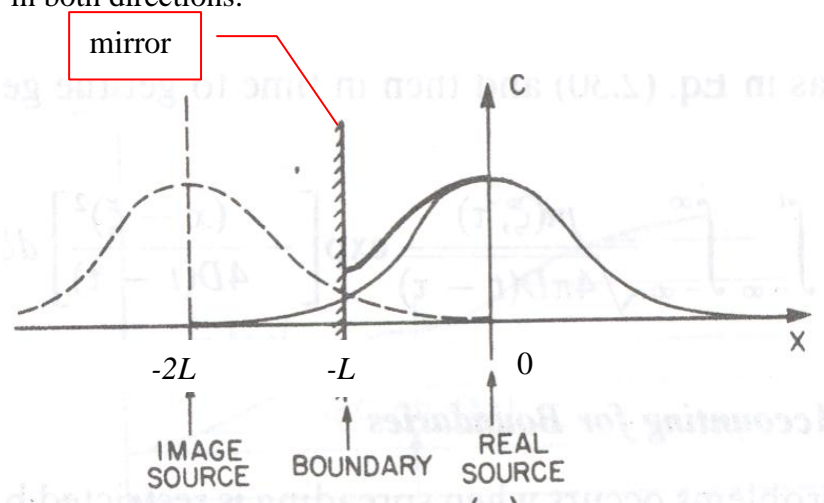
B.C.: wall through which concentration cannot diffuse located at $x = -L$

→ Fick's law for the boundary condition of no transport through the wall is

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

→ Concentration gradient must be zero at the wall.

→ This condition would be met if an additional unit mass of solute (image source) was concentrated at the point $x = -2L$, and if the wall was removed so that both slugs could diffuse to infinity in both directions.



