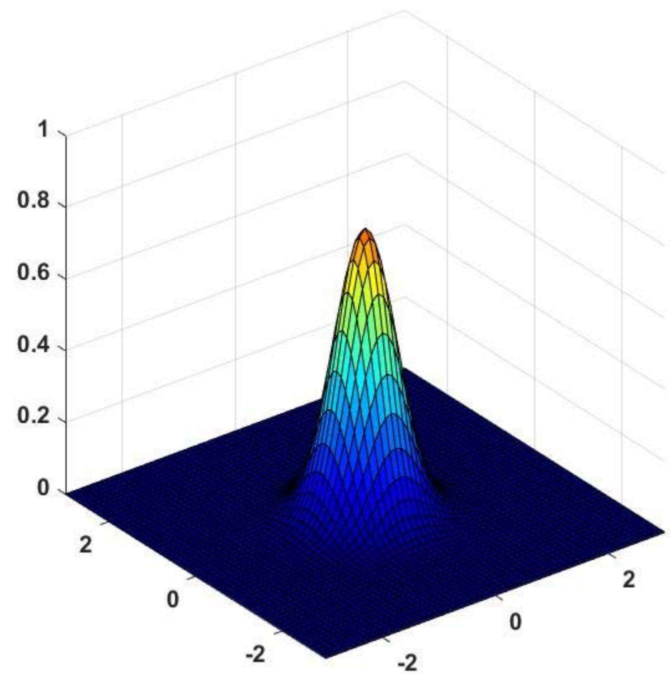
Chapter 2

Diffusion Equation and Its Solutions



Chapter 2 Diffusion Equation and Its Solutions

Contents

Chapter 2 Diffusion Equation and Its Solutions

Objectives

- Present equations and concepts for molecular diffusion processes
- Present two different rationalizations for the molecular diffusion equation
- Introduce statistical aspects of concentration distributions
- Discuss boundary conditions for various inputs of the pollutants in rivers
- Derive analytical solutions to the diffusion equations for different BCs

2.1 Fick's Law for Molecular Diffusion

2.1.1 Diffusion Equation

- **Diffusion and Advection**

  fluids at rest → diffusion

  moving fluids → diffusion + advection

- **molecular diffusion versus turbulent diffusion**

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

- turbulent diffusion ~ large scale; analogous to molecular diffusion

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

	Fourier	Fick
transport	heat	mass
gradient	temp.	conc.

2.1 Fick's Law for Molecular Diffusion

1) Fick's law

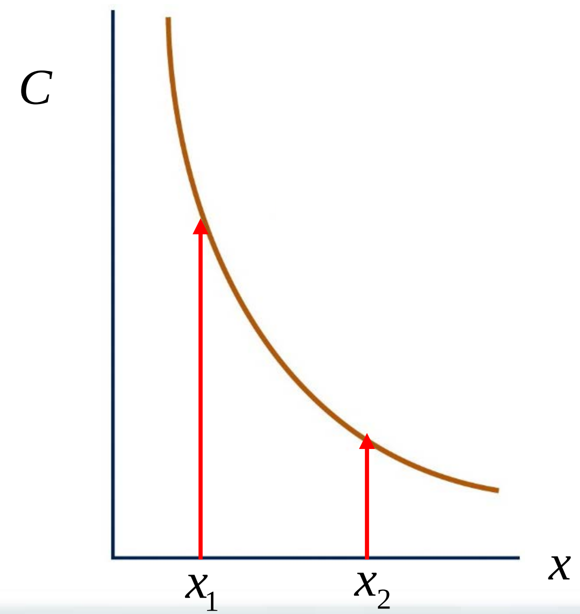
→ flux of solute mass, that is, the mass of a solute crossing a unit area per unit time in a given direction, is proportional to the gradient of solute concentration in that direction.

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

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

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

C = mass concentration of dispersing solute



2.1 Fick's Law for Molecular Diffusion

Since mass transport is from high to low concentrations

따라서 *q*를 양의 값으로 나타내기 위해서는 – 부호를 붙여야 함.

$$q \propto \frac{\Delta C}{\Delta x} = \frac{C_1 - C_2}{x_2 - x_1} = -\frac{C_2 - C_1}{x_2 - x_1} = -\frac{\partial C}{\partial x} = -slope$$

$$\boxed{q = -D\frac{\partial C}{\partial x}} \qquad (2.1)$$

→ Fick's law of diffusion

D = coefficient of proportionality

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

→ distributed parameter

2.1 Fick's Law for Molecular Diffusion

[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_c = mass transfer per unit time per unit volume

2) Mass transfer model

$$q_c = k\Delta C$$

k = mass transfer coefficient → lumped parameter

[Re] Fick's law in 3D

$$\vec{q} = -D\nabla C \qquad (2.1a)$$

$$\vec{q} = \vec{i}q_x + \vec{j}q_y + \vec{k}q_z$$ → vector

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

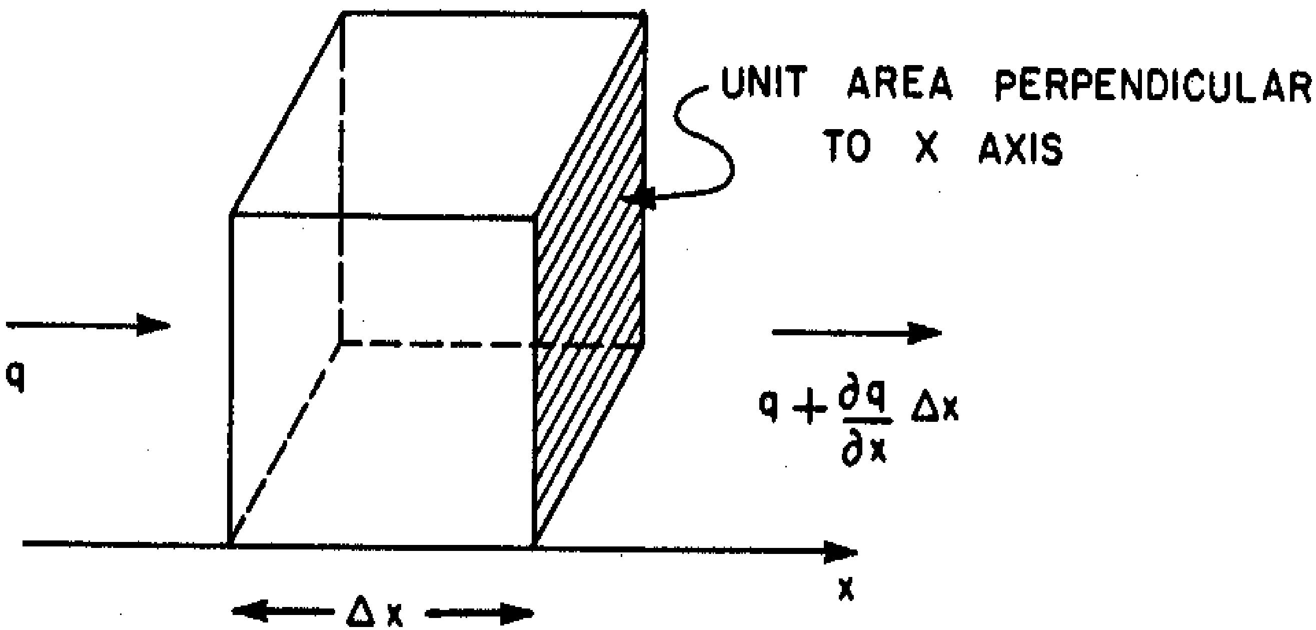
Gradient C

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

2.1 Fick's Law for Molecular Diffusion

2) Conservation of Mass

Consider mass conservation for 1-D transport process of the infinitesimal control volume



Conservation of mass

2.1 Fick's Law for Molecular Diffusion

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

$$\boxed{\Delta M = C\,\Delta V}$$

ii) net change of mass in the volume

$$= \{(flux)_{in} - (flux)_{out}\} \times unit\ \ area$$

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

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

Now, combine (i) and (ii)

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

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

→ Mass conservation equation

2.1 Fick's Law for Molecular Diffusion

3) Diffusion Equation

Combine Eq. (2.1) and (2.2)

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

$$\boxed{\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}} \qquad (2.3)$$

⇒ Diffusion Equation (Heat Equation)

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

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

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

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

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

2.1 Fick's Law for Molecular Diffusion

[Re] Vector and Tensor

Scalar: 크기만 있는 양

~ pressure, density, temperature, concentration

Vector : 크기와 방향이 있는 양

~ velocity, force

Tensor: 스칼라와 벡터를 확장시킨 양, n차 텐서로 표현

0차 텐서 → 스칼라; 1차텐서 → 벡터

2차 텐서: 응력, 변형률, 확산계수

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

2.1 Fick's Law for Molecular Diffusion

(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

$$\overline{V} = \overline{F} \times \overline{G}$$ → 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

2.1 Fick's Law for Molecular Diffusion

(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) → vector

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

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

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

[Re] grad(scalar) → vector

grad(vector) → tensor

grad(F+G) = grad F + grad G

grad CF = C grad F

2.1 Fick's Law for Molecular Diffusion

(6) Divergence of $\overline{F}$ (vector): 벡터의 내적 → scalar

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

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

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

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

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

(7) $$Curl\ \overline{V} = \nabla\times\overline{V} = \begin{vmatrix} \bar{i} & \bar{j} & \bar{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial x} & \frac{\partial}{\partial x} \\ u & v & w \end{vmatrix} = \left(\frac{\partial w}{\partial y} - \frac{\partial v}{\partial z}\right)\vec{i} + \left(\frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}\right)\vec{j} + \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right)\vec{k}$$

2.1 Fick's Law for Molecular Diffusion

(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 Fick's Law for Molecular Diffusion

텐서식의 표기

1차 텐서: 벡터량

$$a_i b_i = a_1 b_1 + a_2 b_2 + a_3 b_3$$

$$\frac{\partial u_i}{\partial x_i} = \frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}$$

2차 텐서

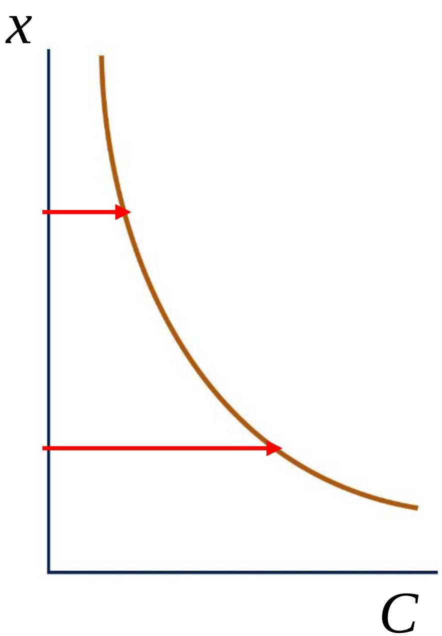
$$a_{ij} b_{ij} = a_{11} b_{11} + a_{12} b_{12} + a_{13} b_{13} + a_{21} b_{21} + a_{22} b_{22} + a_{23} b_{23}$$
$$+ a_{31} b_{31} + a_{32} b_{32} + a_{33} b_{33}$$

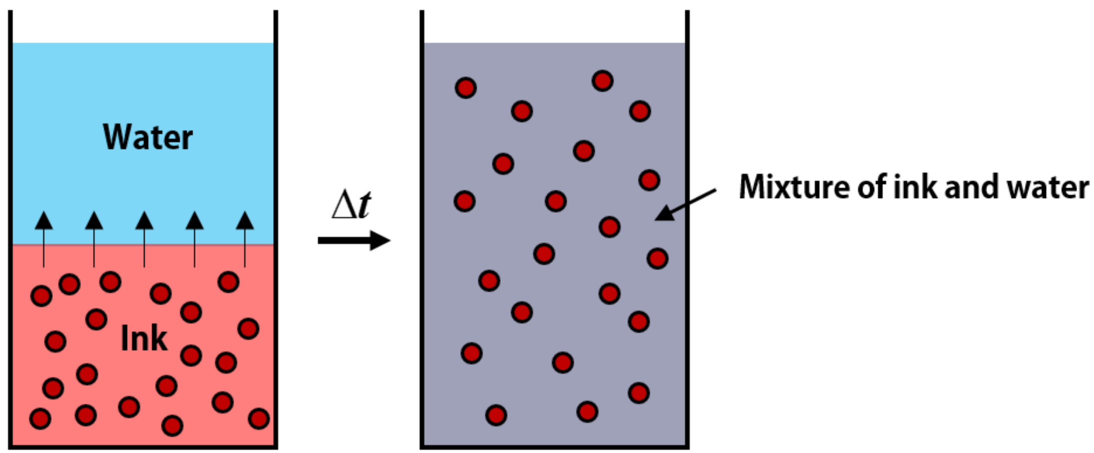
2.1 Fick's Law for Molecular Diffusion

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 <u>random molecular motions</u>





Diffusion process

2.1 Fick's Law for Molecular Diffusion

(i) Watch individual molecules of ink

→ Motion of each molecule is a random one.

→ Each molecule of ink behaves <u>independently of the others</u>.

→ 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 <u>no preferred direction of motion</u>.

→ The motion of a single molecule is described in terms of **<u>random walk model</u>**

→ It is possible to calculate the mean-square distance travelled in given interval of time.

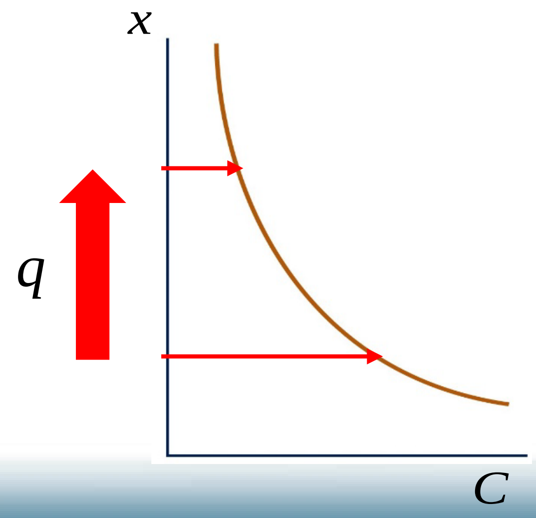
It is not possible to say in what direction a given molecule will move in that time

2.1 Fick's Law for Molecular Diffusion

(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.



2.1 Fick's Law for Molecular Diffusion

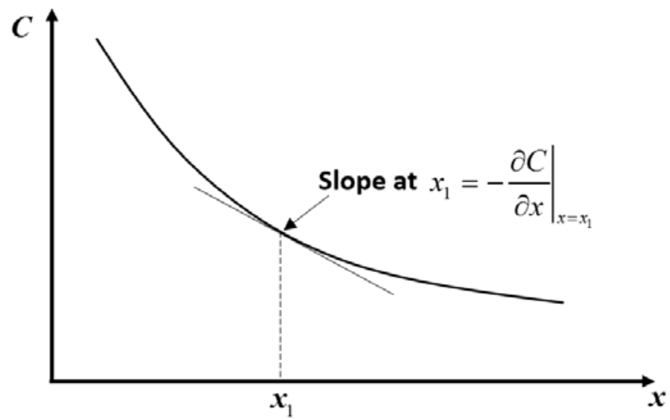
2. Molecular Diffusion

(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.

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

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



Fick's law of molecular diffusion

2.1 Fick's Law for Molecular Diffusion

(ii) Fick's 2nd Law:

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

• 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: $\varepsilon_x, \varepsilon_y, \varepsilon_z$

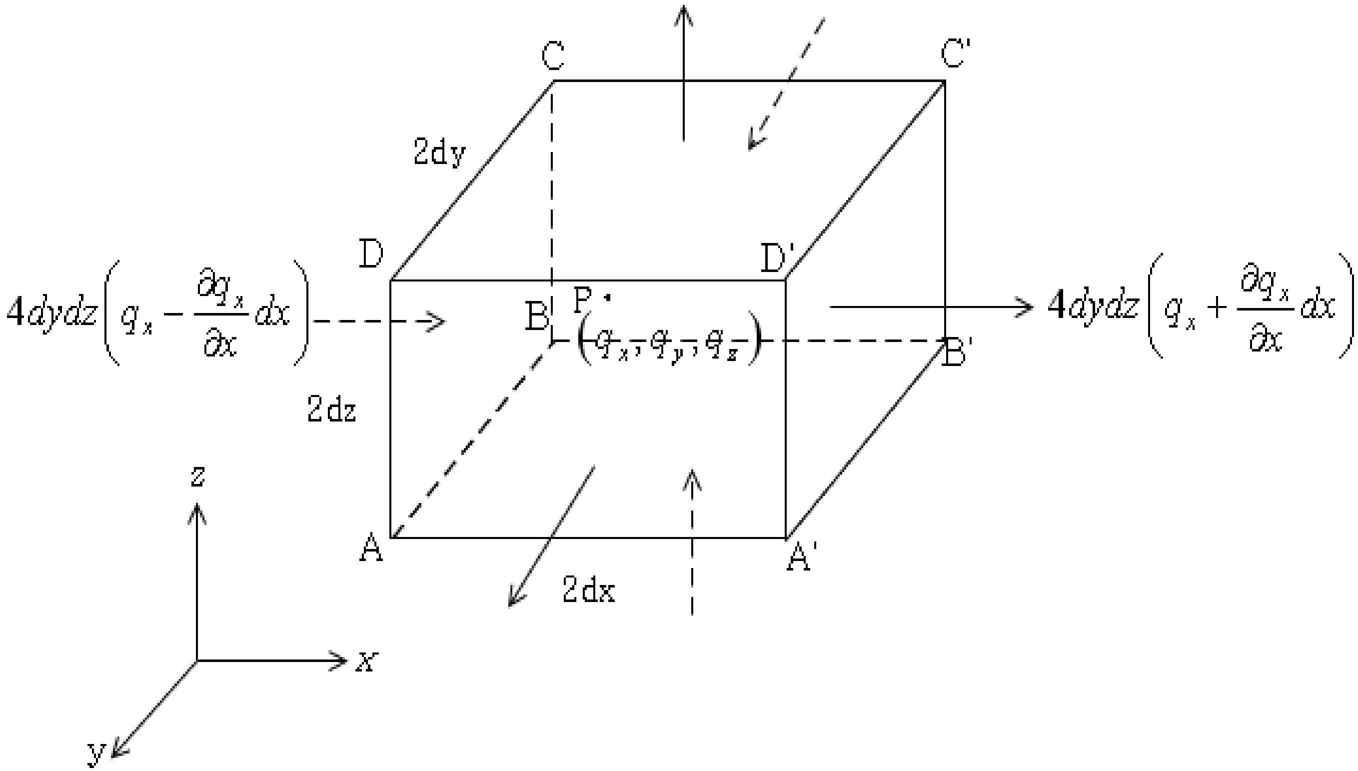
In shear flow dispersion: K_x, K_y, K_z

[Cf] anisotropic medium

→ diffusion properties depend on the direction in which they are measured

2.1 Fick's Law for Molecular Diffusion

3. 3D differential equation of diffusion – point form



3-D differential equation of diffusion (point form)

2.1 Fick's Law for Molecular 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

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

2.1 Fick's Law for Molecular Diffusion

(iv) Similarly from the other faces we obtain

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

(v) Time 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)

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

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

2.1 Fick's Law for Molecular Diffusion

(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; $D \neq f_n\left(x, y, z\right)$

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

→ Fick's 2nd law of diffusion

2.1 Fick's Law for Molecular Diffusion

2.1.3 Advection-Diffusion Equation

Consider 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
- Assume the transports by advection and by diffusion are separate and additive

processes.

