

The Scale Relevant to Life

Most cells are between 1 and 100 μm .
i.e. Three orders of magnitude
difference in size.

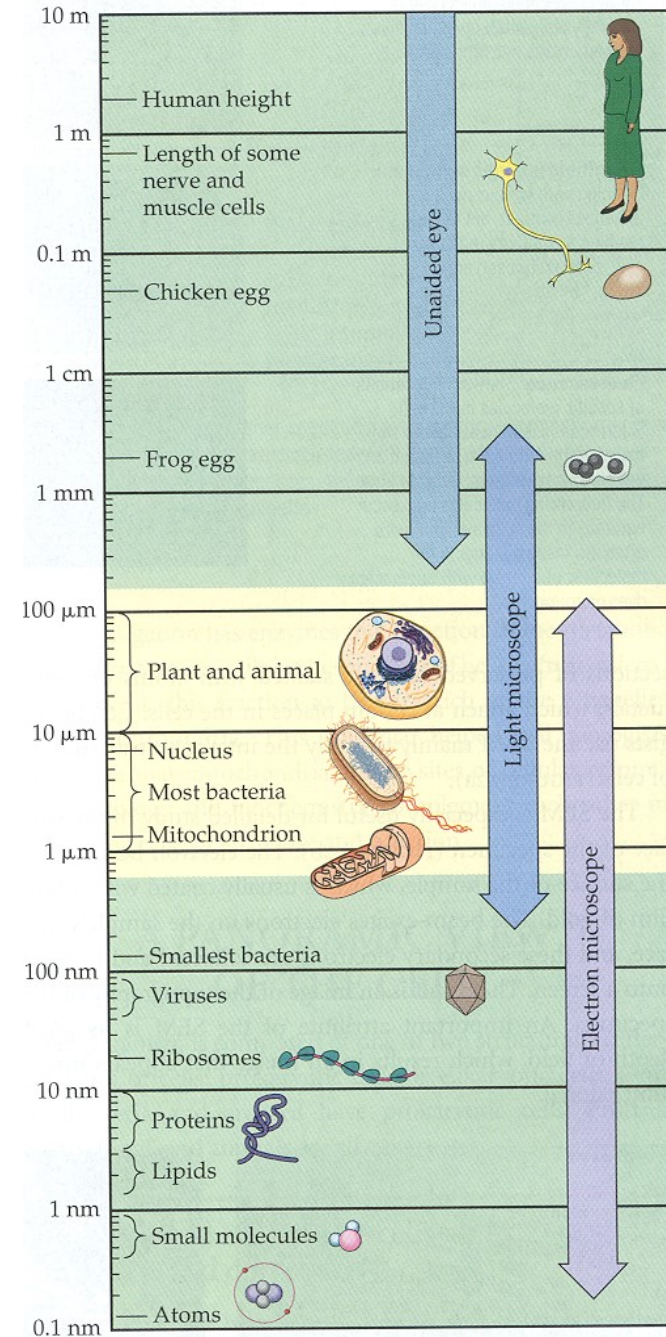
Smallest bacterial cells are
mycoplasmas = 0.1 - 1.0 μm
Bacteria = 1 - 10 μm
Plant and animal cells = 10 - 100 μm

TABLE 1.4

Relevant Length Scales in Biological Systems

Quantity	Length scale (m)
Proteins and nucleic acids	10^{-8}
Organelles	10^{-7}
Cells	10^{-6} to 10^{-6}
Capillary spacing	10^{-4}
Organs	10^{-1}
Whole body	10^0

Source: From Ref. [4].



How many orders of magnitude do living cells span?

1

2

3

4

The speed with which a molecule diffuses in a fluid depends upon: size, shape, temperature, viscosity and chemistry

TABLE 1.1

Range of Values for the Binary Diffusion Coefficient, D_{ij} , at Room Temperature

Diffusing quantity	Diffusion coefficients ($\text{cm}^2 \text{s}^{-1}$)
Gases in gases	0.1 to 0.5
Gases in liquids	1×10^{-7} to 7×10^{-5}
Small molecules in liquids	1×10^{-5}
Proteins in liquids	1×10^{-7} to 7×10^{-7}
Proteins in tissues	1×10^{-7} to 7×10^{-10}
Lipids in lipid membranes	1×10^{-9}
Proteins in lipid membranes	1×10^{-10} to 1×10^{-12}

Be able to estimate
These values

In the x-y plane:

$$D_{ij} = \frac{\langle x^2 \rangle + \langle y^2 \rangle}{4t} \quad i \text{ solute, } j \text{ solvent}$$

What if it is 1-D?

What if it is 2-D?

What if it is 3-D?

How does the equation change?