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

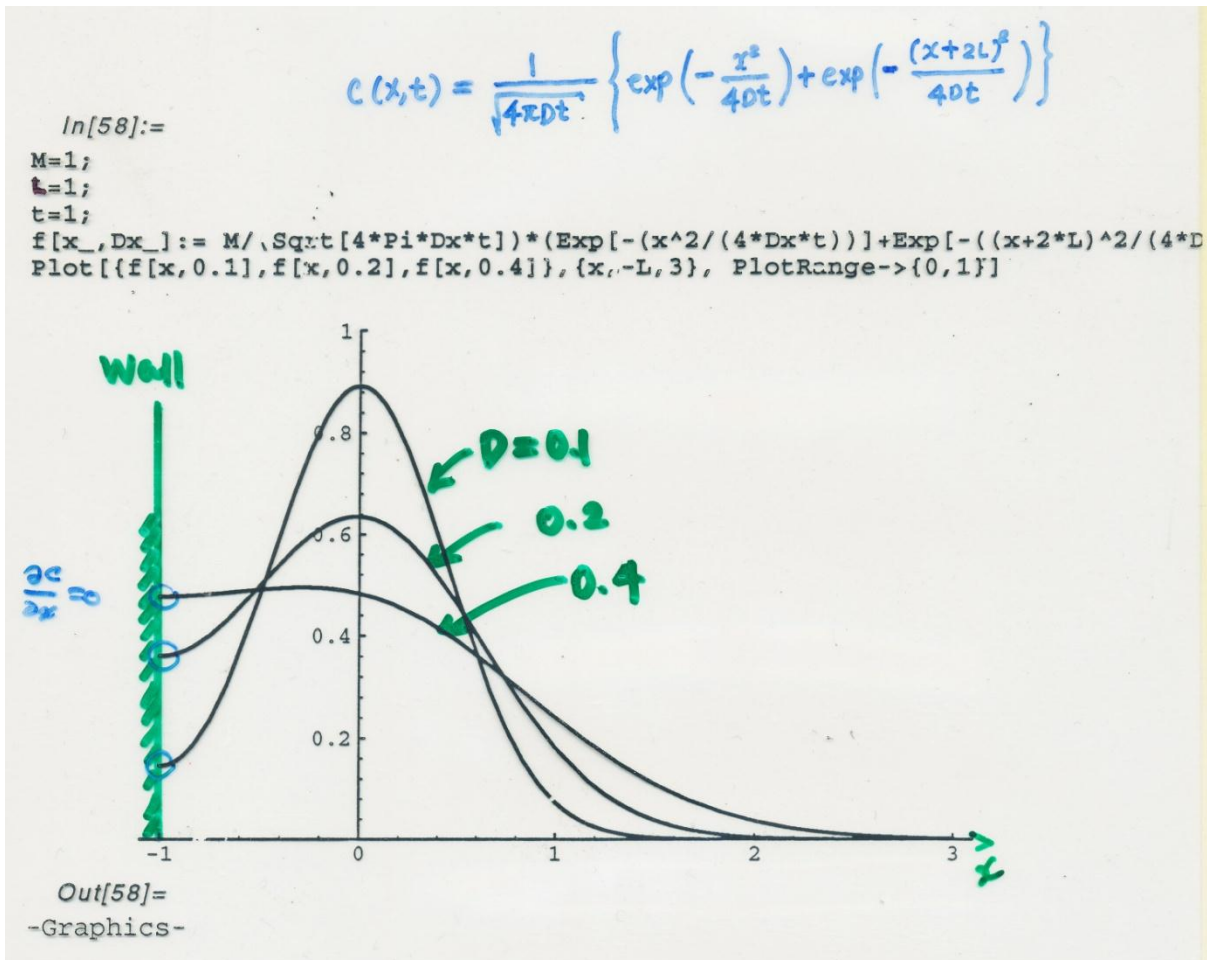
Unit mass;
M = 1

$x - (-2L)$

$$C = \frac{1}{\sqrt{4\pi Dt}} \left\{ \exp\left(-\frac{x^2}{4Dt}\right) + \exp\left(-\frac{(x+2L)^2}{4Dt}\right) \right\} \quad (2.44)$$

real source

image source



(2) Unit mass input $x = 0$ with non-diffusive boundaries at $x = -L$ and at $x = +L$

→ **Problem 3-2**

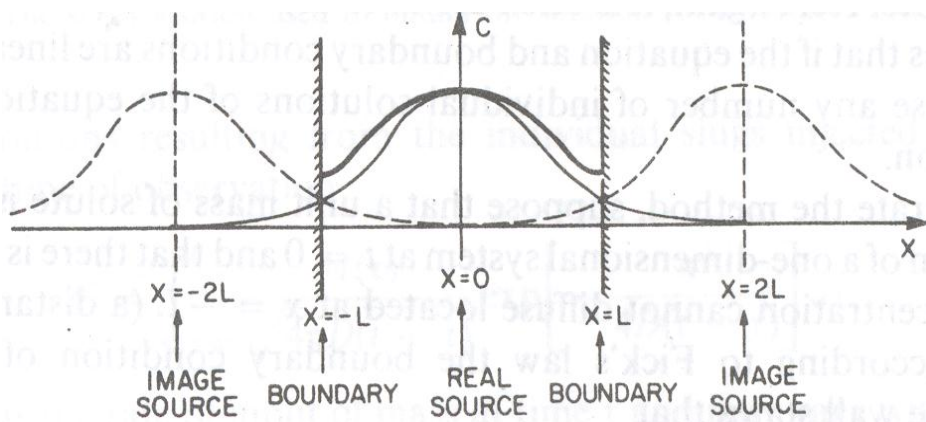
→ put image slugs at $-2L, +2L, 4L, -6L, 8L, \dots$

(∵ 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)

Then, solution is

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

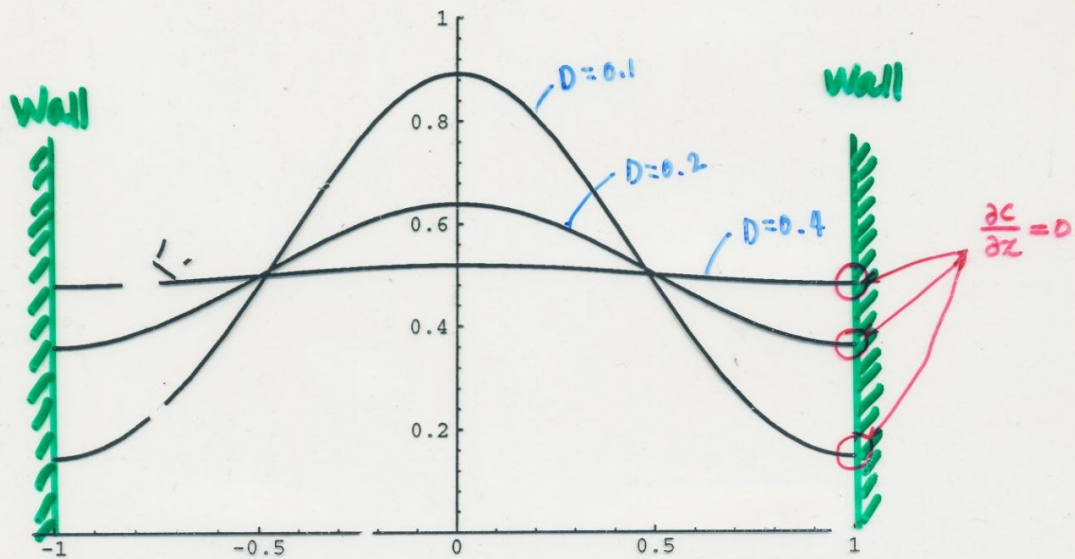
$$n = -2, -1, 0, +1, =2$$



```

In[43]:=
M=1;
L=1;
t=1;
f[x_,Dx_]:= M/(Sqrt[4 Pi Dx t])*(Exp[-(x^2/(4*Dx*t))]
+Exp[-((x+2*L)^2/(4*Dx*t))] +Exp[-((x+4*L)^2/(4*Dx*t))]
+Exp[-((x-2*L)^2/(4*Dx*t))] +Exp[-((x-4*L)^2/(4*Dx*t))])
Plot[{f[x,0.1],f[x,0.2],f[x,0.4]},{x,-L,L},PlotRange->{0,1}]