→ rate of mass transport through unit area (y-z plane) by x component of velocity, q_u

$$q_u = uC \qquad (2.4)$$

[Re] advective flux

mass = volume · concentration

mass rate = volume rate · conc. = discharge · conc. = velocity · area · conc.

advective flux = mass rate /area = velocity · conc.

2.1 Fick's Law for Molecular Diffusion

Total rate of mass transport

$$q = uC + \left(-D\frac{\partial C}{\partial x} \right) \qquad (2.5)$$

= advective flux + diffusive flux

Substitute (2.5) into mass conservation equation, (2.3)

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

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

$$\boxed{\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(uC) = D\frac{\partial^2 C}{\partial x^2}}$$

→ 1-D advection-diffusion equation (1차원 이송-확산 방정식)

→ linear, 2nd order PDE

2.1 Fick's Law for Molecular Diffusion

[Re] Conservation of mass in 3D

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

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

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

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

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

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

Substitute (ii) into (i)

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

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

→ conservative form

2.1 Fick's Law for Molecular Diffusion

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

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

Continuity eq. for incompressible fluid

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

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

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

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

Thus, (iii) becomes

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

→ non-conservative form

2.1 Fick's Law for Molecular Diffusion

write out fully in Cartisian coordinates

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

→ 3D advection-diffusion equation

텐서식으로 표기하면

$$\boxed{\frac{\partial C}{\partial t}+u_i\frac{\partial C}{\partial x_i}=D\frac{\partial^2 C}{\partial x_i{}^2}}$$

2.1 Fick's Law for Molecular Diffusion

[Re] Vector notation of conservation of mass

Consider a fixed volume V with surface area S

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

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

Consider conservation of mass

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

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

<u>Green's theorem</u>

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

Substitute (b) into (a)

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

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

2.2 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 generalize it

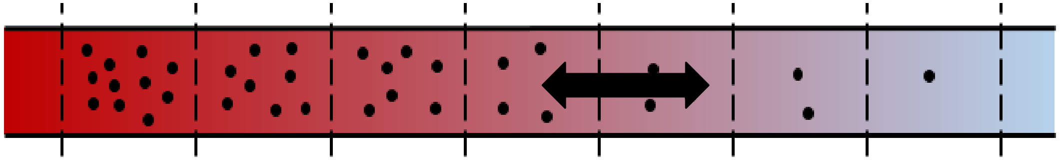
     → random walk model

  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



2.2 The Random Walk and Molecular Diffusion

Use **central limit theorem** → in the limit of many steps, probability of the particle being between $m\Delta x$ and $(m+1)\Delta x$ is the normal distribution

mean: $\mu = 0$

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

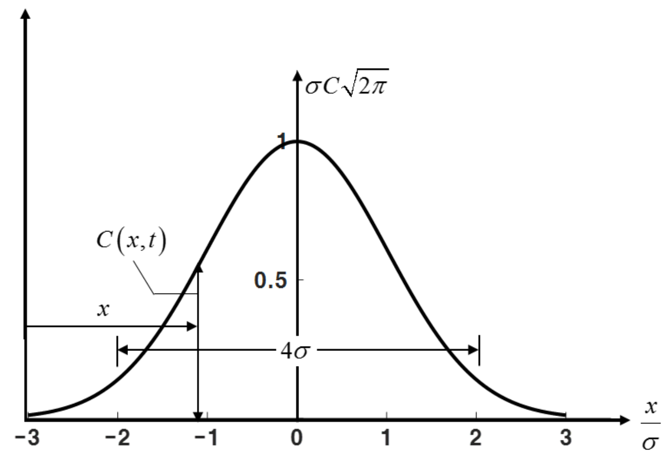
Normal distribution: $p(x,t)dx = \dfrac{1}{\sigma\sqrt{2\pi}}\exp\left(-\dfrac{x^2}{2\sigma^2}\right)$

Designate

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

Then

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



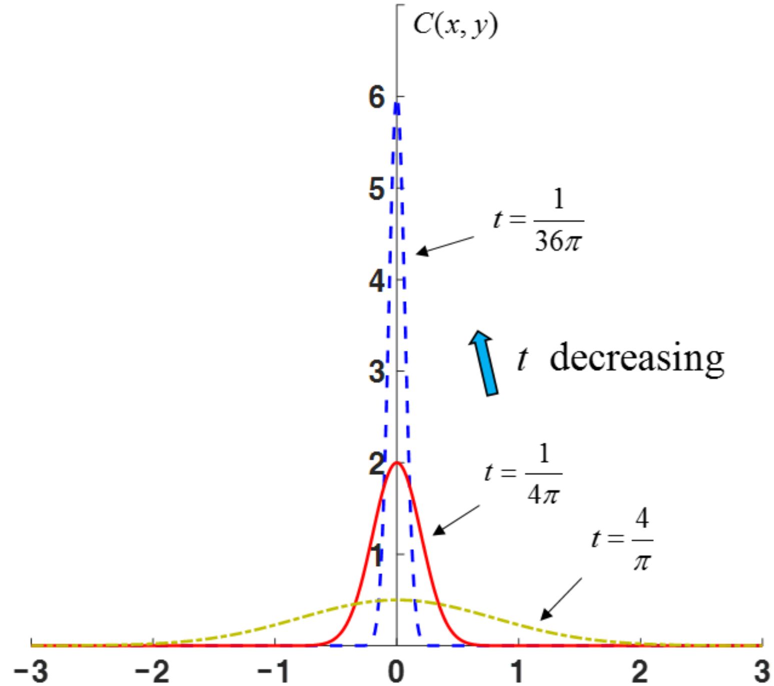
2.2 The Random Walk and Molecular Diffusion

Now think whole group of particles, *N*

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

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

→ Random walk process leads to the same result that a slug of tracer diffuses according to the diffusion equation, Eq. (2.17).



The Gaussian distribution (*M* = 1, *D* =1/4)

2.2 The Random Walk and Molecular Diffusion

2.2.2 The Gradient-Flux Relationship

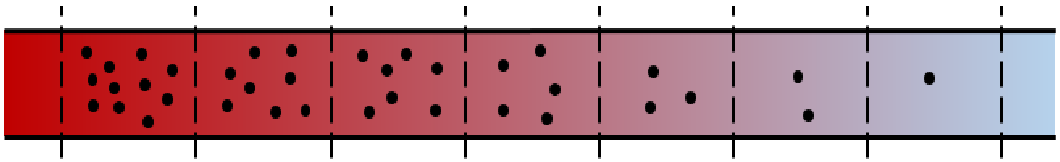
Think random motion of large number of molecules at the same time.

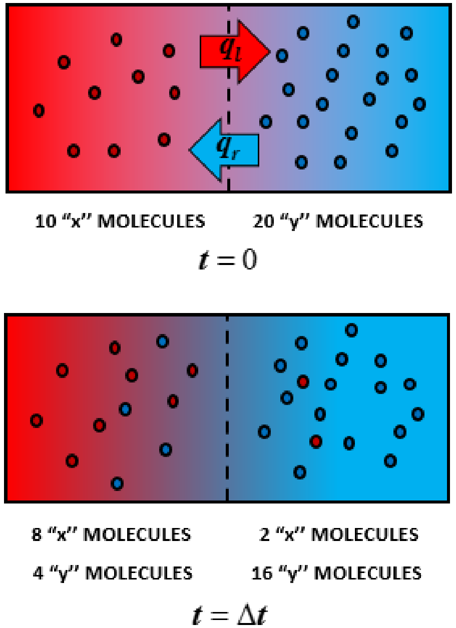
→ probability of a molecule passing through the surface is proportional to the average number of molecule near the surface → mass transfer model

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

Consider flux of material across the bounding surface

2.2 The Random Walk and Molecular Diffusion





Transfer of molecules

2.2 The Random Walk and Molecular Diffusion

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

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

Mass transfer per unit time

where k = transfer probability [1/t] → 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

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

Define

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

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

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

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

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

2.2 The Random Walk and Molecular Diffusion

Combine (b) and (c)

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

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

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

Substitute (d) into (a)

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

$$\boxed{q = -D \frac{\partial C}{\partial x}}$$ ⇒ Fick's law

$D = k(\Delta x)^2$ ⇒ Diffusion coefficient (constant)

→ Convert mass transfer model to diffusion model

2.2 The Random Walk and Molecular Diffusion

[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 $[\mathrm{L}^2/\mathrm{t}]$ → distributed parameter

2) Mass transfer model

$$q_c = k\Delta C$$

q_c = mass transfer per unit time <u>per unit volume</u>

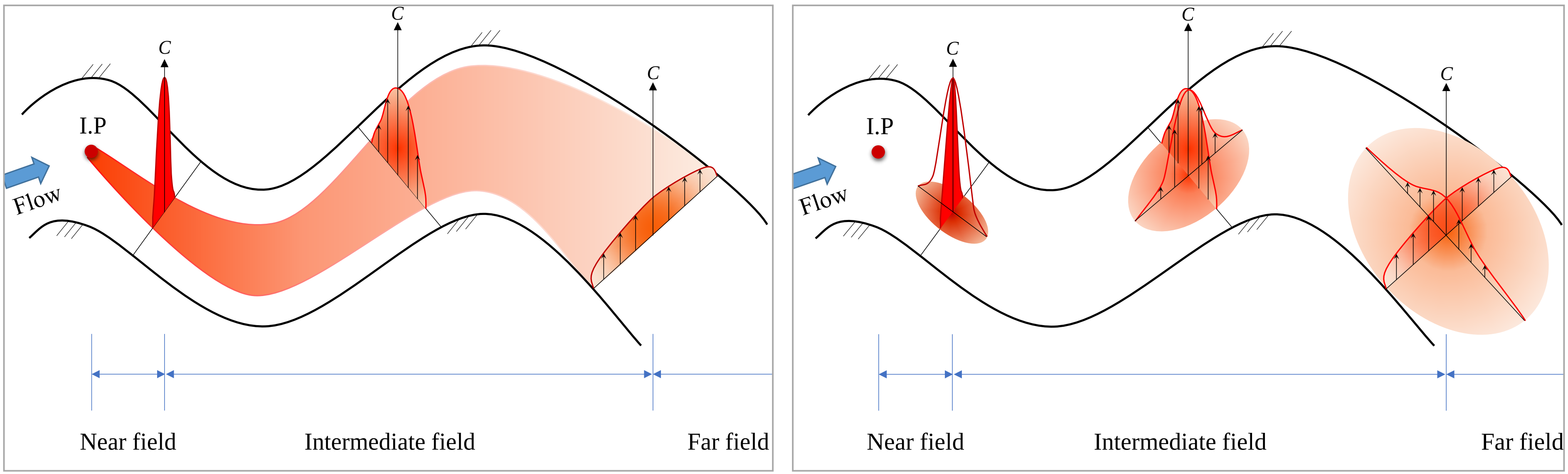
k = mass transfer coefficient $[1/\mathrm{t}]$ → lumped parameter

2.3 Mathematics of Diffusion Equation

2.3.1 Analytical Solution of 1D Diffusion Equation

2.3.1.1 Boundary Conditions for Various Inputs

· Types of pollutants input



(a) Continuous Source (b) Instantaneous Source

Stages of pollutant mixing in natural streams

2.3 Mathematics 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 → initial concentration specified as a function of time

i) Governing equation:

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

ii) Initial & Boundary conditions:

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

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

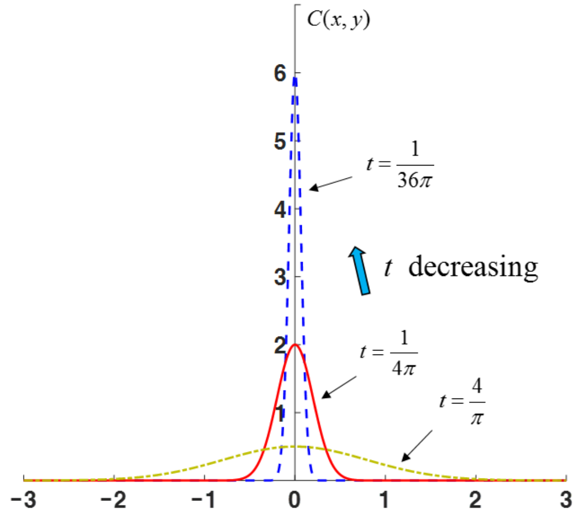
$$C(x=\pm\infty, t) = 0 \qquad (2.11)$$

2.3 Mathematics of Diffusion Equation

where $\delta(x)$ = Dirac delta function

= representing a unit mass of tracer concentrated into an infinitely small space with an infinitely large concentrati

= spike function = $\dfrac{1}{\Delta x}$



· mass M in the 1D model = mass/area

[Re] Boundary conditions

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

$$C(x=0)$$

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

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

2.3 Mathematics of Diffusion Equation

- Types of boundary conditions:

1) Constant concentration → Dirichlet (1st type)

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

2) Constant mass flux → Neumann (2nd type)

a) Finite flux: $J_0=-D\left.\frac{\partial C}{\partial x}\right|_{x=o}$

b) No flux: $\left.\frac{\partial C}{\partial x}\right|_{x=o}=0$ → reflecting (impermeable) boundary

3) Advective mass flux

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

where k_m = mass transfer coefficient

2.3 Mathematics of Diffusion Equation

2.3.1.2 Analytical Solution

To obtain an analytical solution, we can apply

- Dimensional analysis
- Separation of variables
- Laplace transformation

Now, apply dimensional analysis

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

$$C = \frac{M}{\sqrt{4\pi Dt}} f\left(\frac{x}{\sqrt{4Dt}}\right) \qquad (2.12)$$

Now find function f

Set $$\eta = \frac{x}{\sqrt{4Dt}} \qquad (2.13)$$

2.3 Mathematics of Diffusion Equation

Then,

$$\frac{\partial \eta}{\partial t} = \frac{\eta}{2t}$$

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

Substitute Eq. (2.13) into Eq. (2.12) and then into Eq. (2.10)

Eq. (2.12):

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

Thus, each term in Eq. (2.10) become

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

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

2.3 Mathematics of Diffusion Equation

$$\frac{\partial C}{\partial x} = C_p \frac{\partial f}{\partial x} = C_p \frac{\partial f}{\partial \eta}\frac{\partial \eta}{\partial x} = C_p \frac{\partial f}{\partial \eta}\frac{1}{\sqrt{4Dt}} \qquad \text{(b)}$$

$$\frac{\partial^2 C}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial C}{\partial x}\right) = \frac{\partial}{\partial x}\left(C_p \frac{\partial f}{\partial \eta}\frac{1}{\sqrt{4Dt}}\right) = C_p \frac{1}{\sqrt{4Dt}}\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial \eta}\right)$$

$$= C_p \frac{1}{\sqrt{4Dt}}\frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial x}\left(\frac{\partial f}{\partial \eta}\right) = C_p \frac{1}{4Dt}\frac{\partial^2 f}{\partial \eta^2} \qquad \text{(c)}$$

Substitute (a) and (c) into Eq. (2.10)

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

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

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

2.3 Mathematics of Diffusion Equation

Integrate once w.r.t. η

$$2\eta f + \frac{df}{d\eta} = 0 \qquad (2.14)$$

Apply separation of variables to Eq. (2.14)

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

Integrate both sides

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

$$f = e^{-n^2+C} = C_0 e^{-n^2} \qquad (2.15)$$

Total mass, M is

$$\int_{-\infty}^{\infty} C dx = M \qquad (2.16)$$

Substituting Eq. (2.12) and Eq. (2.15) into Eq. (2.16) yields $C_0 = 1$

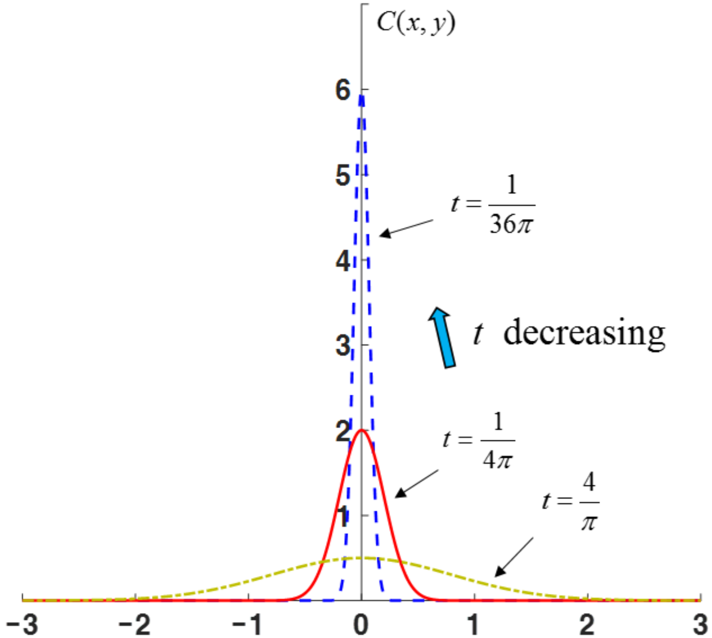
2.3 Mathematics of Diffusion Equation

Then, (2.12) becomes

$$C(x,t)=\frac{M}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right) \tag{2.17}$$