```



```

Out[43]=
-Graphics-

```

(3) Zero concentration at $x = \pm L \rightarrow$ **Problem 3-3**

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

\rightarrow $\left\{ \begin{array}{l} \text{negative image slugs at } x = \pm 2L \\ \text{positive image slugs at } x = \pm 4L \text{ etc.} \end{array} \right.$

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

(4) Mass input $x = 0$ with non-diffusive boundaries at $x = 0 \rightarrow$ **Problem 3-4**

\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

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

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

• Summary of solutions for instantaneous inputs with boundary walls (Series 3)

Case	Initial and boundary conditions	Solution
3-1	Mass input at $x = 0$ with non-diffusive boundary at $x = -L$	$C(x,t) = \frac{1}{\sqrt{4\pi Dt}} \left\{ \exp\left(-\frac{x^2}{4Dt}\right) + \exp\left(-\frac{(x+2L)^2}{4Dt}\right) \right\}$
3-2	Mass input $x = 0$ with non-diffusive boundaries at $x = \pm L$	$C(x,t) = \sum_{n=-\infty}^{\infty} \frac{1}{\sqrt{4\pi Dt}} \exp\left[\frac{-(x+2nL)^2}{4Dt}\right]$
3-3	Zero concentration at $x = \pm L$	$C(x,t) = \frac{1}{\sqrt{4\pi Dt}} \sum_{n=-\infty}^{\infty} \left\{ \begin{array}{l} \exp\left[\frac{-(x+4nL)^2}{4Dt}\right] \\ -\exp\left[\frac{-[x+(4n-2)L]^2}{4Dt}\right] \end{array} \right\}$
3-4	Mass input $x = 0$ with non-diffusive boundaries at $x = 0$	$C(x,t) = \frac{1}{\sqrt{\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$

2.4.5 Solutions in Two and Three Dimensions

(1) 2-D Fluid

- A mass M [M/L] deposited at $t = 0$ at $x = 0, y = 0 \rightarrow$ **Problem 4-1**

$$\text{G. E.: } \frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} \quad (2.49)$$

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

For molecular diffusion, $D_x = D_y = D$

use Product rule

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

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

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

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

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

Eq. (2.49) 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

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

$$M_x$$

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

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

$$M = \int \int_{-\infty}^{\infty} C \, dx dy$$

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

→ lines of constant concentration = set of concentric ellipses

▪ Iso-concentration lines

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

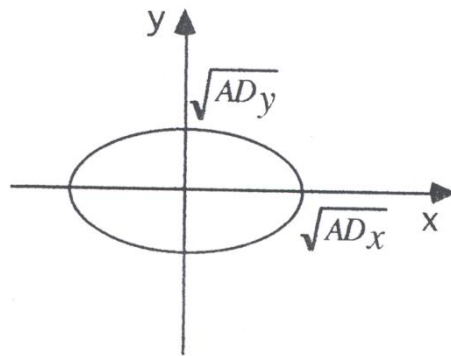
$$e^{\left(-\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t}\right)} = \frac{4\pi t \sqrt{D_x D_y} C}{M}$$

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

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

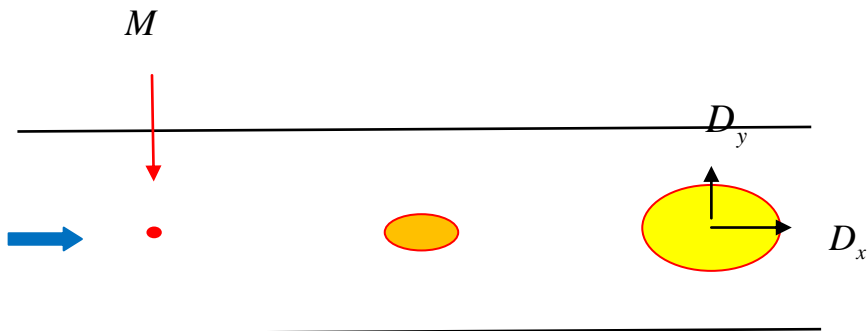
$$\frac{x^2}{(\sqrt{D_x})^2} + \frac{y^2}{(\sqrt{D_y})^2} = A$$

$$\frac{x^2}{(\sqrt{AD_x})^2} + \frac{y^2}{(\sqrt{AD_y})^2} = 1 \rightarrow \text{ellipses}$$



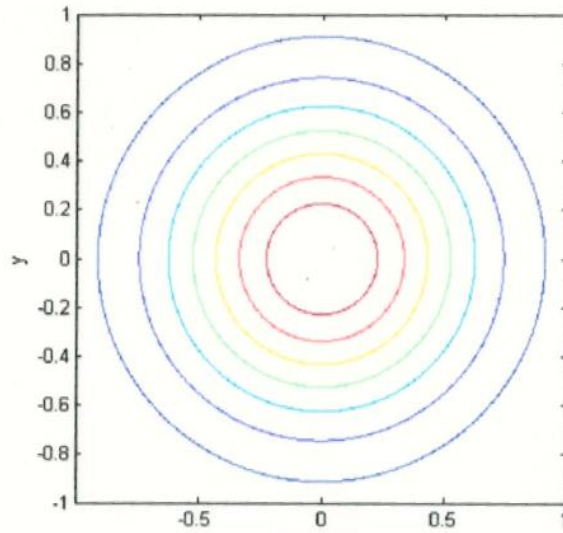
If $D_x = D_y$

Then, $x^2 + y^2 = R^2 \rightarrow \text{circle}$

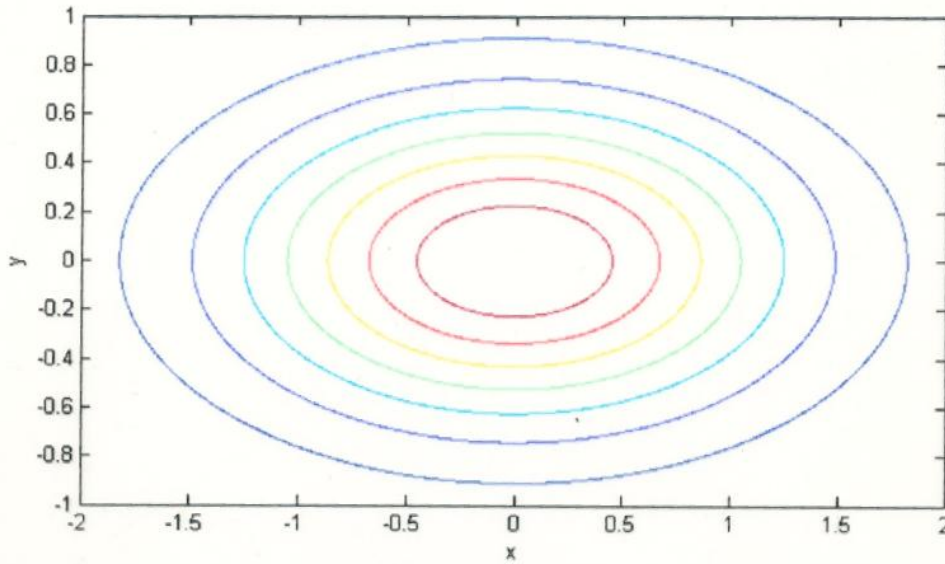


-Contour Graphics-

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



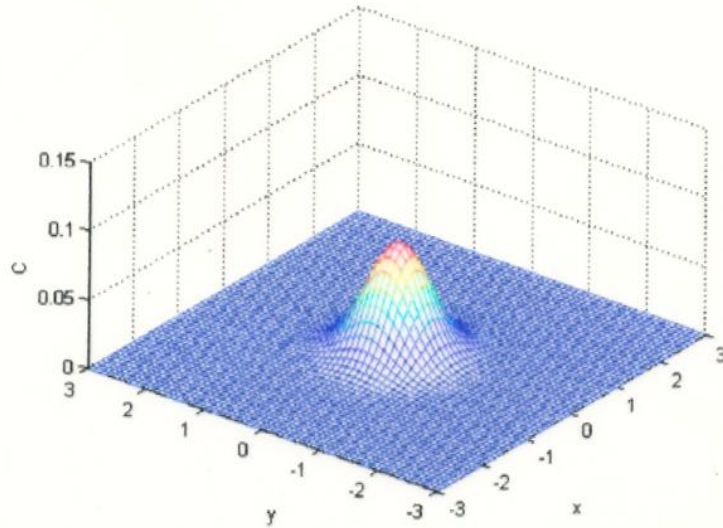
$(D_x = D_y = 0.1, M = 1)$



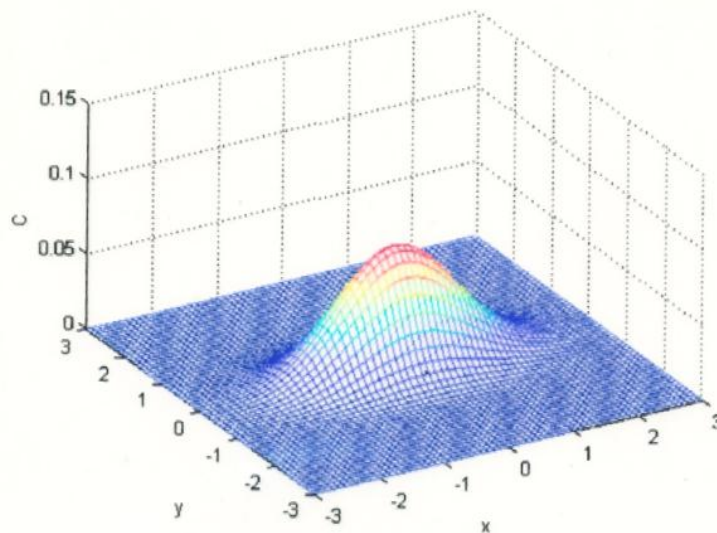
$(D_x = 0.4, D_y = 0.1, M = 1)$

-Mesh Graphics-

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



$(D_x = D_y = 0.1, M = 1)$



$(D_x = 0.4, D_y = 0.1, M = 1)$

(2) 3-D fluid

- A mass M [M] deposited at $t = 0$ at $x = 0, y = 0, z = 0 \rightarrow$ **Problem 4-2**