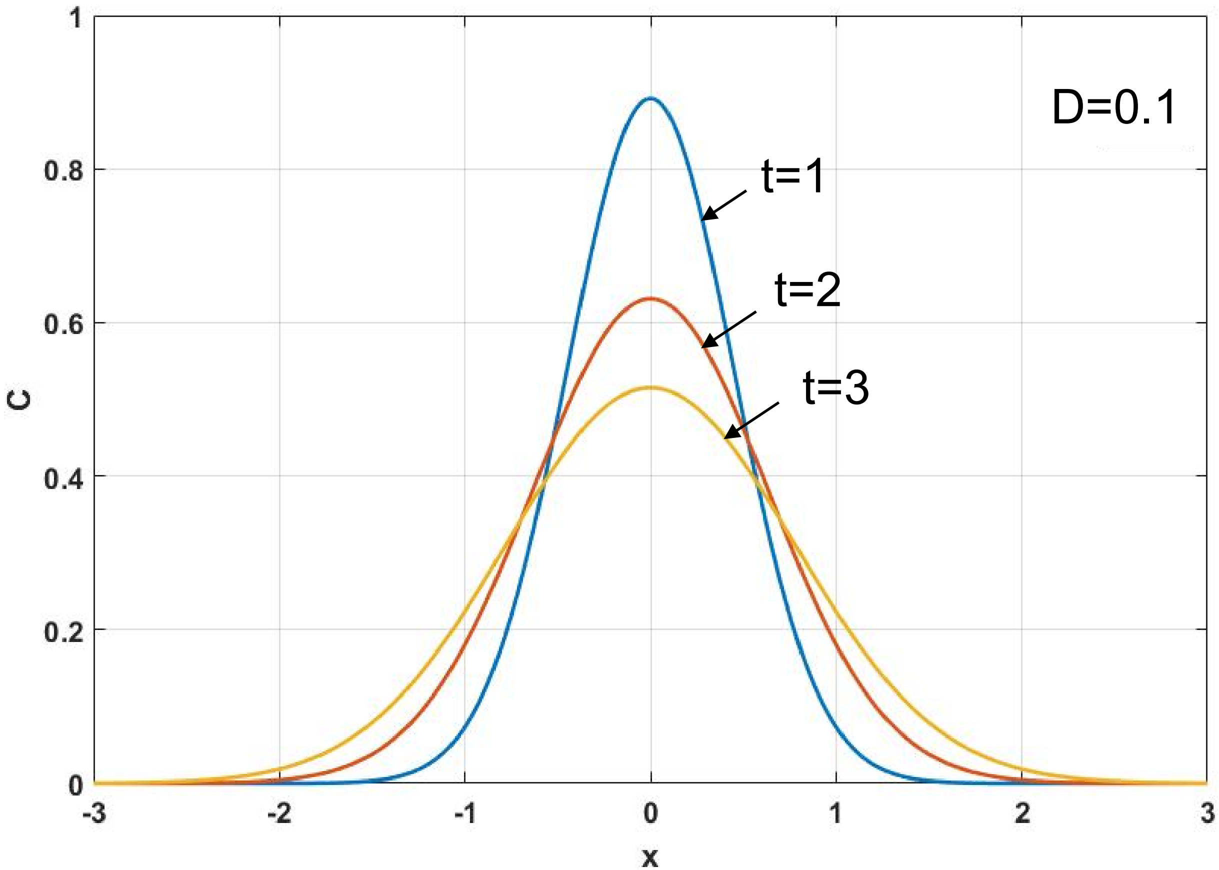
C_p- peak

exponential decay



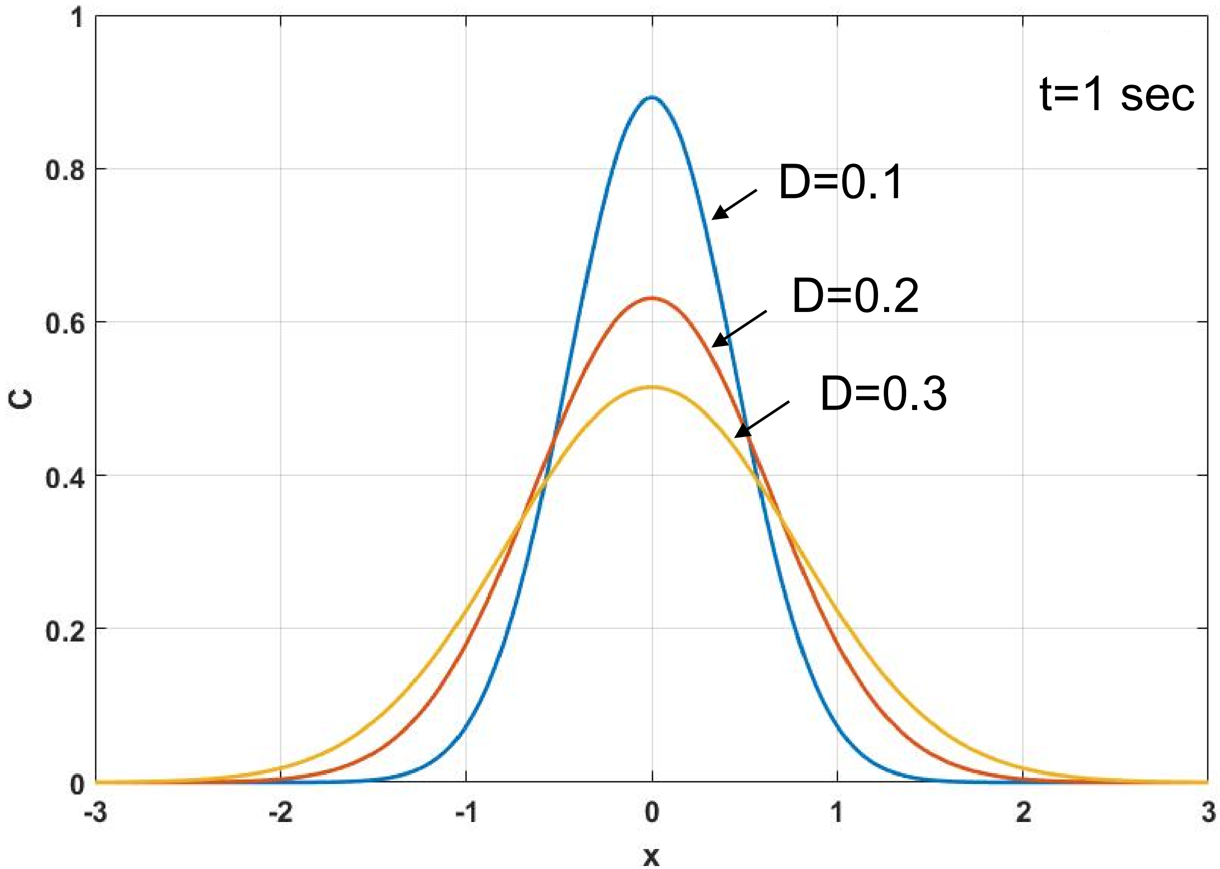
Gaussian distribution ($M = 1$, $D = 1/4$)

2.3 Mathematics of Diffusion Equation



Gaussian concentration distributions with elapsed time

2.3 Mathematics of Diffusion Equation



Gaussian concentration distributions with varying dispersion coefficient

$$\boxed{C(x,t) = \underbrace{\frac{M}{\sqrt{4\pi Dt}}}_{\boxed{C_p}} \underbrace{\exp\left(-\frac{x^2}{4Dt}\right)}_{\text{Decay (exponential)}}}$$

- Peak concentration occurs at x=0 (when advection does not exist)
- Gaussian distribution → symmetrical shape

$$\boxed{\int_{-\infty}^{\infty} c_1 dx = \int_{-\infty}^{\infty} c_2 dx = \int_{-\infty}^{\infty} c_3 dx = M}$$

(for conservative substance)

2.3 Mathematics of Diffusion Equation

[Re] Analytical solution by separation of variables

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \qquad (2.18)$$

$$C(x, t=0) = M\delta(x) \qquad (2.19a)$$

$$C(x = \pm\infty, t) = 0 \qquad (2.19b)$$

$$M = \lim_{\varepsilon \to 0} \int_{-\varepsilon}^{\varepsilon} f(x)dx \qquad M = \lim \qquad (2.19c)$$

Separation of variables

$$C(x,t) = F(x)G(t) \qquad (2.20)$$

Substitute Eq. (2.20) into Eq. (2.10)

$$F(x)\frac{\partial G}{\partial t} = DG(t)\frac{\partial^2 F}{\partial x^2} \qquad FG' = DGF''$$

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

$$F'' - \omega^2 F = 0$$

$$G' - D\omega^2 g = 0$$

2.3 Mathematics of Diffusion Equation

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

$i)$ $k > 0$

$$k = \omega^2$$

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

$$\rightarrow \begin{cases} F'' - \omega^2 F = 0 & (2.21a) \\ G' - D\omega^2 g = 0 & (2.21b) \end{cases}$$

Solution of (2.21a) is $F = C_1 e^{wx} + C_2 e^{-wx}$ (a)

Substituting (2.19b) into (a) yields $C_1 = 0$

Then

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

2.3 Mathematics of Diffusion Equation

Solution of (2.21b) is $G = C_3 e^{\sqrt{D\omega}t}$

Substituting B.C. (2.19b) gives $C_3 = 0$

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

Therefore, $k \le 0$

$ii)\ k = 0$

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

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

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

Therefore, $k < 0$

2.3 Mathematics of Diffusion Equation

$iii)\ k < 0$

$$k = -p^2$$

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

$$F'' + p^2 F = 0 \qquad (2.21c)$$

$$G' + Dp^2 G = 0 \qquad (2.21d)$$

Assume solution of Eq. (2.21c) as $F = e^{\lambda x}$

Substitute this into Eq. (2.21c) and derive characteristic equation (2.22)

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

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

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

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

$$= A \cos px + B \sin px \qquad (2.22)$$

2.3 Mathematics of Diffusion Equation

Assume solution of Eq. (2.21d) as and $G = e^{\lambda x}$

Substitute this into Eq. (2.21d) and derive characteristic equation

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

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

$$\therefore G = C_1 e^{-Dp^2 t} \qquad (2.23)$$

Substitute Eq. (2.22) and (2.23) into Eq. (2.20)

$$C(x,t) = F(x)G(t) = (A\cos px + B\sin px)e^{-Dp^2 t} \qquad (2.24)$$

Use Fourier integral for non-periodic function.

Assume

$$A, B = f_n(p)$$

$$C(x,t,p) = \{A(p)\cos px + B(p)\sin px\}(-Dp^2 t) \qquad (2.25)$$

2.3 Mathematics of Diffusion Equation

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

$$= \int_0^\infty \{A(p)\cos px + B(p)\sin px\}\exp(-Dp^2 t)\,dp \qquad (2.26)$$

Since Eq. (2.10) is linear and homogeneous, integral of Eq. (2.26) exists

I.C.: Eq. (2.19a) and Eq. (2.19c)

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

Where $f(x)$= Fourier integral

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

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

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

2.3 Mathematics of Diffusion Equation

Use Trigonometric rule

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

$$=\frac{1}{\pi}\int_{-\infty}^{\infty}\left\{\int_{-\infty}^{\infty} f(v)\cos(px-pv)dv\right\}dp \tag{2.27}$$

Substitute Eq. (2.27) into Eq. (2.26)

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

Switch order of integral

$$C(x,t)=\frac{1}{\pi}\int_0^{\infty} f(v)\underbrace{\left\{\int_{-\infty}^{\infty}\exp(-Dp^2t)\cos(px-pv)dv\right\}}_{(e)}dp \tag{2.28}$$

Let

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

2.3 Mathematics of Diffusion Equation

Use Residue theorem to get integral of *(e)*

$$\int_{-\infty}^{\infty} e^{-s^2} \cos 2bsds = \frac{\sqrt{\pi y}}{2} e^{-b^2} \qquad (2.29)$$

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

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

(e) becomes

$$\int_{0}^{\infty} \exp(-Dp^2 t)\cos(px - pv)dp = \frac{\sqrt{x}}{2\sqrt{Dt}} \exp\left\{-\frac{(x-v)^2}{4Dt}\right\} \qquad (2.30)$$

Substitute Eq. (2.30) into Eq. (2.28)

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

$$= \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) \qquad (2.31)$$

2.3.2 Statistical Analysis of the Diffusion Equation

2.3.2.1 Concentration Distribution

G.E. and BCs for instantaneous point source

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$
$$C(x,0) = M\delta(x) \qquad (2.32)$$

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

2.3.2 Statistical Analysis of the Diffusion Equation

The solution is

$$C(x,t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) \tag{2.33}$$

→ Gaussian distribution (Normal distribution if M = 1)

[Re] *M*

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

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

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

2.3.2 Statistical Analysis of the Diffusion Equation

2.3.2.2 Moments of Concentration Distribution

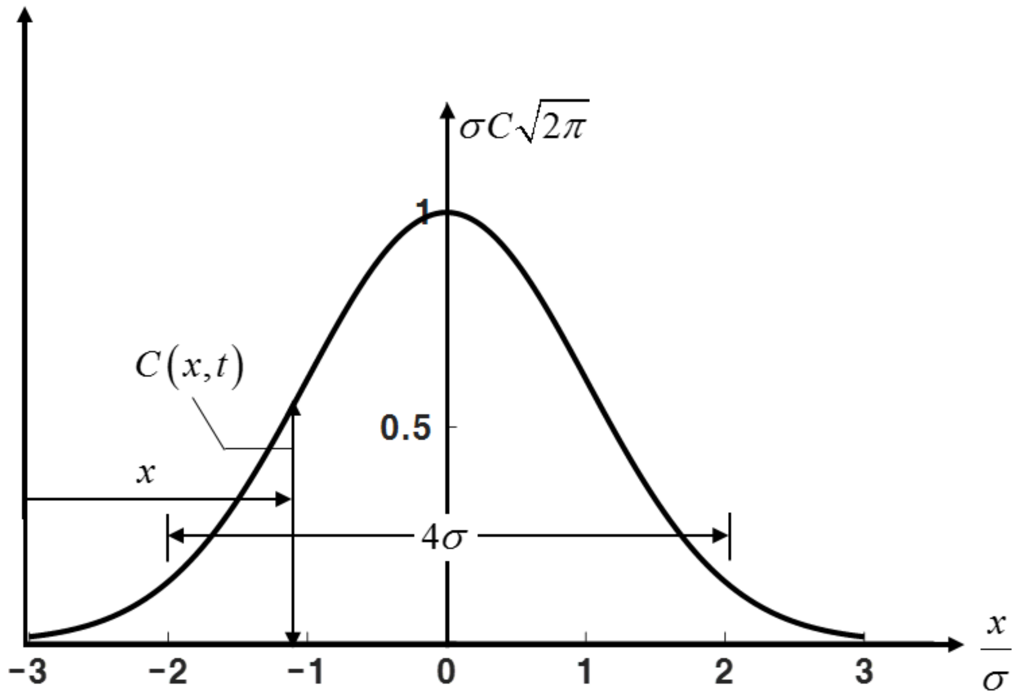
Moments of concentration distributions are defined as

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

1st 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 = $M_p = \int_{-\infty}^{\infty} C(x,t)\,x^p\,dx$



2.3.2 Statistical Analysis of the Diffusion Equation

i) Mass: $M = M_0$

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

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

iv) Skewness
$$S_1 = \frac{\frac{M_3}{M_0} - 3\mu \frac{M_2}{M_0} + 2\mu^3}{(\sigma^2)^{3/2}}$$

- measure of skew
- For normal dist., $S_t = 0$

Normal distribution is given as

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

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

2.3.2 Statistical Analysis of the Diffusion Equation

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, $M_0 = 1$

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

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

2.3.2 Statistical Analysis of the Diffusion Equation

2.3.2.3 Calculation of Diffusion Coefficients

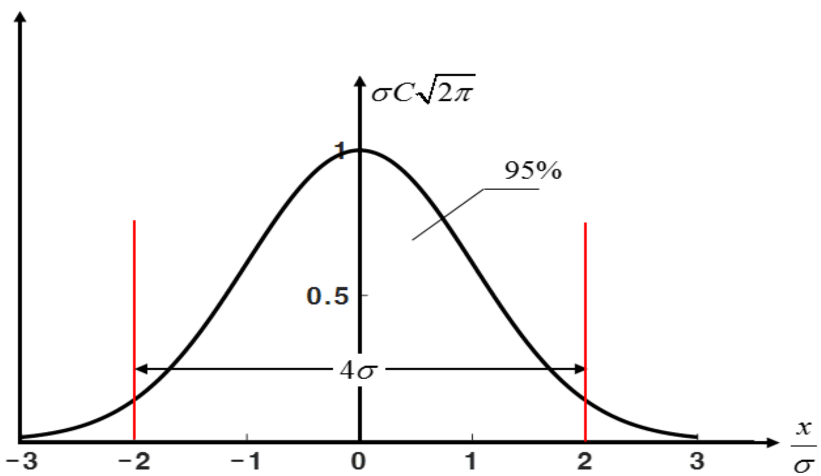
(1) Measure of spread of dispersing tracer

$\sigma = \sqrt{2Dt}$ ⇒ standard deviation (a)

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

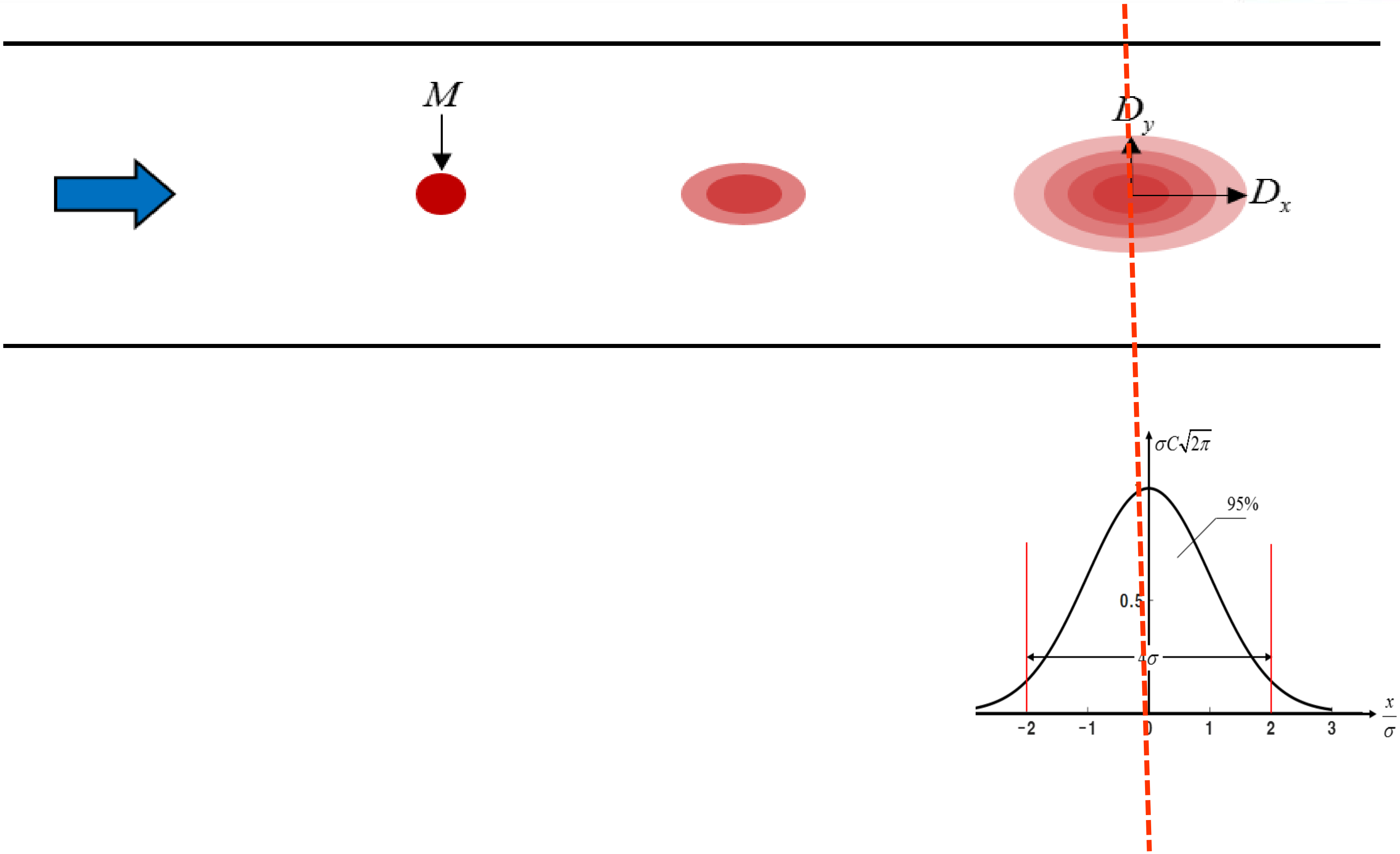
⇒ include 95% of the total mass

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



Width of a dispersing cloud

2.3.2 Statistical Analysis of the Diffusion Equation



2.3.2 Statistical Analysis of the Diffusion Equation

(2) Calculation of diffusion coefficient

→ Change of moment method

Differentiate Eq. (a) w.r.t. time

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

$$\boxed{D = \frac{1}{2}\frac{d\sigma^2}{dt}} \tag{2.34}$$

i) For normal distribution: it is obvious

ii) Eq. (2.34) can be also true for any distribution, provided that it is dispersing in accord with the Fickian diffusion equation.

2.3.2 Statistical Analysis of the Diffusion Equation

Proof: Start with Fickian diffusion equation

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \qquad \text{(a)}$$

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 integration by parts into right hand side

$$\boxed{\int uv' = uv - \int u'v}$$

2.3.2 Statistical Analysis of the Diffusion Equation

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

$$\left(\because \left.\frac{\partial C}{\partial x}\right]_{\pm\infty} \approx 0\right)$$

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

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

$$= 2D\int_{-\infty}^{\infty} Cdx$$

$$\left(\because C]_{-\infty}^{\infty} \approx 0\right)$$

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

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

2.3.2 Statistical Analysis of the Diffusion Equation

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

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

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

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

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

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

$\rightarrow$ μ is independent of time.