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

$$\text{I.C.: } C(x, y, z, 0) = M \delta(x) \delta(y) \delta(z) \rightarrow \text{point source}$$

Use product rule

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

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

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

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

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

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

Substituting these relations into (b) yields

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

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

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

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

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

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

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

• Summary of solutions for instantaneous inputs in 2D & 3D fluids (Series 4)

Case	Initial and boundary conditions	Solution
4-1	M (mass/L) deposited at $t = 0$ at $x = 0, y = 0$	$C = \frac{M}{4\pi t \sqrt{D_x D_y}} \exp\left(-\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t}\right)$
4-2	M deposited at $t = 0$ at $x = 0, y = 0, z = 0$	$C = \frac{M}{(4\pi t)^{\frac{3}{2}} (D_x D_y D_z)^{\frac{1}{2}}} \exp\left(-\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t} - \frac{z^2}{4D_z t}\right)$

2.4.6 Advective Diffusion

(1) Governing Equation

Fluid moving with velocity \vec{u}

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

linear

- Advection = transport by the mean motion of the fluid
- Assume the transports by advection and by diffusion are separate and additive processes.

→ rate of mass transport through unit area (yz plane) by x 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

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

= 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

→ Linear, 2nd order PDE

• In 3-D

i) Mass conservation equation

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

ii) Rate of mass transport

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

Substitute (b) into (a)

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

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

Rearrange 2nd term of LHS

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

By the way

$$\nabla \cdot \vec{u} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad \leftarrow \text{continuity eq. for incompressible fluid}$$

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

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

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

(2.57) becomes

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

→ 3-D Advection-Diffusion Equation

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

(2) Analytical Solutions

1) Instantaneous mass input in 1D uniform flow → **Problem 5-1**

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

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

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

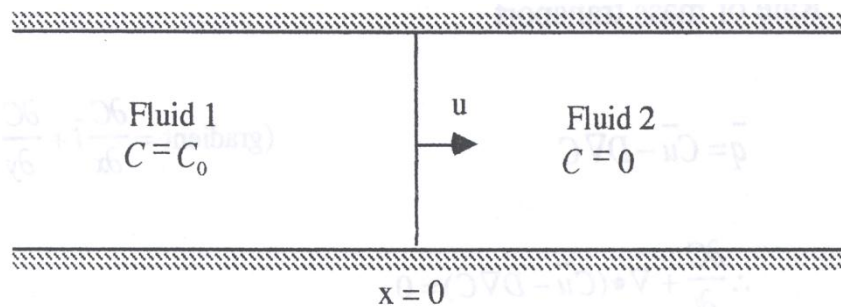
$$C(x, t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x-ut)^2}{4Dt}\right)$$

2) Instantaneous concentration input over $x < 0 \rightarrow$ **Problem 5-2**

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

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

$$\frac{\partial t}{\partial x} = 0, \quad \frac{\partial t}{\partial t} = 1$$

Use chain rule

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

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

Substitute this into G.E.

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

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

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

Then G.E. becomes

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

→ This problem is identical to diffusion of distributed source with step function

C_0 for $x < 0$ in a stagnant fluid (Problem 1-5).