2.3.2 Statistical Analysis of the Diffusion Equation

By the way,

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

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

Combine Eq.(b) and Eq.(c)

$$D = \frac{1}{2}\frac{\partial \sigma^2}{\partial t} \qquad (2.35)$$

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

→ Property of the Fickian diffusion equation: any finite initial distribution eventually decays into Gaussian distribution.

2.3.2 Statistical Analysis of the Diffusion Equation

(3) Change of moment method

a) Calculate diffusion coefficient from two concentration curves

Start from Eq. (2.36)

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

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

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

Subtract (1) from (2)

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

Rearrange

$$D = \frac{1}{2}\frac{\sigma_2{}^2 - \sigma_1{}^2}{t_2 - t_1} \qquad (2.36)$$

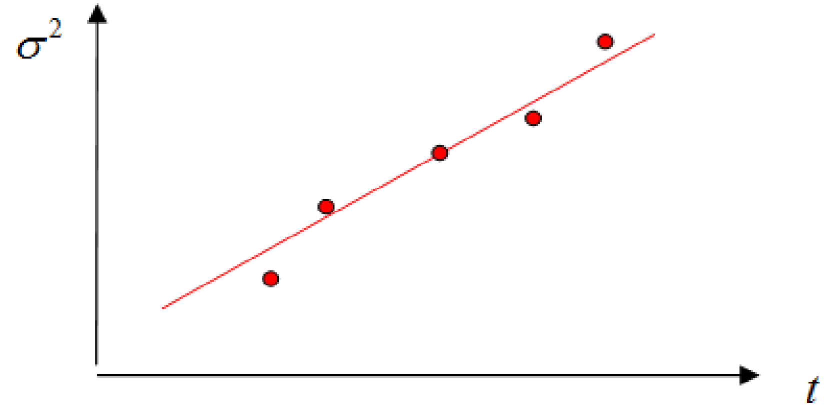
$\sigma_1{}^2$ = variance of concentration distribution at $t = t_1$

$\sigma_2{}^2$ = variance of concentration distribution at $t = t_2$

2.3.2 Statistical Analysis of the Diffusion Equation

b) Calculate diffusion coefficient from more than 2 curves

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

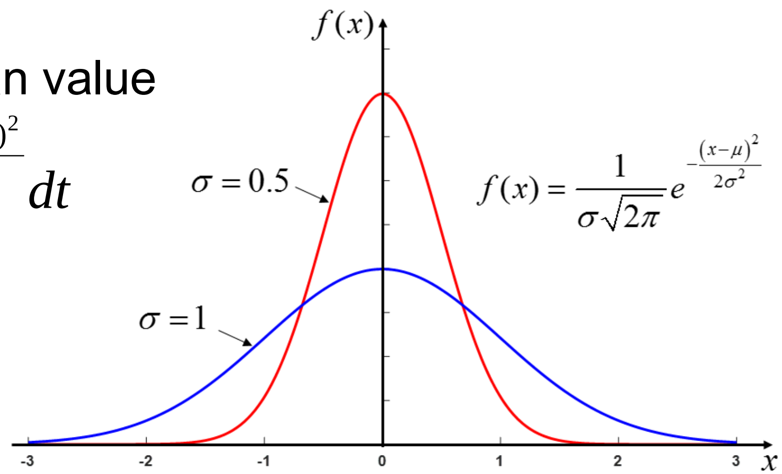


Plot of σ^2 with t

[Re] Normal (Gaussian) distribution

- bell-formed distribution occur around a mean value

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



Normal distribution

Homework #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 2.34 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?

2.3.3 Solutions of the Diffusion Equation

G.E.:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \qquad (2.37)$$

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

Series 7: Pollutant Mixing in Rivers

2.3.3 Solutions of the Diffusion Equation

Problem 1-1:

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

$$C(x=0,t=0)=M\delta(x) \tag{2.38}$$

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

Solution is

$$C(X,t)=\frac{M}{\sqrt{4\pi Dt}}\exp\left[\frac{-x^2}{4Dt}\right] \tag{2.39}$$

2.3.3 Solutions of the Diffusion Equation

2.3.3.1 An Initial Spatial Distribution C(x, 0)

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

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

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

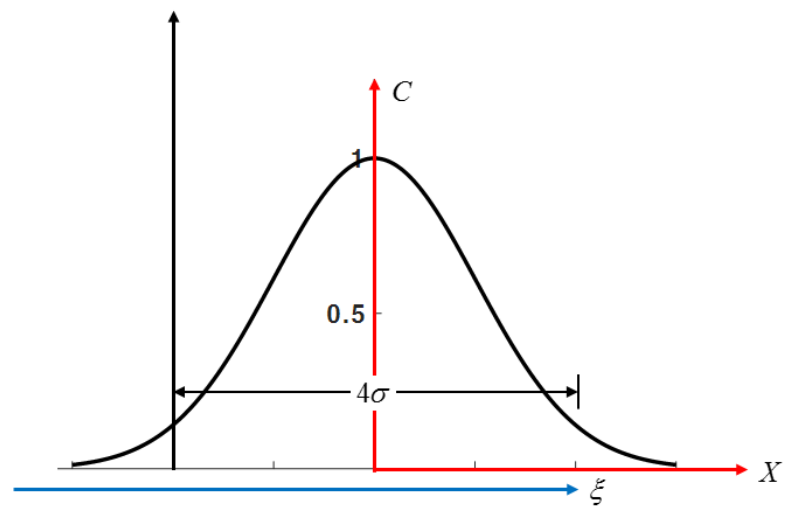
For the coordinate transformation, set $X = x - \xi$

Then, I.C. becomes

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

The solution is

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



Coordinate transformation

Convert X into x

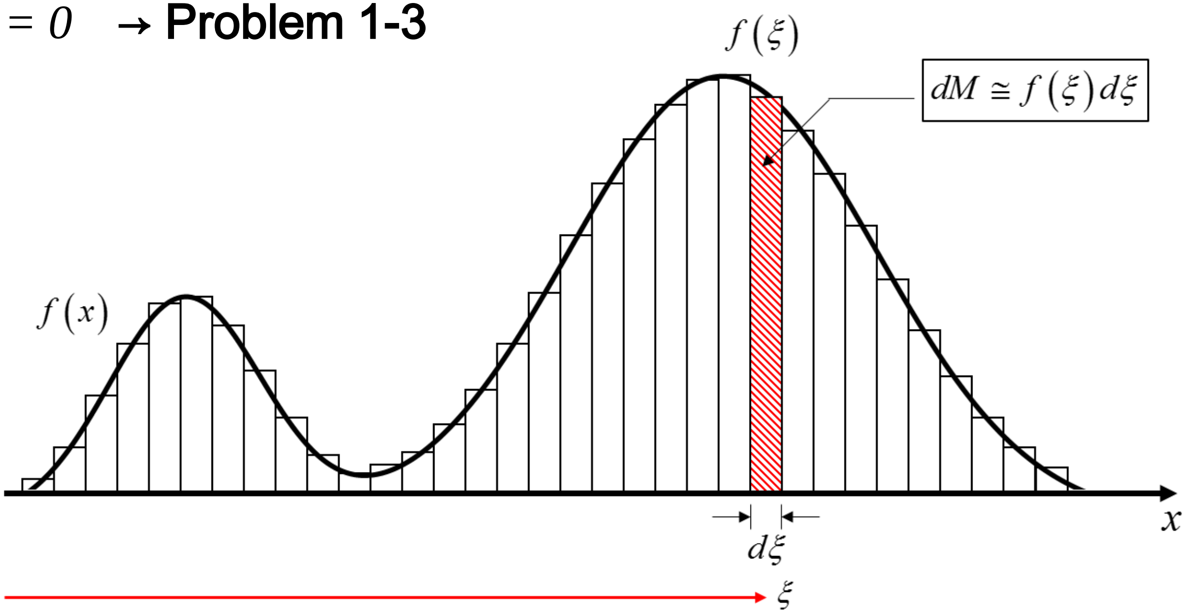
$$C(x,t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left[\frac{-(x-\xi)^2}{4Dt}\right] \qquad (2.40)$$

2.3.3 Solutions of the Diffusion Equation

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

$$I.C.: C(x,0) = f(x),$$

$$-\infty < x < \infty$$



$f(x)$ ~ arbitrary function

Distributed sources along x axis

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

2.3.3 Solutions of the Diffusion Equation

Concentration resulting from the slug containing the mass $\boxed{dM = f(\xi)d\xi}$ is given as

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

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

$$C(x,t)=\int_{-\infty}^{\infty}\frac{f(\xi)}{\sqrt{4\pi Dt}}\exp\left[\frac{-(x-\xi)^2}{4Dt}\right]d\xi \qquad (2.41)$$

→ superposition integral

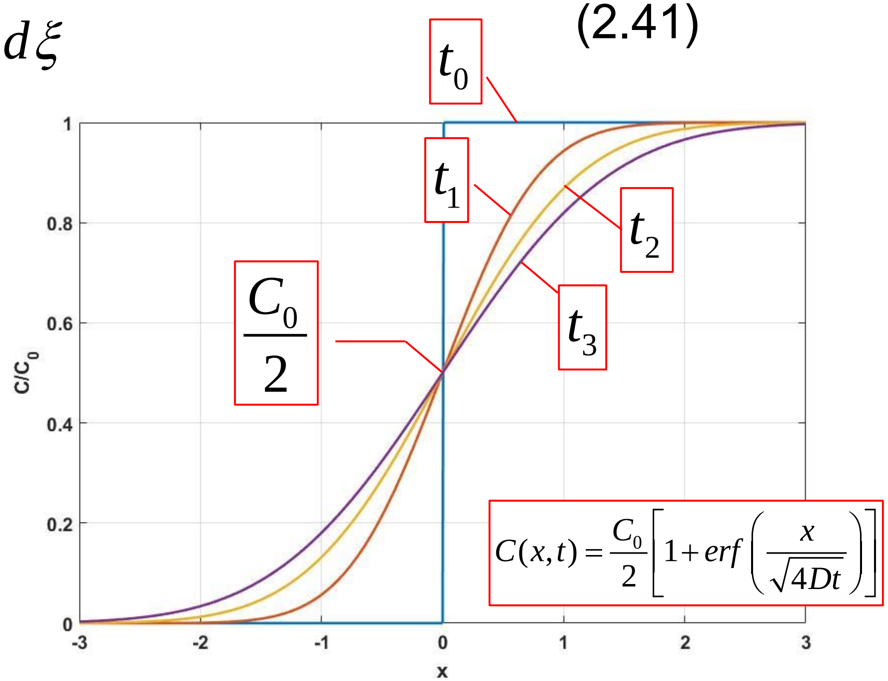
(3) Distributed source with step function,

→ Problem 1−4

Consider a particular case

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

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



Distributed source with step function

2.3.3 Solutions of the Diffusion Equation

According to (2.41), solution is given as

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

Set $u=\dfrac{(x-\xi)}{\sqrt{4Dt}}$ $\quad \xi=0:\ u=\dfrac{x}{\sqrt{4Dt}}$ $\quad \xi=\infty:\ u=-\infty$

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

Substitute (b) into (a)

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

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

$$C(x,t)=\frac{C_0}{2}\left[1+erf\left(\frac{x}{\sqrt{4Dt}}\right)\right] \qquad (2.42)$$

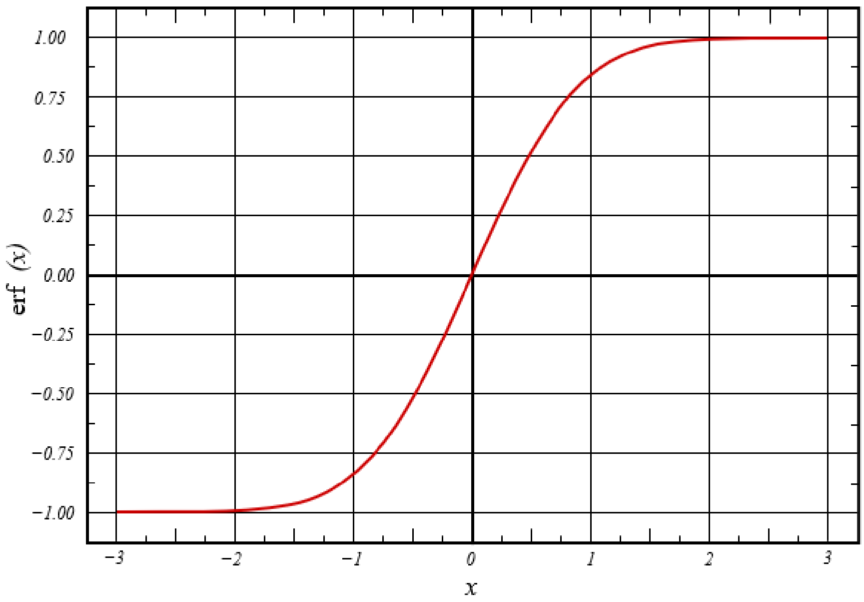
2.3.3 Solutions of the Diffusion Equation

[Re] Error function (오차함수)

~ a special function of "S" shaped curve (sigmoid curve)

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

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



- complementary error function

$$erfc\,x = 1 - erf\ x$$

2.3.3 Solutions of the Diffusion Equation

[Re] Normal distribution

- Most important distribution in statistical application since many measured (random) data 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

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

2.3.3 Solutions of the Diffusion Equation

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

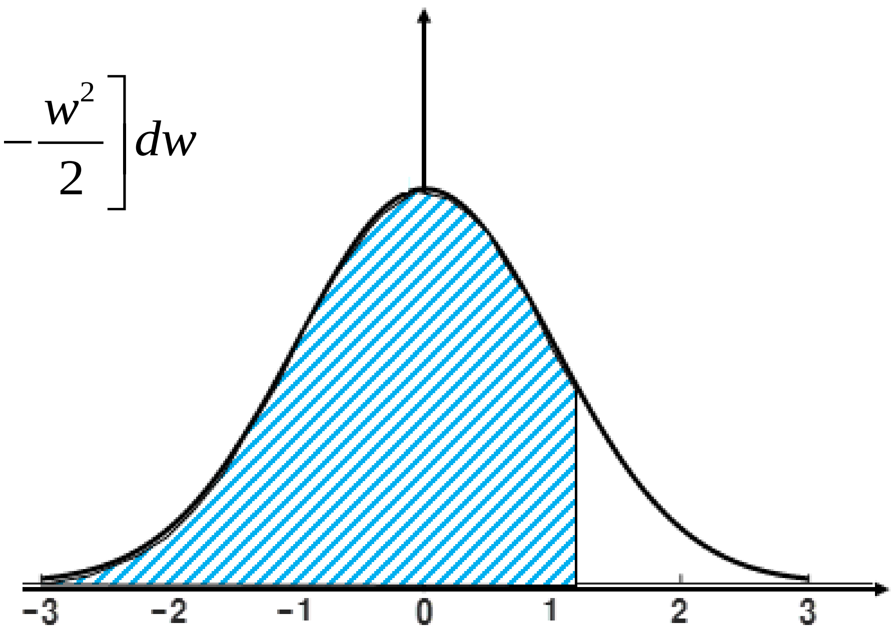
Then,

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

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

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

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



Normalized distribution

2.3.3 Solutions of the Diffusion Equation

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

Consider instantaneous input of step function

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

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

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

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

Then $\quad d\eta = -\dfrac{d\xi}{\sqrt{4Dt}} \quad \xi = -\infty \rightarrow \eta = \infty \quad \xi = 0 \rightarrow \eta = \dfrac{x}{\sqrt{4Dt}}$

2.3.3 Solutions of the Diffusion Equation

Substituting this relation yields

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

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

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

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

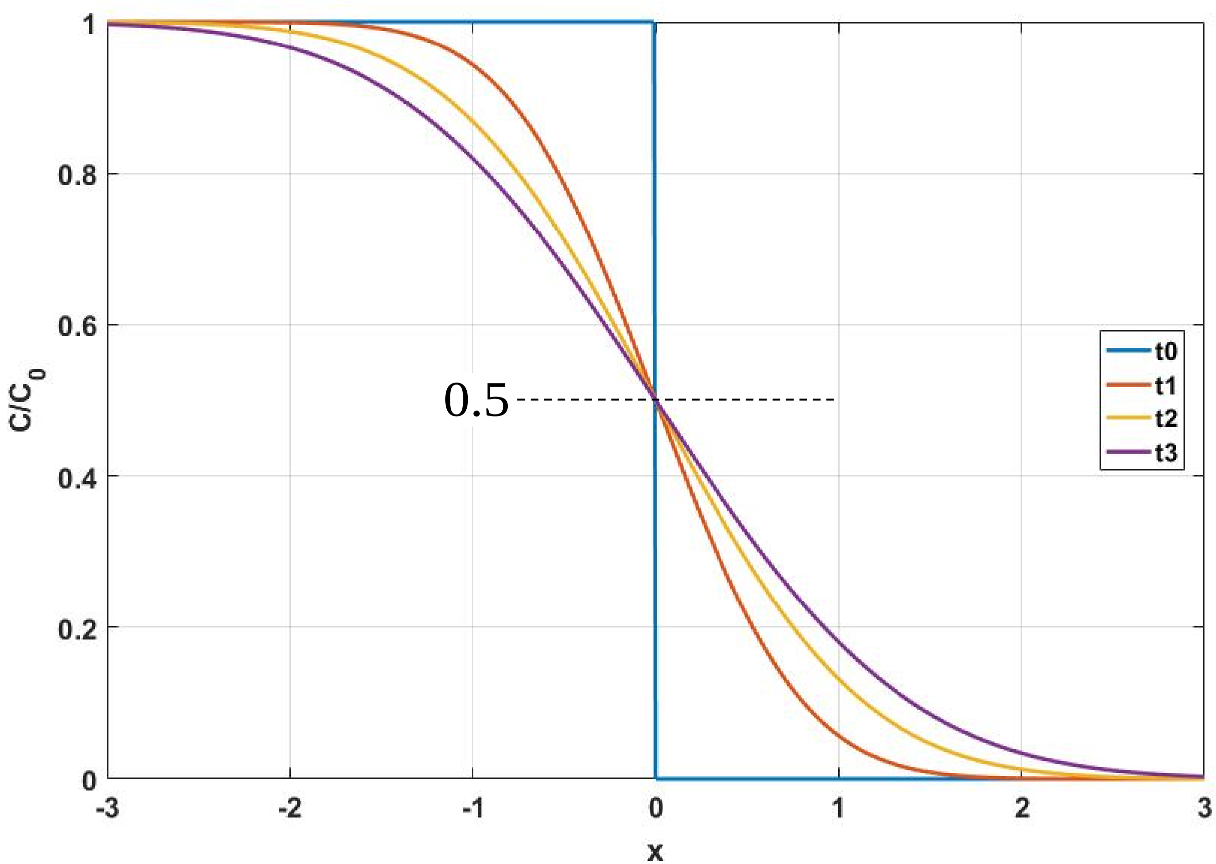
$$C(x,t)=\frac{C_0}{2}\left[1-erf\left(\frac{x}{\sqrt{4Dt}}\right)\right]=\frac{C_0}{2}erfc\left(\frac{x}{\sqrt{4Dt}}\right),\ -\infty\le x\le\infty \qquad (2.43)$$

→ complementary error function

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

2.3.3 Solutions of the Diffusion Equation

[Re] complementary error function



Analytical solution for step function

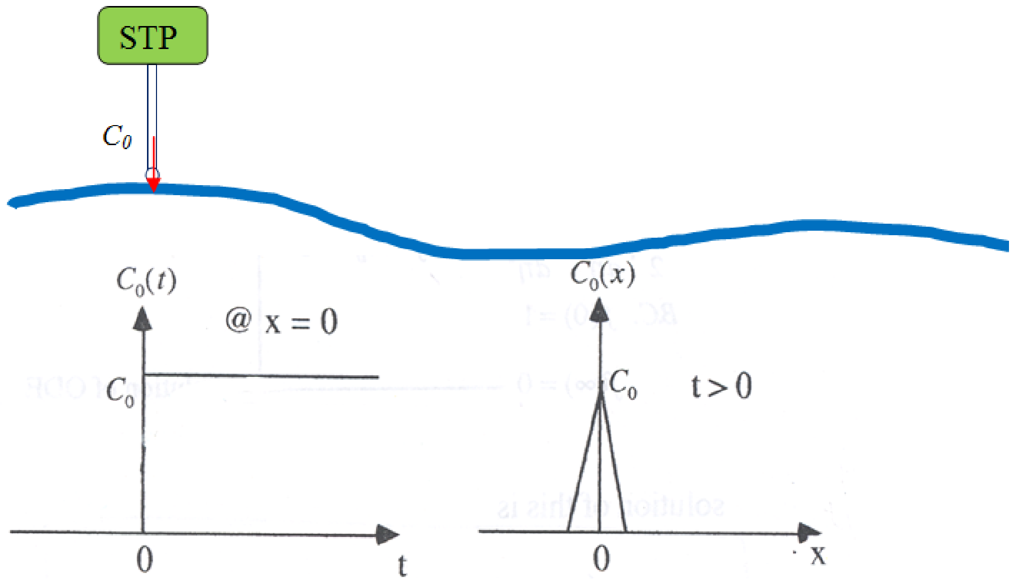
2.3.3 Solutions of the Diffusion Equation

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 $C(x,0)=C_0\ \ for\ x>0$	$C(x,t)=\frac{C_0}{2}\left[1+erf\left(\frac{x}{\sqrt{4Dt}}\right)\right]$
1-5	Distributed source with step function $C(x,0)=C_0\ \ for\ x<0$	$C(x,t)=\frac{C_0}{2}\left[1-erf\left(\frac{x}{\sqrt{4Dt}}\right)\right]$

Summary of solutions for instantaneous inputs (Series 1)

2.3.4 Concentration Specified as a Function of Time

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



Continuous input with step function

Consider continuous input with step input at $x = 0$

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

$$B.C. \qquad \boxed{C(x=0, t>0) = C_0}$$

2.3.4 Concentration Specified as a Function of Time

Solution by dimensional analysis

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

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

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

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

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

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

2.3.4 Concentration Specified as a Function of Time

Substitute these into Eq. (2.10) to obtain O.D.E.

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

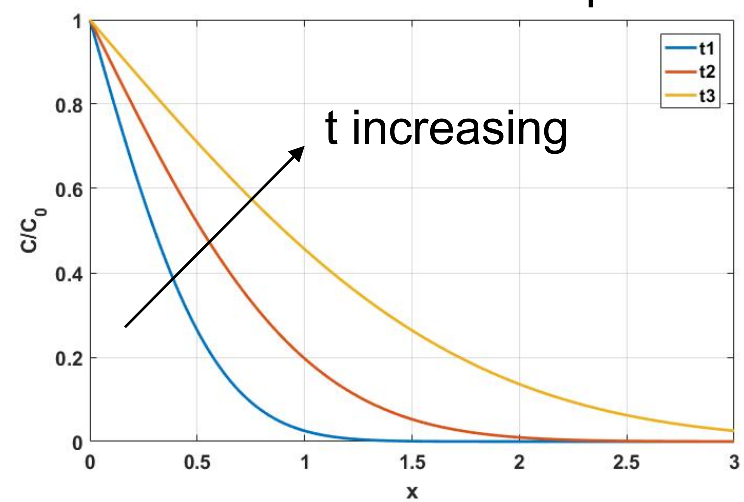
$$\boxed{2f''+\eta f'=0} \qquad \text{(a)}$$

B.C. $\quad f(0)=1 \qquad f(\infty)=0$

Solution of Eq. (a) is

$$\boxed{C=C_0\left[1-erf\left(\frac{x}{\sqrt{4Dt}}\right)\right]=C_0 erfc\left(\frac{x}{\sqrt{4Dt}}\right),\quad x>0 \qquad (2.44)}$$

Solution for continuous step function



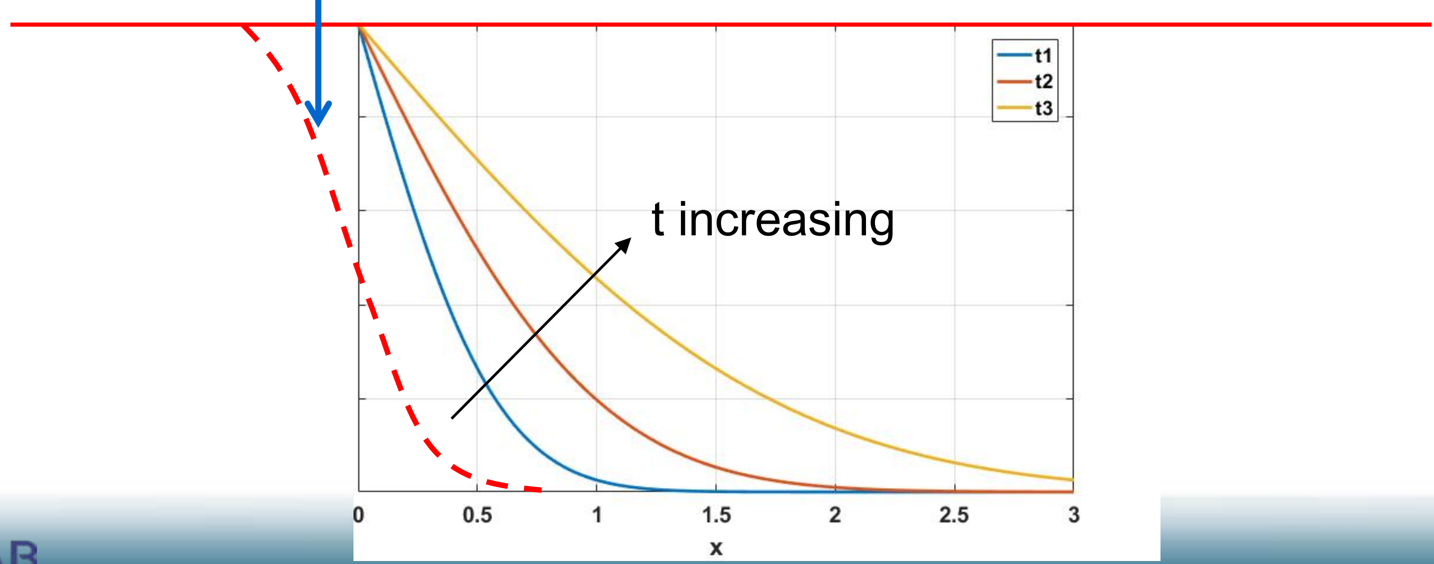
2.3.4 Concentration Specified as a Function of Time

Solution of Prob. 1-5

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

Solution of Prob. 2-1

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



2.3.4 Concentration Specified as a Function of Time

[Re] Laplace transformation

For ODE, it transforms ODE into algebraic problem.

For PDE, it transforms PDE into ODE.

i) Laplace transformation ("operational calculus")

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

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

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

ii) Inverse transform

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

iii) Linearity of Laplace transformation

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

iv) Integration of f(t)

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

2.3.4 Concentration Specified as a Function of Time

[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

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

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

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

Rewrite G.E.

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

2.3.4 Concentration Specified as a Function of Time

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, $\overline{C'} = \dfrac{\partial \overline{C}}{\partial x}$, $\overline{C''} = \dfrac{\partial^2 \overline{C}}{\partial x^2}$ Then $\overline{C''} - \dfrac{U}{D}\overline{C'} - \dfrac{s}{D}\overline{C} = 0$

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

Derive <u>characteristic equation</u> as

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

Solution is

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

2.3.4 Concentration Specified as a Function of Time

Then, $\overline{C}$ is

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

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

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

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

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

If we apply this to Eq. (1)

$$\lim_{x\to\infty}\overline{C}(x,s) = \lim_{x\to\infty}\left[C_1(s)\exp\left\{\frac{U \pm \sqrt{U^2+4sD}}{2D}x\right\}\right] + \lim_{x\to\infty}\left[C_2(s)\exp\left\{\frac{U \pm \sqrt{U^2+4sD}}{2D}x\right\}\right] = 0$$

$\therefore C_1(s)$ should be zero

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

2.3.4 Concentration Specified as a Function of Time

Apply B.C., Eq. (a)

Laplace transformation

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

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

$$\therefore\therefore\overline{C}=\frac{C_0}{s}\exp\left(\frac{U\pm\sqrt{U^2+4sD}}{2D}x\right)$$

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

Get inverse Laplace transformation using Laplace transform table

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

2.3.4 Concentration Specified as a Function of Time

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

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

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

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

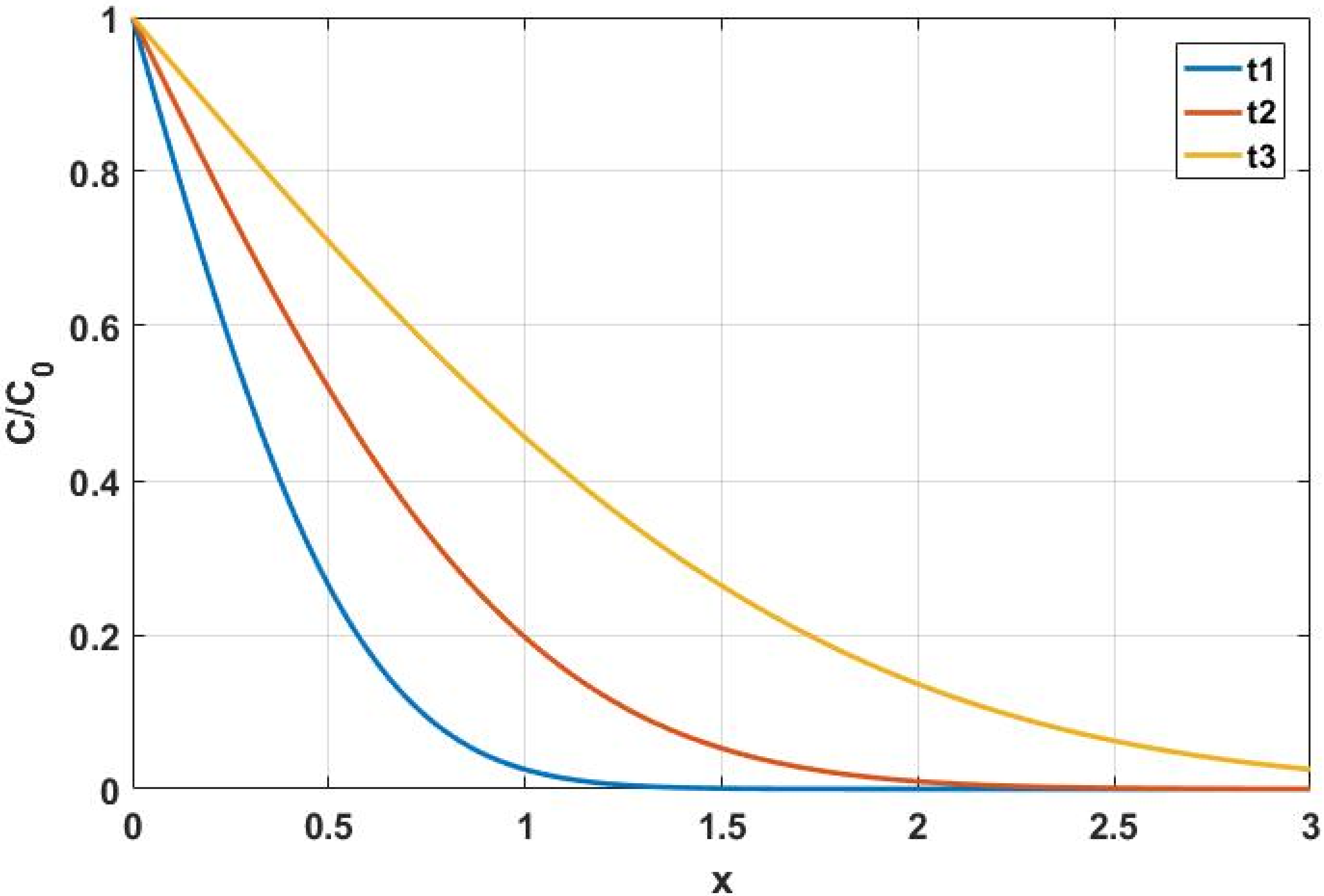
$$\therefore C = \frac{C_0}{2}\exp\left(\frac{Ux}{2D}\right)\left\{\exp\left(\frac{-Ux}{2D}\right)erfc\left(\frac{x-Ut}{\sqrt{4Dt}}\right) + \exp\left(\frac{Ux}{2D}\right)erfc\left(\frac{x+Ut}{\sqrt{4Dt}}\right)\right\}$$

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

In case U=0

$$C = \frac{C_0}{2}\left\{erfc\left(\frac{x}{\sqrt{4Dt}}\right) + erfc\left(\frac{x}{\sqrt{4Dt}}\right)\right\} = C_0 erfc\left(\frac{x}{\sqrt{4Dt}}\right) \qquad (2.45)$$

2.3.4 Concentration Specified as a Function of Time

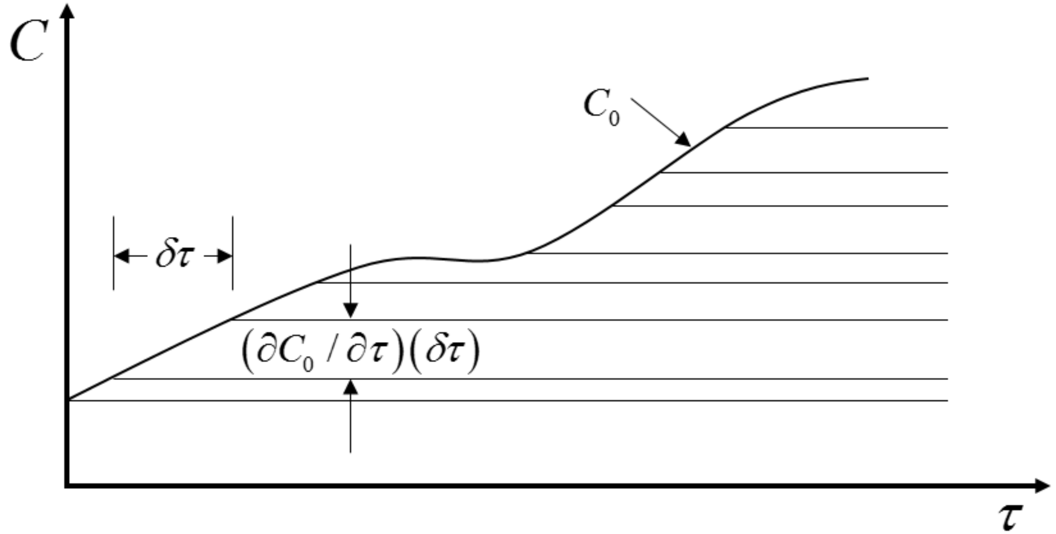


Solution for continuous step function

2.3.4 Concentration Specified as a Function of Time

(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 $x = 0$



Continuous input with step function

I.C. and B.C. are

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

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

2.3.4 Concentration Specified as a Function of Time

The solution is obtained by a superposition of solution, (2.44).

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

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

Then, total contribution is

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

2.3 Mathematics of Diffusion Equation

2.3.5 Input of mass specified as a function of time

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

$$C = \int_{-\infty}^{t} \frac{\dot{M}(\tau)\tau}{\sqrt{4\pi D(t-\tau)}}\exp\left[-\frac{x^2}{4D(t-\tau)}\right]d\tau \qquad (2.46)$$

where $\dot{M}(\tau)$ = rate of input mass at time τ and may vary with time = [$ML^{-2}t^{-1}$]

2.3 Mathematics of Diffusion Equation

(2) Continuous injection of mass of constant strength $\dot{M}$, $t > 0$ → Problem 2-4

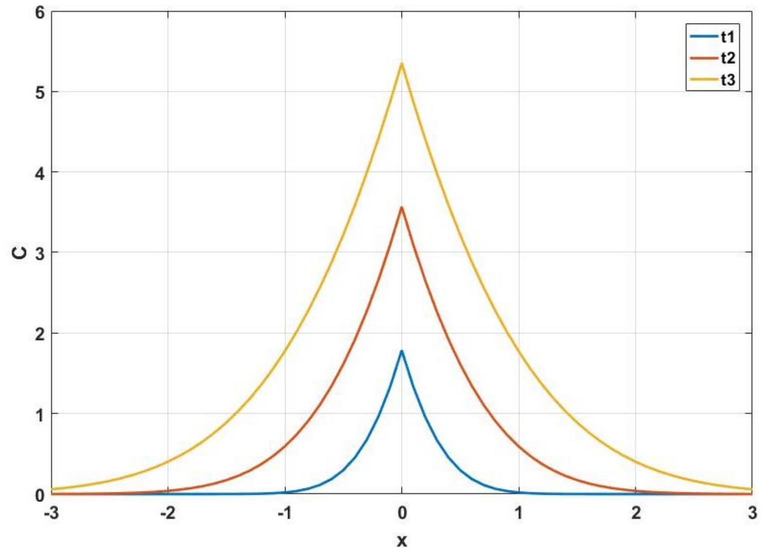
Eq. (2.46) gives

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

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

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

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



Continuous injection of mass of constant strength

Then, substituting this into (1) yields

$$\boxed{C(x,t) = \frac{\dot{M}x}{4D\sqrt{\pi}} \int_0^{\frac{4Dt}{x^2}} u^{-\frac{1}{2}} \exp\left[-\frac{1}{u}\right] du} \qquad (2.47)$$

2.3 Mathematics of Diffusion Equation

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

→ superposition in space and then in time to get solution

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

$$C(x,t) = \int_{-\infty}^{t}\int_{-\infty}^{\infty} \frac{m(\xi,\tau)}{\sqrt{4\pi D(t-\tau)}} \exp\left[-\frac{(x-\xi)^2}{4D(t-\tau)}\right] d\xi d\tau \tag{2.48}$$

2.3 Mathematics of Diffusion Equation

Case	Initial and boundary conditions	Solution
2-1	Continuous input with step function $C_0 = C_0(t)$	$C(x,t) = C_0\left[1 - erf\left(\frac{x}{\sqrt{4Dt}}\right)\right] = C_0 erfc\left(\frac{x}{\sqrt{4Dt}}\right)$
2-2	$C_0(\tau)$ as a time variable concentration at $x = 0$	$C(x,t) = \int_{-\infty}^{t} \frac{\partial C_0}{\partial \tau} erfc\left(\frac{x}{\sqrt{4D(t-\tau)}}\right) d\tau$
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 $m(x, t)$	$C(x,t) = \int_{-\infty}^{t} \int_{-\infty}^{\infty} \frac{m(\xi,\tau)}{\sqrt{4\pi D(t-\tau)}} \exp\left[-\frac{(x-\xi)^2}{4D(t-\tau)}\right] d\xi d\tau$

Summary of solutions for continuous inputs (Series 2)

Homework # 2

Due: 1 week from today

Consider pulse input of concentration specified as a step function

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

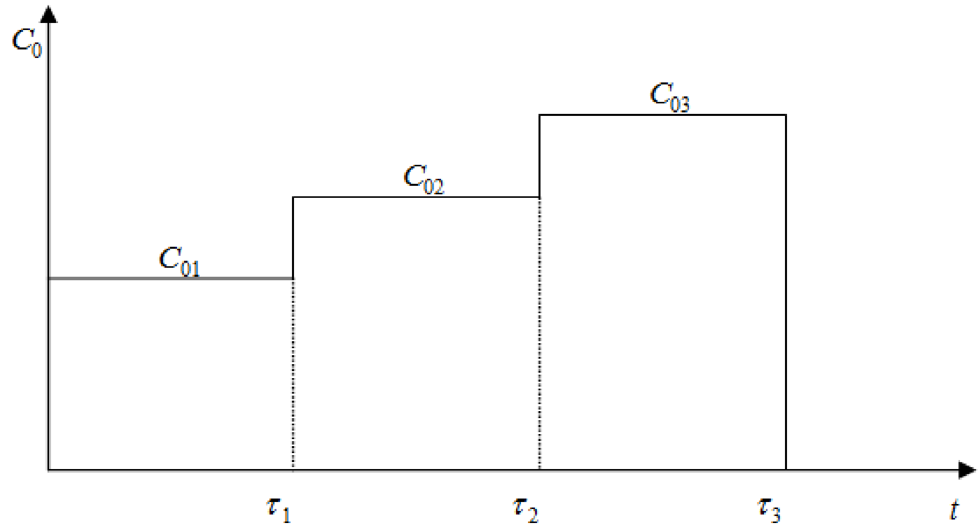
I.C.: $\mathrm{C}\left(x,\ t=0\right)=0$

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

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

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

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



a) Derive analytical solution using Laplace transformation.

b) Plot C vs x for various time t with assumed C_0s,

for example, $C_{01} = C_0/2$; $C_{02} = C_0$; $C_{03} = 3/2C_0$.

c) Plot C vs t for various distance x.