There, solution is

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

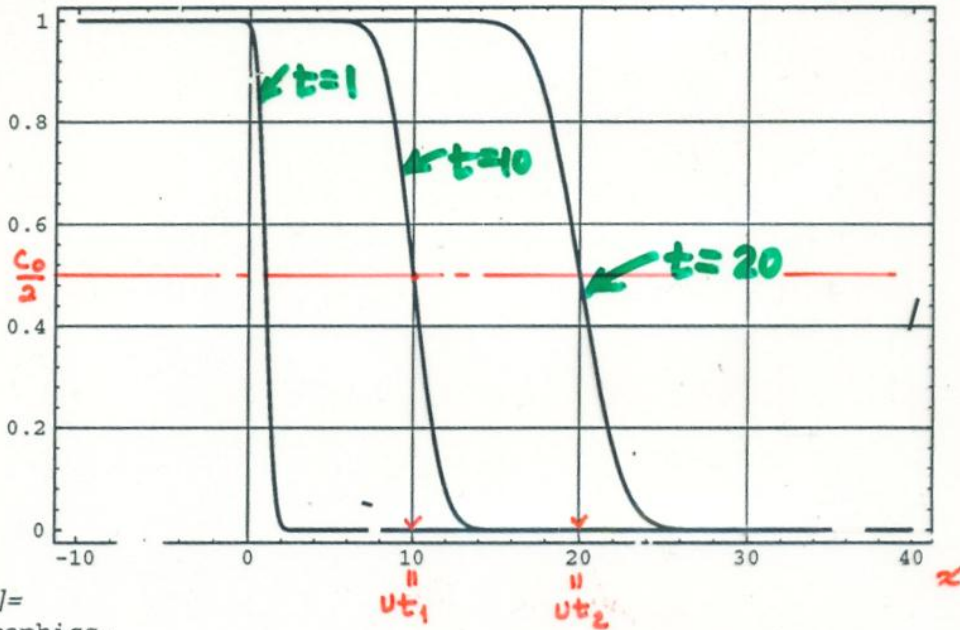
Adjust for the moving coordinates

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

$$c = \frac{c_0}{2} \operatorname{erfc} \left\{ \frac{z-ut}{\sqrt{4Dt}} \right\}$$

```
In[24]:=
Dx=0.1;
C0=1;
U=1;
f[x_,t_]:= C0/2 Erfc[(x-U*t)/Sqrt[4*Dx*t]]
Plot[{f[x,1],f[x,10],f[x,20]}, {x,-10,40}, Frame->True, GridLines->Automat
```

Advective Diffusion

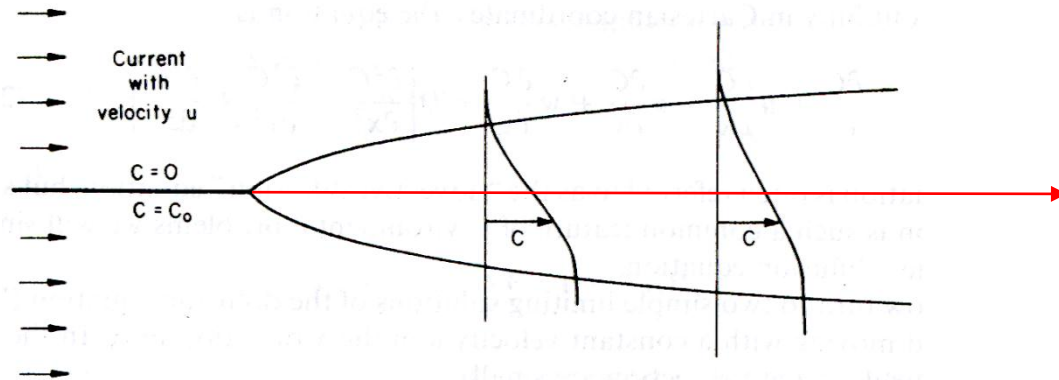


Out[24]=
-Graphics-

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-SurfaceGraphics-

3) Lateral (transverse) diffusion → **Problem 5-3**

- 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) continuous input: $\frac{\partial C}{\partial t} \rightarrow 0$

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

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

Then, G.E. becomes

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

→ similar to 1-D diffusion equation

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

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

→ Now, this problem is similar to Problem 1-4 with $t = x/u$; $x' = y$

Solution is

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

Convert to x-y coordinates

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

4) Continuous plane source → Problem 5-4

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

$$\text{B.C.: } C(0, t) = C_0 \quad 0 < t < \infty \rightarrow \text{steady continuous input}$$

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

→ identical to continuous input with step function $C_0 = C_0(t)$ (Problem 2-1).

The solution is

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

Set

$$P_e = \text{Peclet number} = \frac{ux}{D}$$

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

Then,

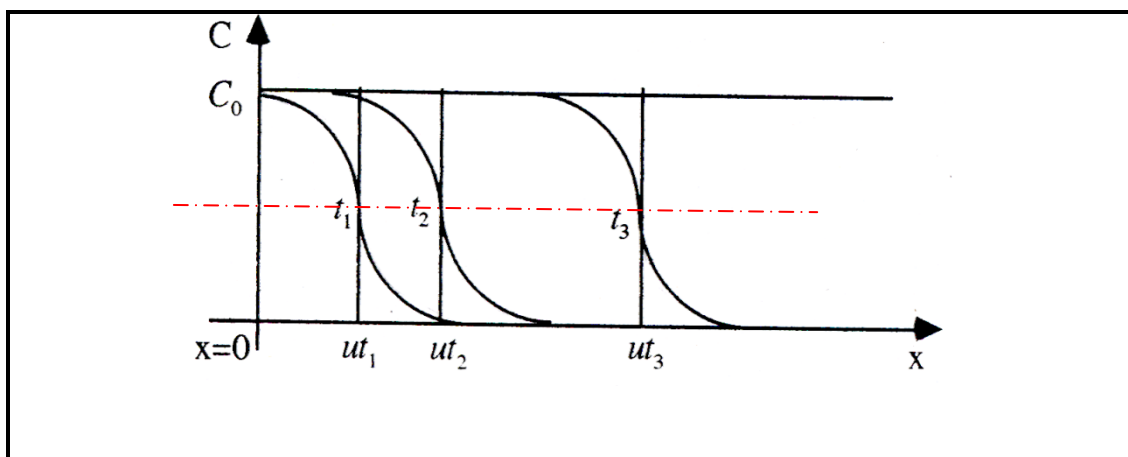
$$\frac{C(x,t)}{C_0} = \frac{1}{2} \operatorname{erfc} \left[\left(\frac{P_e}{4t_R} \right)^{\frac{1}{2}} (1 - t_R) \right] + \frac{1}{2} \operatorname{erfc} \left[\left(\frac{P_e}{4t_R} \right)^{\frac{1}{2}} (1 + t_R) \right] \exp(P_e)$$