2.3 Mathematics of Diffusion Equation

2.3.6 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 $x = -L$

2.3 Mathematics of Diffusion Equation

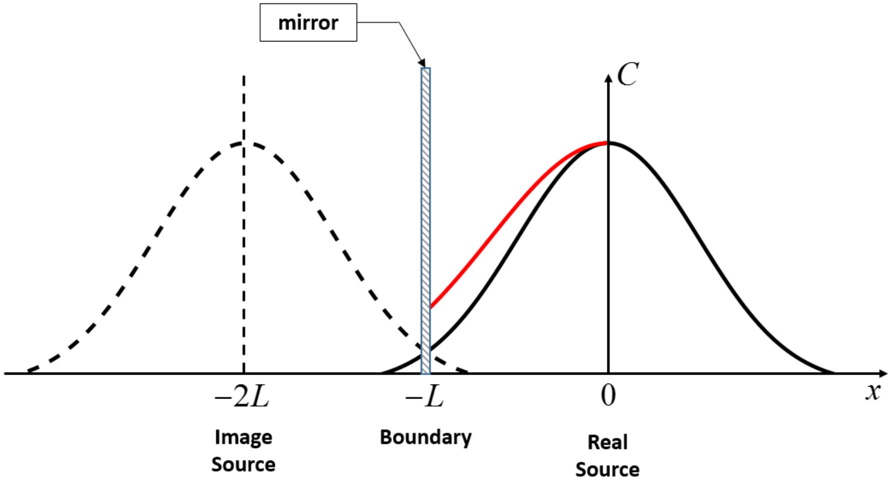
→ Fick's law for the boundary condition of no transport through the wall is

$$\boxed{q\big|_{x=-L} = -D\frac{\partial c}{\partial x}\bigg|_{x=-L} = 0}$$

→ 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.



Mass input at $x = 0$ with non-diffusive boundary

2.3 Mathematics of Diffusion Equation

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

x - (- 2 L)

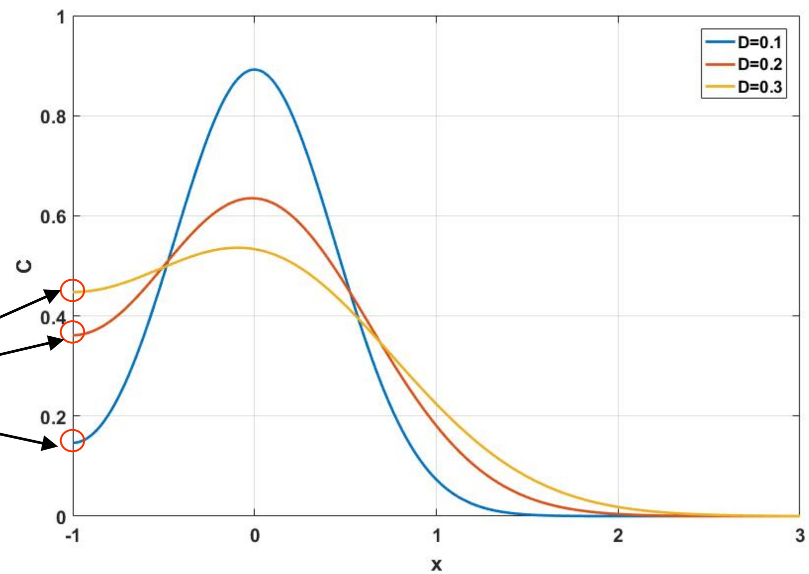
$$C = \frac{1}{\sqrt{4\pi D t}}\left\{\exp\left(-\frac{x^2}{4Dt}\right) + \exp\left(-\frac{(x+2L)^2}{4Dt}\right)\right\} \tag{2.49}$$

Unit mass: $M = 1$

Real source

Image source

$$\frac{\partial C}{\partial x} = 0$$



Solution with varying diffusion coefficient

2.3 Mathematics of Diffusion Equation

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

→ Problem 3-2

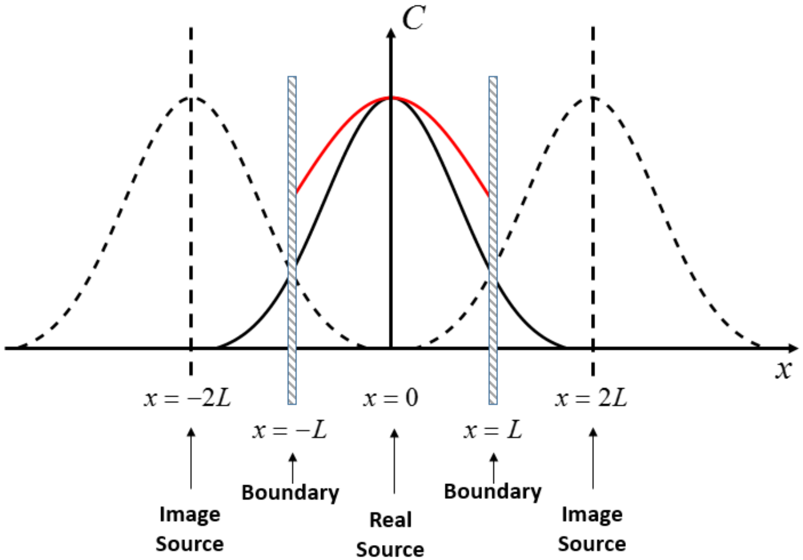
→ put image slugs *at* $-2L, +2L, 4L, -6L, 8L, \ldots\ldots$

(∵ 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

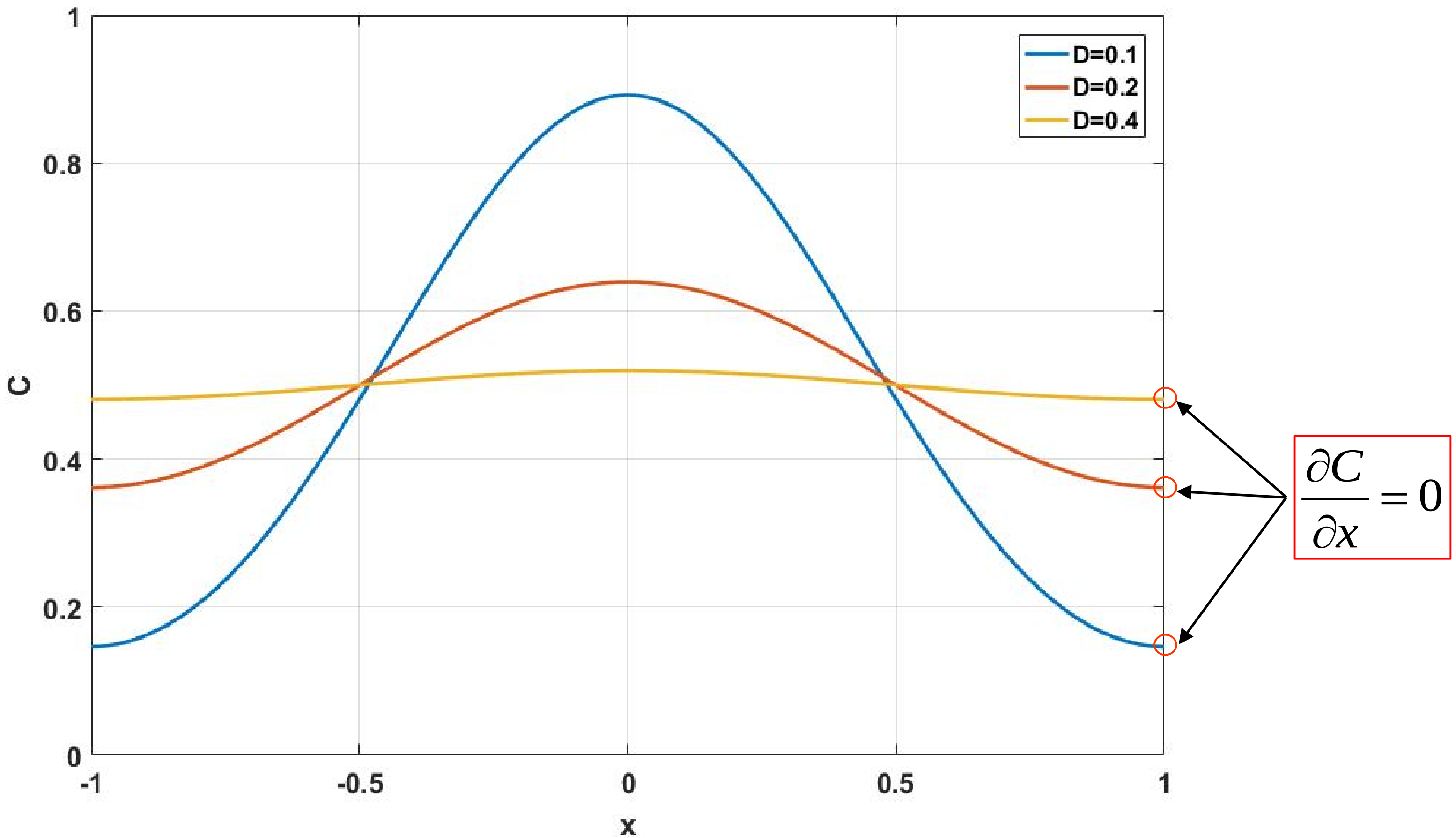
$$\boxed{C(x,t) = \sum_{n=-\infty}^{\infty} \frac{1}{\sqrt{4\pi Dt}} \exp\left[-\frac{(x+2nL)^2}{4Dt} \right]}$$

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



Mass input at $x = 0$
with non-diffusive boundaries

2.3 Mathematics of Diffusion Equation



Solution for mass input at $x = 0$ with non-diffusive boundaries

2.3 Mathematics of Diffusion Equation

(3) Zero concentration at $x = \pm L$ (absorbing boundary) → **Problem 3-3**

→ $\boxed{C(x = \pm L, t) = 0}$ → Dirichlet type B.C.

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

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

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

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

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

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

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

2.3 Mathematics of Diffusion Equation

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 $x = \pm L$	$C(x,t)=\frac{1}{\sqrt{4\pi Dt}}\sum_{n=-\infty}^{\infty}\left\{\begin{matrix}\exp\left[\frac{-(x+4nL)^2}{4Dt}\right] \\ -\exp\left[\frac{-\left[x+(4n-2)L\right]^2}{4Dt}\right]\end{matrix}\right\}$
3-4	Mass input $x = 0$ with non-diffusive boundaries at $x = 0$	$C(x,t)=\frac{1}{\sqrt{\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)$

2.3 Mathematics of Diffusion Equation

2.3.7 Solutions in Two and Three Dimensions

(1) 2D Fluid

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

G. E.: $$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} \qquad (2.50)$$

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

For molecular diffusion, $D_x = D_y = D$

Use Product rule

$$\boxed{C(x, y, t) = C_1(x, t)C_2(y, t)}$$

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

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial t}(C_1 C_2) = C_1 \frac{\partial C_2}{\partial t} + C_2 \frac{\partial C_1}{\partial t} \; ; \quad \frac{\partial^2 C}{\partial x^2} = \frac{\partial^2}{\partial x^2}(C_1 C_2) = C_2 \frac{\partial^2 C_1}{\partial x^2}$$

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

2.3 Mathematics of Diffusion Equation

Eq. (2.50) becomes

$$C_1\frac{\partial C_2}{\partial t}+C_2\frac{\partial C_1}{\partial t}=D_xC_2\frac{\partial^2 C_1}{\partial x^2}+D_yC_1\frac{\partial^2 C_2}{\partial y^2}$$

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

$$\frac{\partial C_1}{\partial t}=D_x\frac{\partial^2 C_1}{\partial x^2}$$

$$\frac{\partial C_2}{\partial t}=D_y\frac{\partial^2 C_2}{\partial y^2}$$

→ 1-D diffusion equation

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

$$\boxed{M_x}$$

$$\therefore C_1=\frac{\int_{-\infty}^{\infty}Cdx}{\sqrt{4\pi D_xt}}\exp\left(-\frac{x^2}{4D_xt}\right)\qquad C_2=\frac{\int_{-\infty}^{\infty}Cdy}{\sqrt{4\pi D_yt}}\exp\left(-\frac{y^2}{4D_yt}\right)$$

$$\therefore C=C_1C_2=\frac{M}{4\pi t\sqrt{D_xD_y}}\exp\left(-\frac{x^2}{4D_xt}-\frac{y^2}{4D_yt}\right)\tag{2.51}$$

2.3 Mathematics of Diffusion Equation

- Iso-concentration lines

→ lines of constant concentration = set of concentric ellipses

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

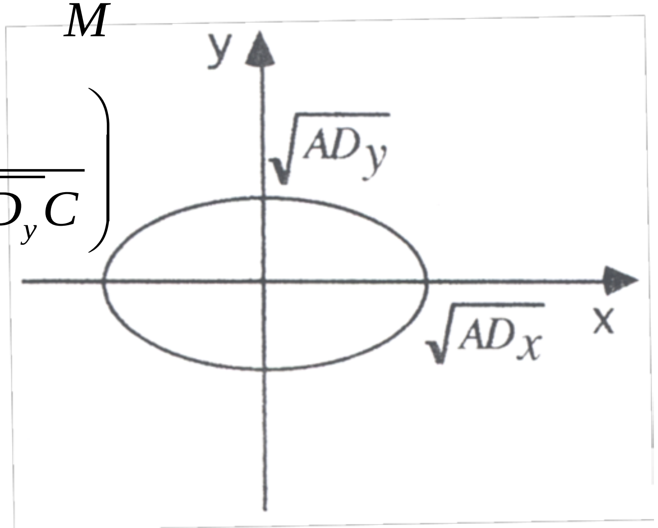
$$\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t} = -\ln\left(\frac{4\pi t\sqrt{D_x D_y}C}{M}\right) = \ln\left(\frac{M}{4\pi t\sqrt{D_x D_y}C}\right)$$