For advection-dominated case (large u)

$$P_e > 500; \quad \frac{C}{C_0} \approx \frac{1}{2} \operatorname{erfc} \left(\frac{x - ut}{\sqrt{4Dt}} \right)$$

Diffusion problem ($u = 0$)

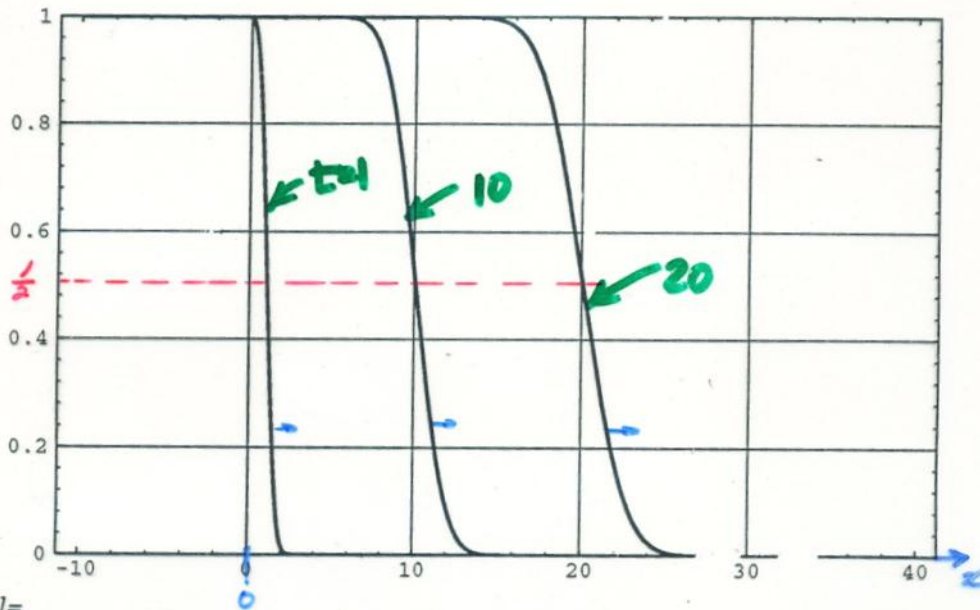
$$\frac{C}{C_0} = \operatorname{erfc} \left(\frac{x}{\sqrt{4Dt}} \right)$$



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

In[47]:=

```
Dx=0.1;
C0=1;
U=1;
f[x_,t_]:= C0/2 'Erfc[(x-U*t)/Sqrt[4*Dx*t]]
+Erfc[(x+U*t)/Sqrt[4*Dx*t]]*Exp[U*x/Dx])
Plot[{f[x,1],f[x,10],f[x,20]},{x,-10,40},Frame->True,GridLines->Autom
```



Out[47]=

-Graphics-

SurfaceGraphics::optx:
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-SurfaceGraphics-

• Summary of solutions for advective diffusion (Series 5)

Case	Initial and boundary conditions	Solution
5-1	Instantaneous mass input in 1D uniform flow	$C(x,t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x-ut)^2}{4Dt}\right)$
5-2	Instantaneous concentration input over $x < 0$	$C(x,t) = \frac{C_0}{2} \left[1 - \operatorname{erf}\left(\frac{x-ut}{\sqrt{4Dt}}\right) \right]$
5-3	Transverse mixing of two streams of different uniform concentrations flowing side by side	$C = \frac{C_0}{2} \left[1 - \operatorname{erf}\left(\frac{y}{\sqrt{4Dx/u}}\right) \right]$
5-4	Continuous plane source in 1D uniform flow	$C(x,t) = \frac{C_0}{2} \left[\operatorname{erfc}\left(\frac{x-ut}{\sqrt{4Dt}}\right) + \operatorname{erfc}\left(\frac{x+ut}{\sqrt{4Dt}}\right) \exp\left(\frac{ux}{D}\right) \right]$

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

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

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

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

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

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

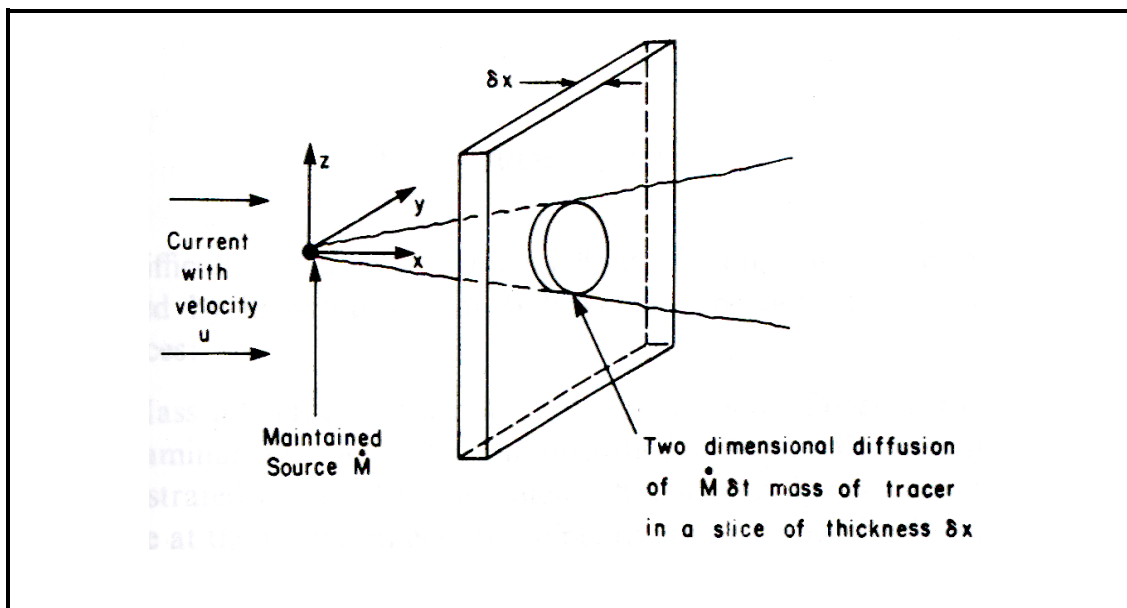
2.4.7 Maintained point source

(1) Constant point source in 3D → **Problem 6-1**

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

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

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



• 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 bounded by infinite parallel y - z planes

→ 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 = $\dot{M} \delta t = \dot{M} \frac{\delta x}{u}$

2-D solution ← Eq. (2.53)

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

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

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

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

Eq. (2.67) was derived by neglecting diffusion in the direction of flow.

$$\rightarrow ut \gg \sqrt{2Dt} \quad \text{or} \quad t \gg 2D/u^2$$

(2) Maintained point source in 2D flow → **Problem 6-2**

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

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

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

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

• Summary of solutions for maintained point discharges in 2D & 3D flows (Series 6)

Case	Initial and boundary conditions	Solution
6-1	Mass input at the rate \dot{M} at the origin (x, y, z) in 3D flow	$C(x, y, z) = \frac{\dot{M}}{4\pi Dx} \exp\left(-\frac{(x^2 + y^2)u}{4Dx}\right)$
6-2	Maintained point source in 2D flow	$C(x, y) = \frac{\dot{M}}{u\sqrt{4\pi Dx/u}} \exp\left(-\frac{y^2 u}{4Dx}\right)$

2.4.8 Solutions for Pollutant Mixing in Rivers

(1) 2-D Instantaneous Input



Assume rapid vertical mixing

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

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

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

i) Case A: Right-bank input

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

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

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

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

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

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

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

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

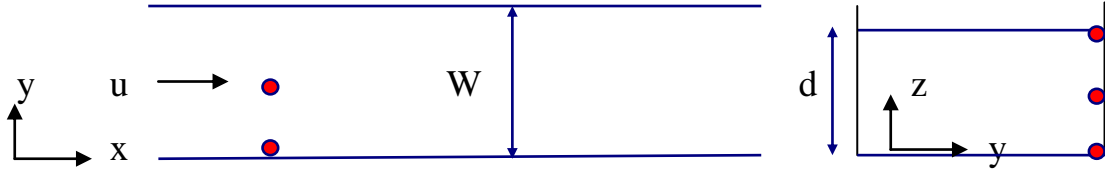
$$C = \frac{M}{4\pi t \sqrt{D_x D_y}} \exp\left(-\frac{(x-ut)^2}{4D_x t}\right) \sum_{n=-\infty}^{\infty} \left[\exp\left\{-\frac{(y+nW)^2}{4D_y t}\right\} \right]$$

[Re] Decaying substance

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

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

(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
$$\left. \frac{\partial C}{\partial z} \right|_{z=d} = 0 \text{ impermeable, non-diffusive}$$

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

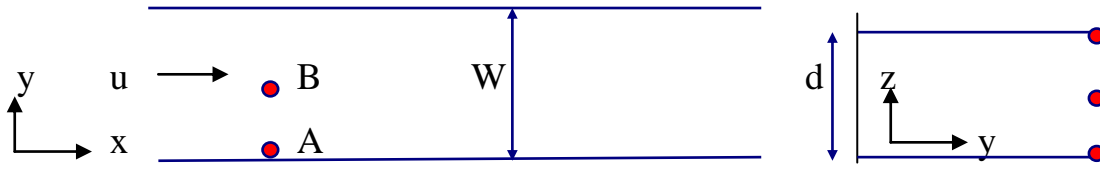
$$C_2 = \sum_{n=-\infty}^{\infty} \frac{M_2}{\sqrt{4\pi D_y t}} \left[\exp \left\{ -\frac{(y + (2n-1)\frac{W}{2})^2}{4D_y t} \right\} \right]$$

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

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

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

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



* Governing Equation

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

Case I: side injection

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

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

Case II: centerline injection

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

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

* Product Rule

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

Then, the governing equation will be modified as

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

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

After that, we must to solve two equations

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

and

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

i) Case I:

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

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

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

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

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

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

ii) Case II:

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

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

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

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