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

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

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

→ ellipses

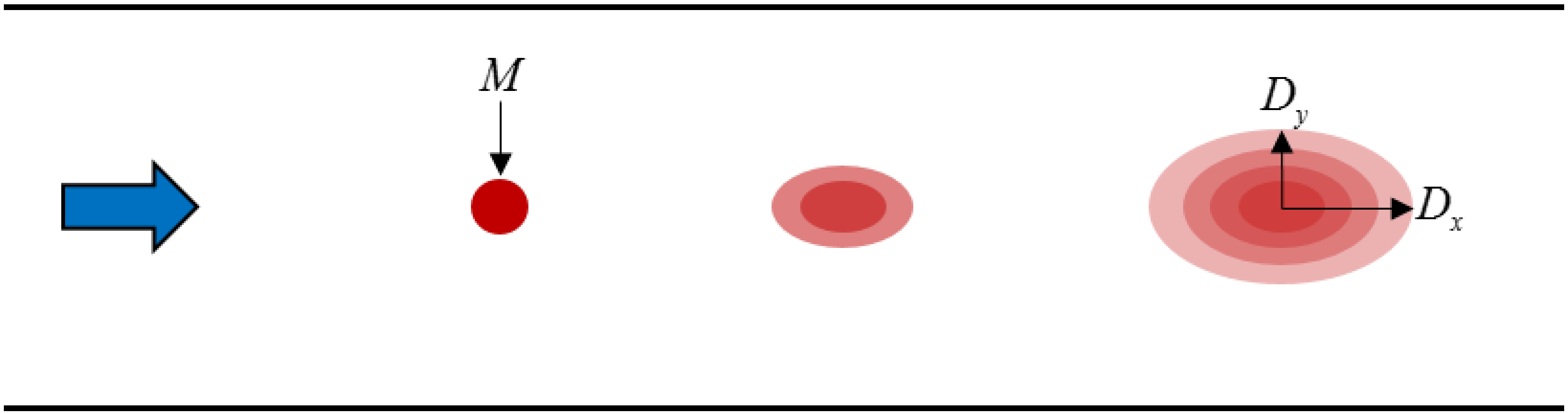


Iso-concentration lines

2.3 Mathematics of Diffusion Equation

If $D_x = D_y$

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

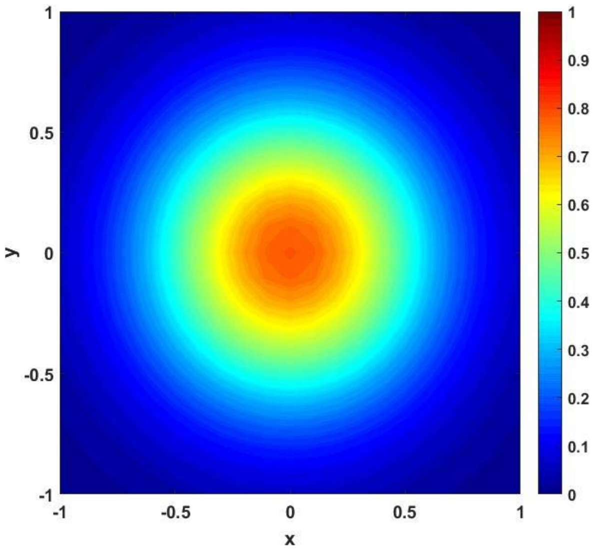


Two-dimensional advection and diffusion in open channels

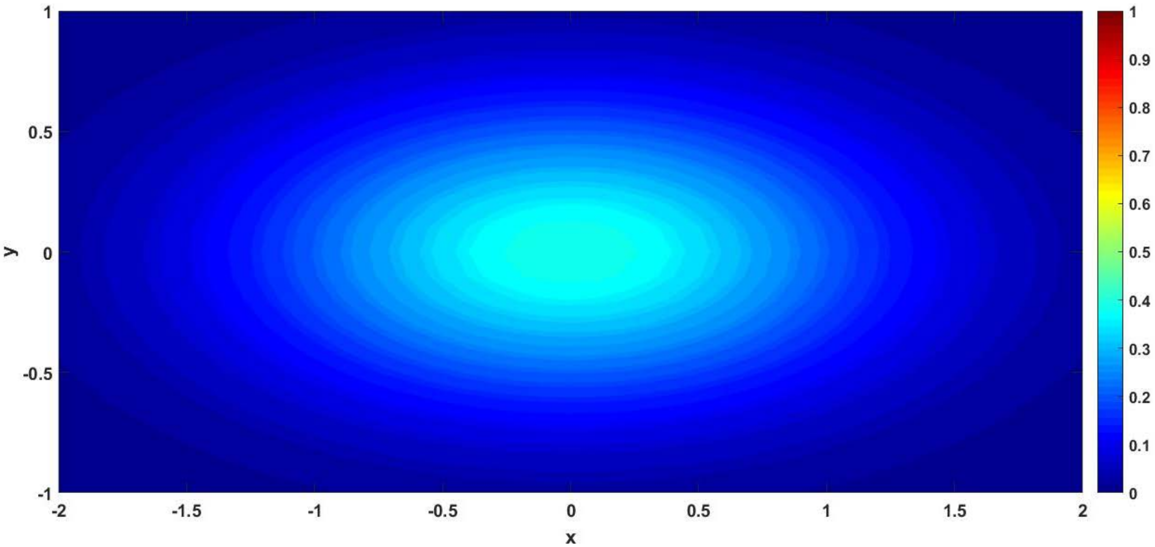
2.3 Mathematics of Diffusion Equation

-Contour Graphics-

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



$\left(D_x = D_y = 0.1,\ M = 1\right)$



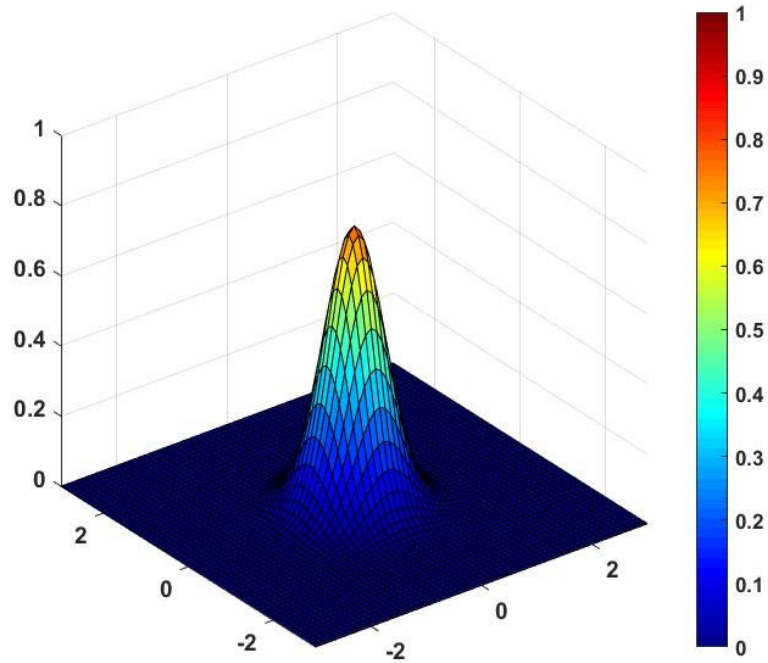
$\left(D_x = 0.1, D_y = 0.4,\ M = 1\right)$

Contour graphics for different cases of D_x and D_y

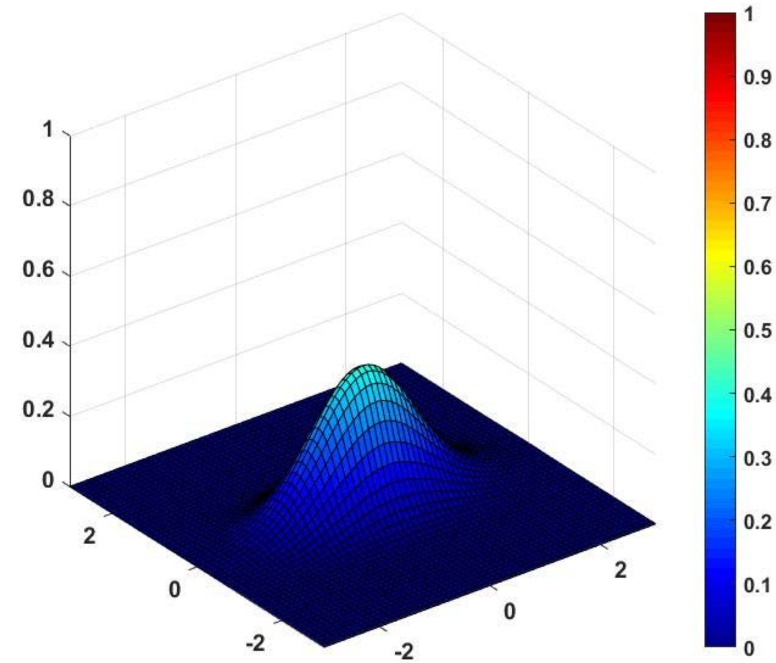
2.3 Mathematics of Diffusion Equation

-Mesh Graphics-

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



$\left(D_x = D_y = 0.1,\ M = 1\right)$



$\left(D_x = 0.1, D_y = 0.4,\ M = 1\right)$

3D graphics of concentration distributions

2.3 Mathematics of Diffusion Equation

(2) 3D fluid

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

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

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

Use product rule

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

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

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

2.3 Mathematics of Diffusion Equation

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

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

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

Substituting these relations into (b) yields

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

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

2.3 Mathematics of Diffusion Equation

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

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

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

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

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

2.3 Mathematics of Diffusion Equation

2.3.8 Advective Diffusion

1D Advection-Diffusion Equation is

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(uC) = D\frac{\partial^2 C}{\partial x^2} \qquad (2.52)$$

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

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

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

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

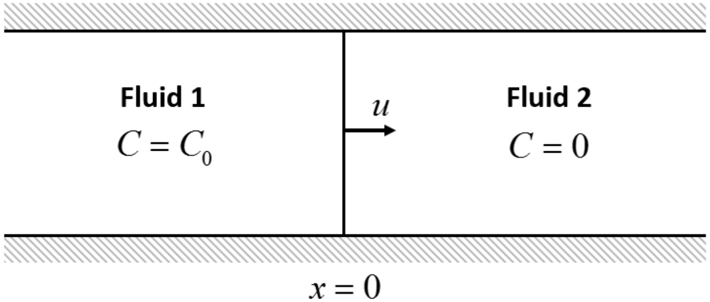
$$\boxed{C(x,t) = \frac{M}{\sqrt{4\pi D\, t}} \exp\left(-\frac{(x-ut)^2}{4Dt} \right)}$$

2.3 Mathematics of Diffusion Equation

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.: $C(x,0)=0, \quad x>0 \quad ; \quad C(x,0)=C_0, \quad x<0$



Fluid being displaced at a mean velocity u by another fluid

Transform coordinate system whose origin moves at velocity u

Let $\quad x' = x - ut, \; t = t \quad \rightarrow \dfrac{\partial x'}{\partial x} = 1, \dfrac{\partial x'}{\partial t} = -u$

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

2.3 Mathematics of Diffusion Equation

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

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

2.3 Mathematics of Diffusion Equation

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

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

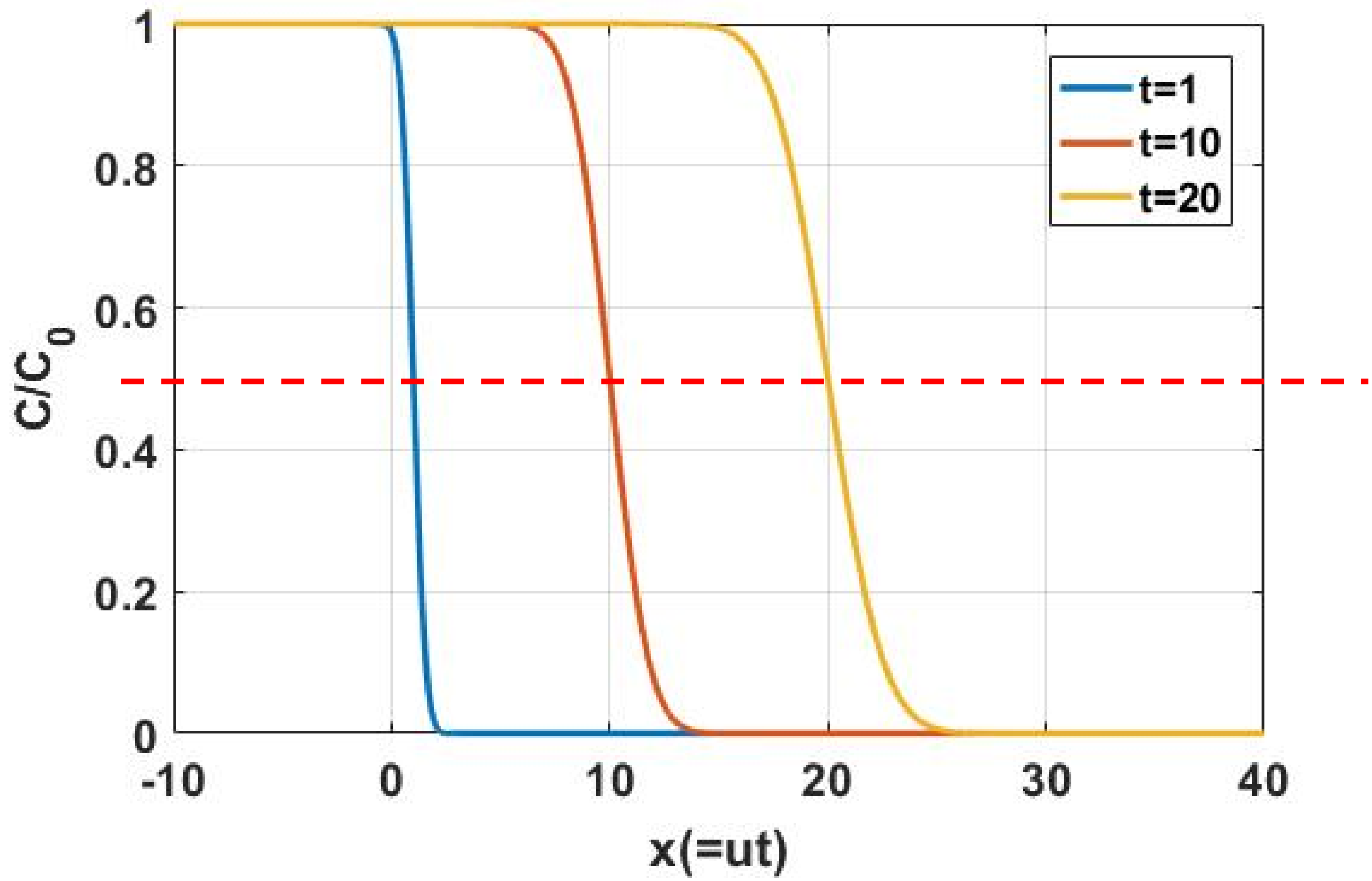
There, solution is

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

Adjust for the moving coordinates

$$\boxed{C(x,t) = \frac{C_0}{2}\left[1 - erf\left(\frac{x-ut}{\sqrt{4Dt}}\right)\right]} \qquad (2.53)$$

2.3 Mathematics of Diffusion Equation

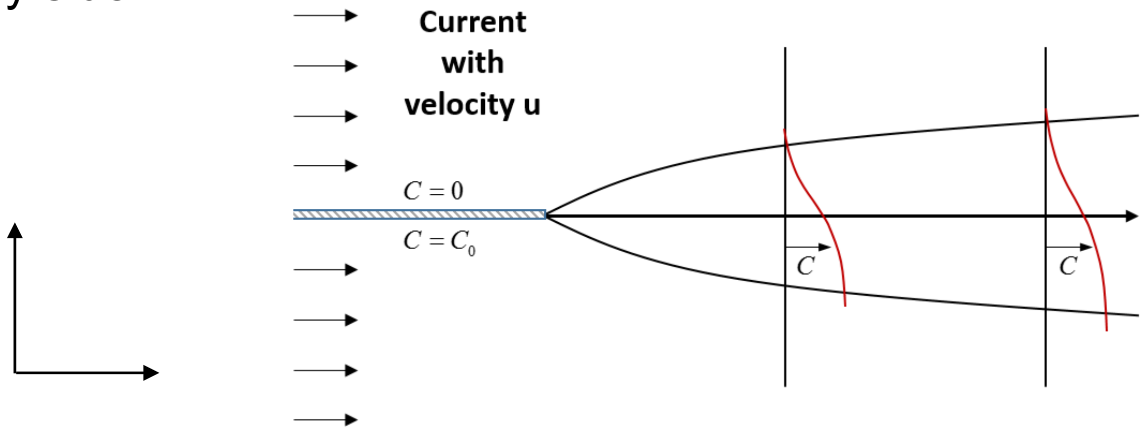


Solution of instantaneous concentration input over $x < 0$

2.3 Mathematics of Diffusion Equation

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

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



Transverse mixing of two streams

Start with 2-D advection-diffusion equation

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

2.3 Mathematics of Diffusion Equation

Assumptions:

i) continuous input: $\frac{\partial C}{\partial t} \to 0$

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

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

Then, G.E. becomes

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

→ similar to 1-D diffusion equation

B. C.: $C(0, y) = 0 \quad y > 0 \quad ; \quad C(0, y) = C_0, \quad y < 0$

→ Now, this problem is similar to <u>Problem 1-5</u> with $t = x/u; x' = y$

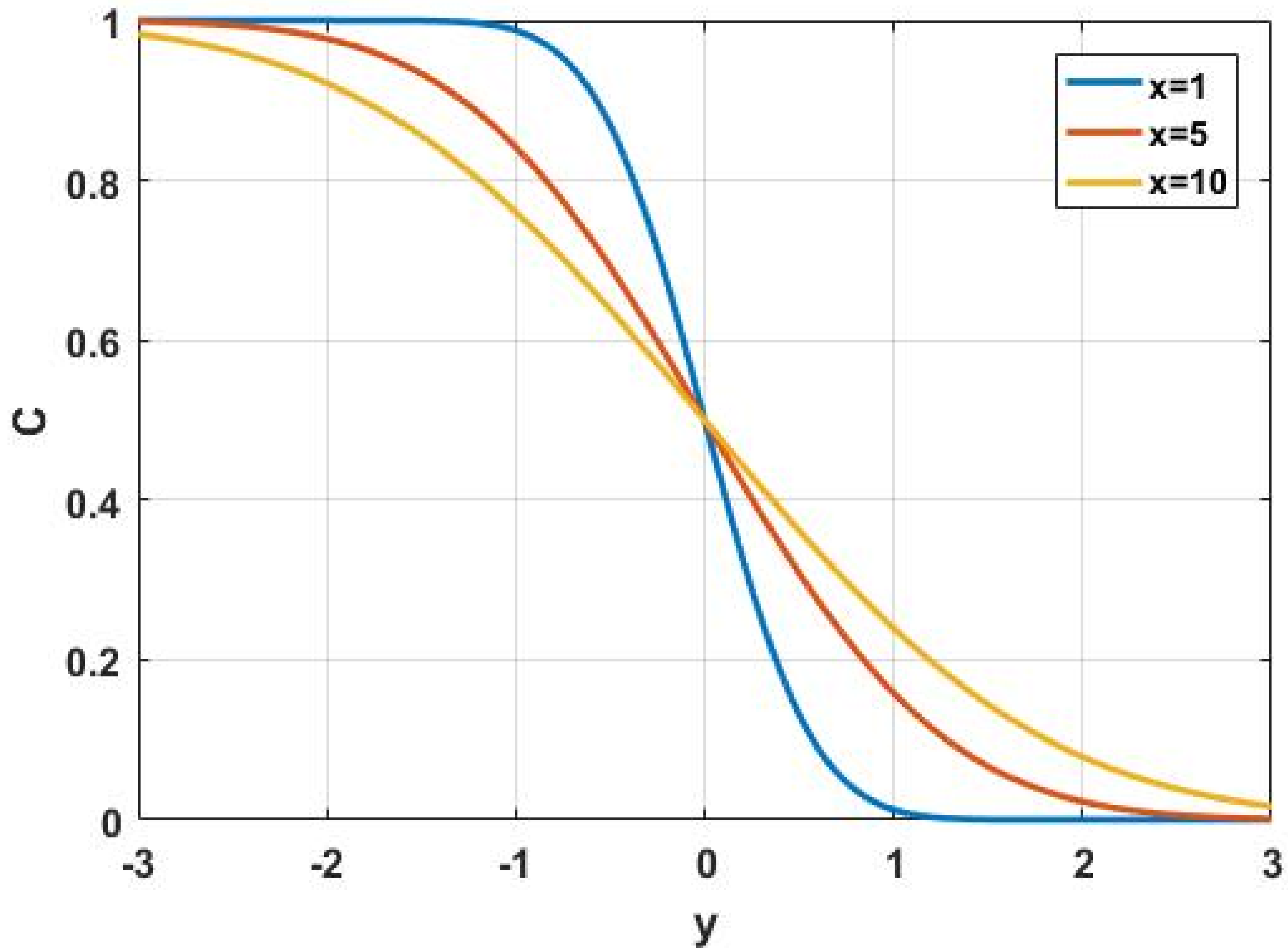
Solution is

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

Convert to *x*-*y* coordinates

$$C = \frac{C_0}{2}\left[1 - erf\left(\frac{y}{\sqrt{4Dx/u}}\right)\right] \qquad (2.54)$$

2.3 Mathematics of Diffusion Equation



2.3 Mathematics of Diffusion Equation

4) Continuous plane source → **Problem 5-4**

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

B.C.: $$\boxed{C(0,t)=C_0 \qquad 0<t<\infty}$$ → steady continuous input

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

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

The solution is

$$\boxed{C(x,t)=\frac{C_0}{2}\left[erfc\left(\frac{x-ut}{\sqrt{4Dt}}\right)+erfc\left(\frac{x+ut}{\sqrt{4Dt}}\right)\exp\left(\frac{ux}{D}\right)\right]} \qquad (2.55)$$

Set

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

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

2.3 Mathematics of Diffusion Equation

Then,

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

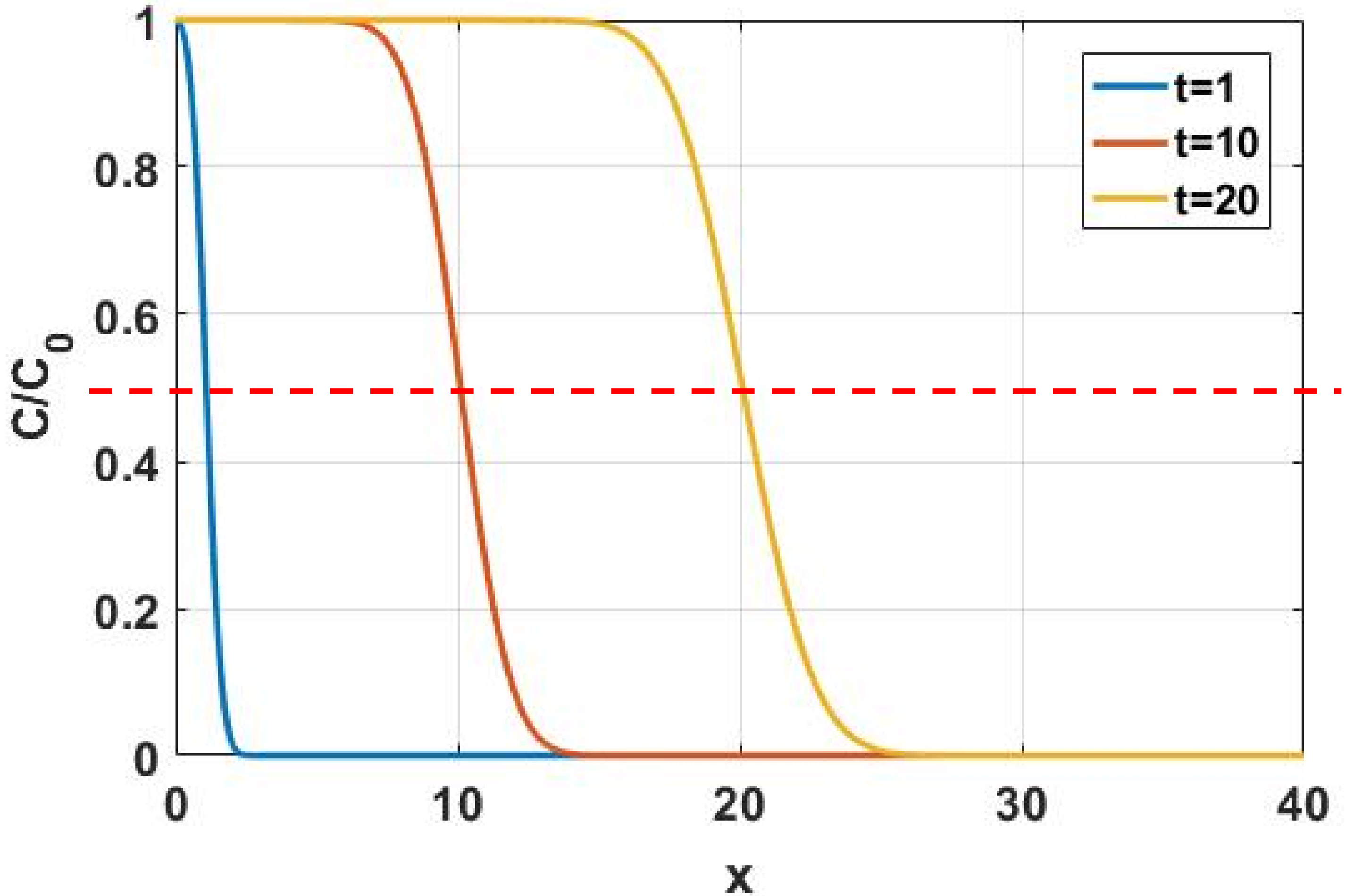
For advection-dominated case (large u)

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

Diffusion problem ($u = 0$)

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

2.3 Mathematics of Diffusion Equation



Solution for continuous plane source with elapsed time

2.3 Mathematics of Diffusion Equation

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

Summary of solutions for advective diffusion (Series 5)

Homework Assignment #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 P_e of and t.

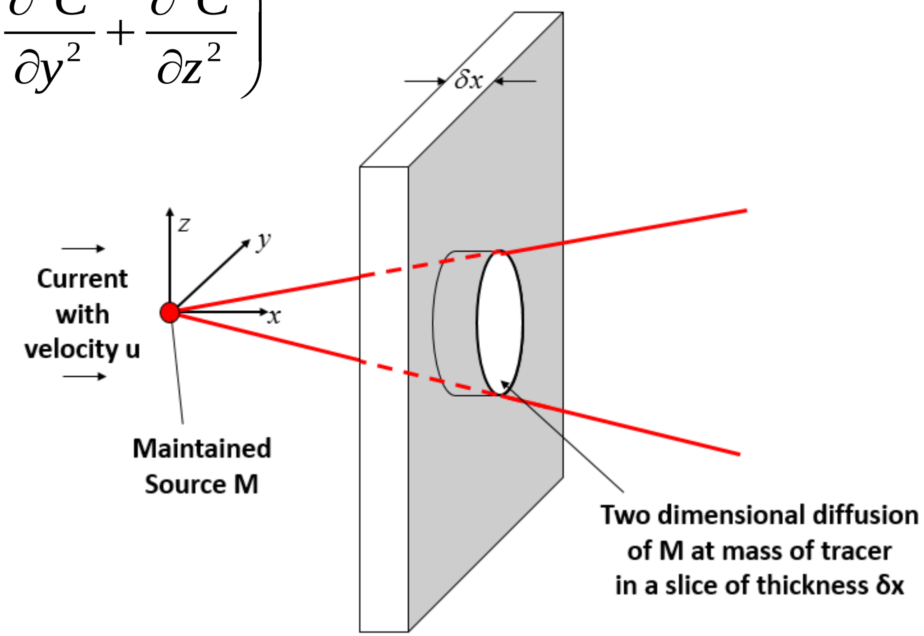
2.3 Mathematics of Diffusion Equation

2.3.9 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

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



Constant point source in 3D flows

2.3 Mathematics of Diffusion Equation

- 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 with velocity u, and during the passage each one receives a slug of mass of amount $\dot{M}\delta t$

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

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

→ This is identical to 2-D solution of Eq. (2.51).

$$C = \frac{mass / l}{4\pi t\sqrt{D_y D_z}} \exp\left(-\frac{y^2}{4D_y t} - \frac{z^2}{4D_z t} \right) \quad ; \quad C = \frac{\left(\dot{M}\dfrac{\delta x}{u} \right) \Big/ \delta x}{4\pi D t} \exp\left(-\frac{(y+z)^2}{4Dt} \right)$$

2.3 Mathematics of Diffusion Equation

Substitute $t = \dfrac{x}{u}$

$$\boxed{C(x,y,z) = \frac{\dot{M}}{4\pi D x}\exp\left(-\frac{\left(y^2+z^2\right)u}{4Dx}\right)} \qquad (2.55)$$

Eq. (2.56) was derived by neglecting diffusion in the direction of flow.

→ $ut >> \sqrt{2Dt}$ or $\boxed{t >> 2D/u^2}$

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

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

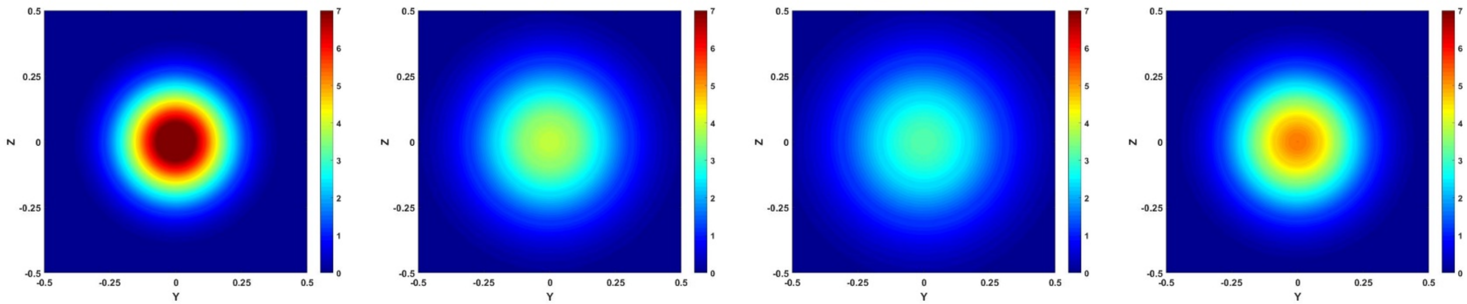
Substitute $t = \dfrac{x}{u}$

$$C(x,y) = \frac{\dot{M}}{u\sqrt{4\pi D x/u}}\exp\left(-\frac{y^2 u}{4Dx}\right) \qquad (2.57)$$

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

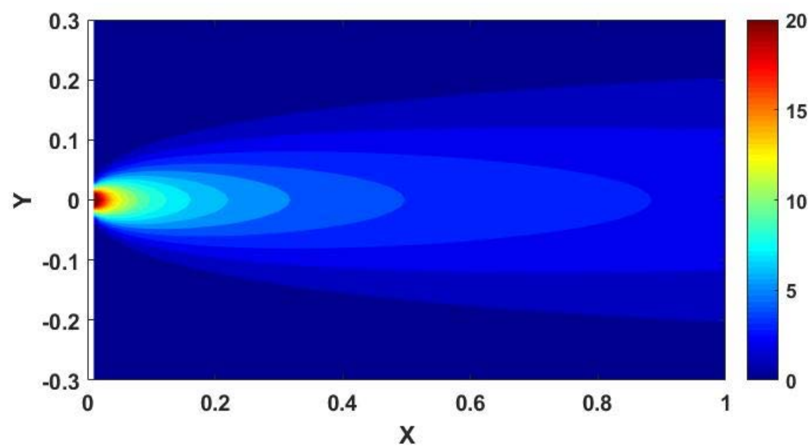
2.3 Mathematics of Diffusion Equation

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



$x = x_1$ $x = x_2$ $x = x_3$ $x = x_4$

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



$\dot{M}$

2.3 Mathematics of Diffusion Equation

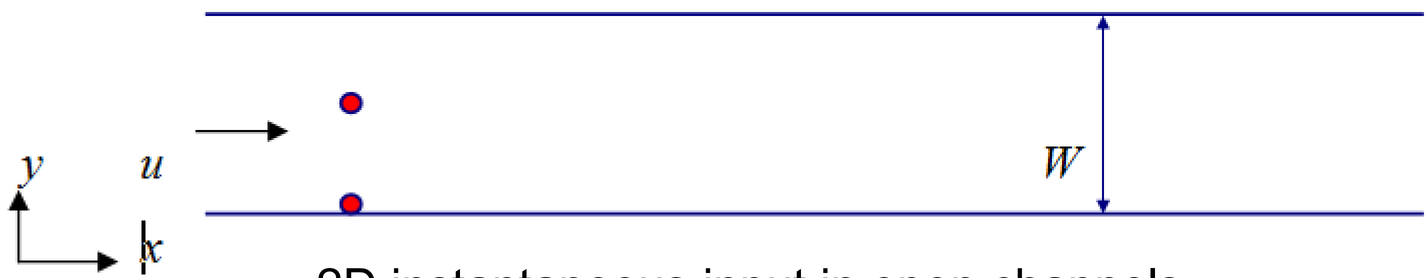
Case	Initial and boundary conditions	Solution
6-1	Mass input at the rate $\dot{M}$ at the origin (x, y, z) in 3D flow	$\boxed{C(x,y,z)=\frac{\dot{M}}{4\pi Dx}\exp\left(-\frac{\left(y^2+z^2\right)u}{4Dx}\right)}$
6-2	Maintained point source in 2D flow	$C(x,y)=\frac{\dot{M}}{u\sqrt{4\pi Dx/u}}\exp\left(-\frac{y^2u}{4Dx}\right)$

Solutions for maintained point discharges in 2D & 3D flows (Series 6)

2.3 Mathematics of Diffusion Equation

2.3.10 Solutions for Pollutant Mixing in Rivers

(1) 2D Instantaneous Input



2D instantaneous input in open channels

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

2.3 Mathematics of Diffusion Equation

i) Case A: Right-bank input

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

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

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

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

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

2.3 Mathematics of Diffusion Equation

ii) Case B: Centerline input

a) For axis at right bank

$$C_1 = \frac{M_1}{\sqrt{4\pi D_x t}} \exp\left(-\frac{(x-ut)^2}{4D_x t}\right) \qquad C_2 = \sum_{n=-\infty}^{\infty} \frac{M_2}{\sqrt{4\pi D_y t}} \exp\left[-\frac{\left\{y+(2n-1)\frac{W}{2}\right\}^2}{4D_y t}\right]$$

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

b) For axis at centerline

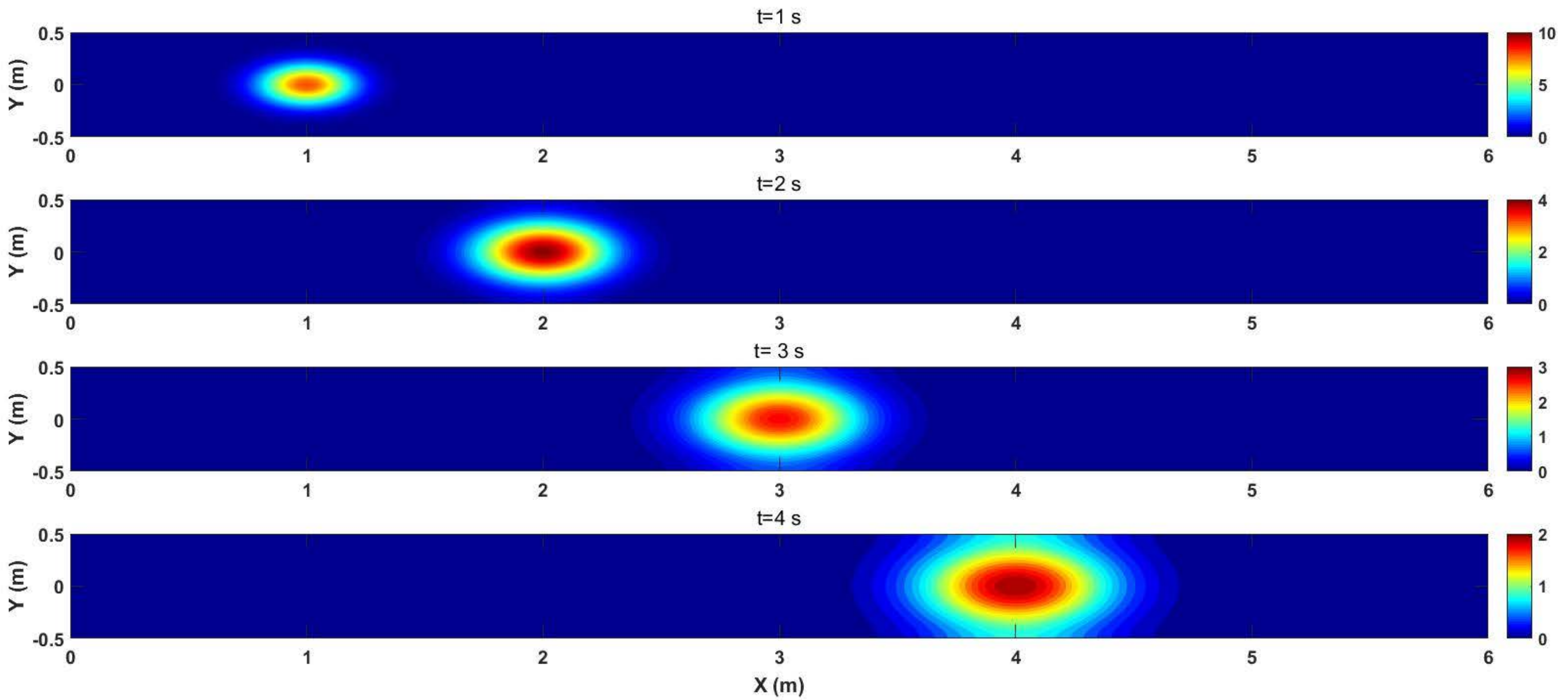
$$C_1 = \frac{M_1}{\sqrt{4\pi D_x t}} \exp\left(-\frac{(x-ut)^2}{4D_x t}\right) \qquad C_2 = \sum_{n=-\infty}^{\infty} \frac{M_2}{\sqrt{4\pi D_y t}} \left[\exp\left\{-\frac{y+nW^2}{4D_y t}\right\}\right]$$

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

2.3 Mathematics of Diffusion Equation

ii) Case B: Centerline input

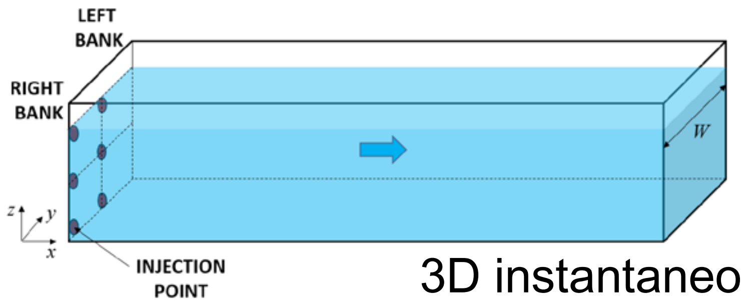
b) For axis at centerline

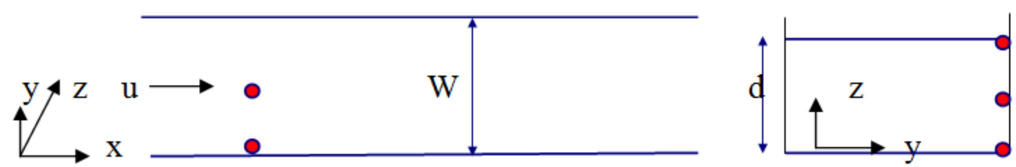


2.3 Mathematics of Diffusion Equation

(2) 3D Instantaneous Input

Fig. 2.40 3D instantaneous input in open channels





3D instantaneous input in open channels

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

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

2.3 Mathematics of Diffusion Equation

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

Use product rule

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

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

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

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

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

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

2.3 Mathematics of Diffusion Equation

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

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

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

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

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

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

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

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

2.3 Mathematics of Diffusion Equation

iv) Case D: Centerline input – bottom input

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

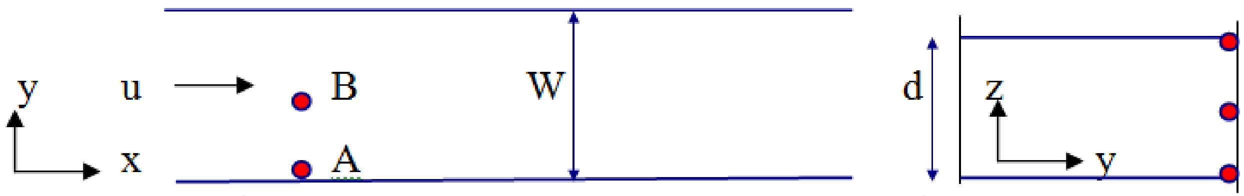
$$C_3 = \sum_{n=-\infty}^{\infty} \frac{M_3}{\sqrt{4\pi D_z t}} \left[\exp\left\{ -\frac{(z+2nd)^2}{4D_z t} \right\} \right]$$

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

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

2.3 Mathematics of Diffusion Equation

(3) 2D Analytical Solutions for continuous point injection



Continuous point injection in 2D flows

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

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

Case II: centerline injection

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

2.3 Mathematics of Diffusion Equation

◈ Product Rule

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

Then, the governing equation will be modified as

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

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

After that, we must to solve two equations

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

and

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

2.3 Mathematics of Diffusion Equation

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

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

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

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

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

2.3 Mathematics of Diffusion Equation

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

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

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

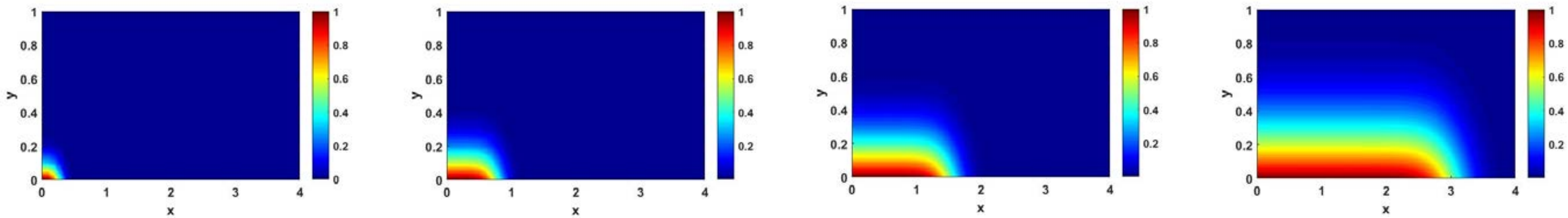
[Re] Decaying substance in 2D flow

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

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

2.3 Mathematics of Diffusion Equation

Case I: side injection



$t = t_1$ $t = t_2$ $t = t_3$ $t = t_4$

[Re] Decaying substance in 2D flow