How do you calculate the root mean square versus the geometric mean? What happens to outliers in each case?

Diffusion / Convection

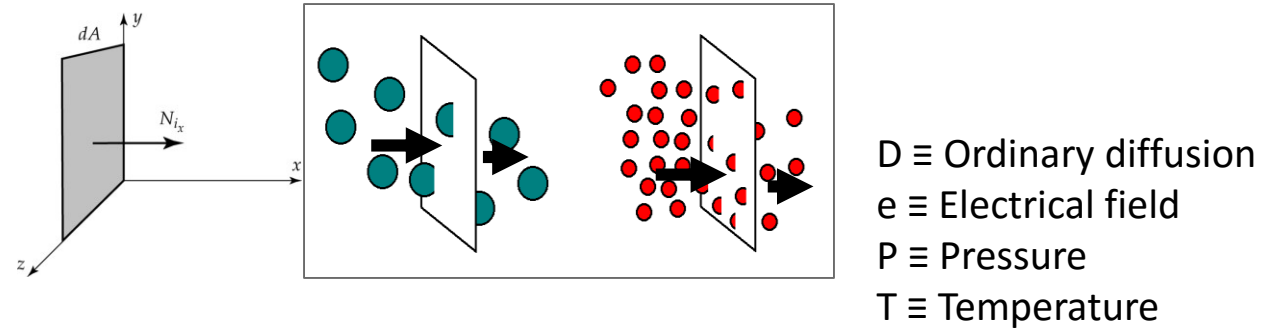
- A protein molecule of diffusion coefficient 10^{-7} cm² /s will diffuse from edge to center of a 20 um diameter cell in 2.5 s.
- A protein molecule of diffusion coefficient 10^{-7} cm² /s will diffuse through 2mm thick tissue in 27.7 h.
- Diffusion – short distances
 - How far from blood vessel can oxygen transport by diffusion
- Convection – long distances
 - Do all bugs need a pumping heart?
 - Are there bugs without hearts?
 - What kind of hearts are there in bugs?

How do you calculate the distance something diffuses in 1D, 2D and 3D?

A protein molecules with a D of $1e-7 \text{ cm}^2/\text{s}$ will diffuse from the edge to the center of a 20 μm diameter cell in how many seconds?

How do you estimate the diameter of particles using nanoparticle tracking analysis software?

Flux of i in the x -direction.



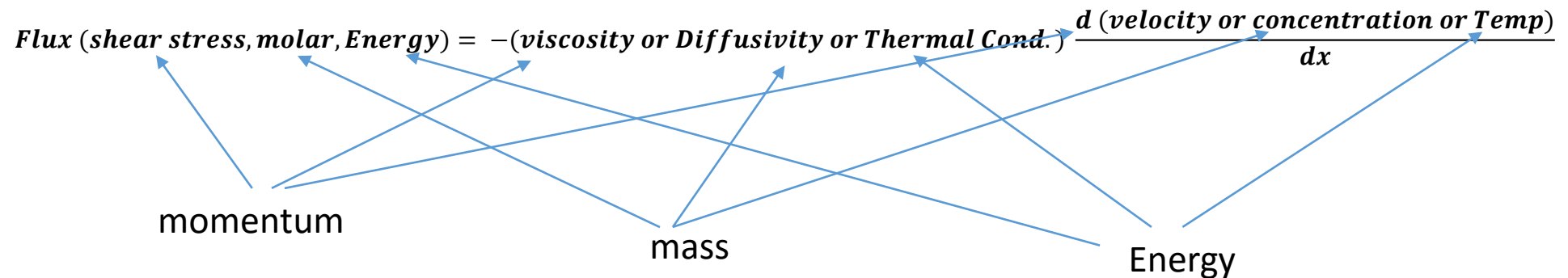
$$J_i^* = J_i^{*D} + J_i^{*e} + J_i^{*p} + J_i^{*T}$$

These different fluxes can be used for separation purposes (i.e., ultracentrifugation, electrophoresis, isoelectric focusing, the usage of membranes)...

TABLE 1.3

Relations between Fluxes and Gradients for Molecular Transport			
Molecular transport mechanism	Flux	Gradient	Coefficient of proportionality
Momentum	Shear stress	Velocity	Viscosity
Mass	Mass or molar flux	Concentration ^a	Diffusion coefficient
Energy	Energy	Temperature	Thermal conductivity

^aFor charged molecules, transport is down an electrochemical gradient, defined as the sum of the concentration gradient plus the potential field gradient. This kind of transport is discussed in detail in Section 7.4.



8.28.18: Some of the arrows were shifted somehow on slide 10. I made sure the arrows were pointing to the correct word.

What is the i and what is the j ?

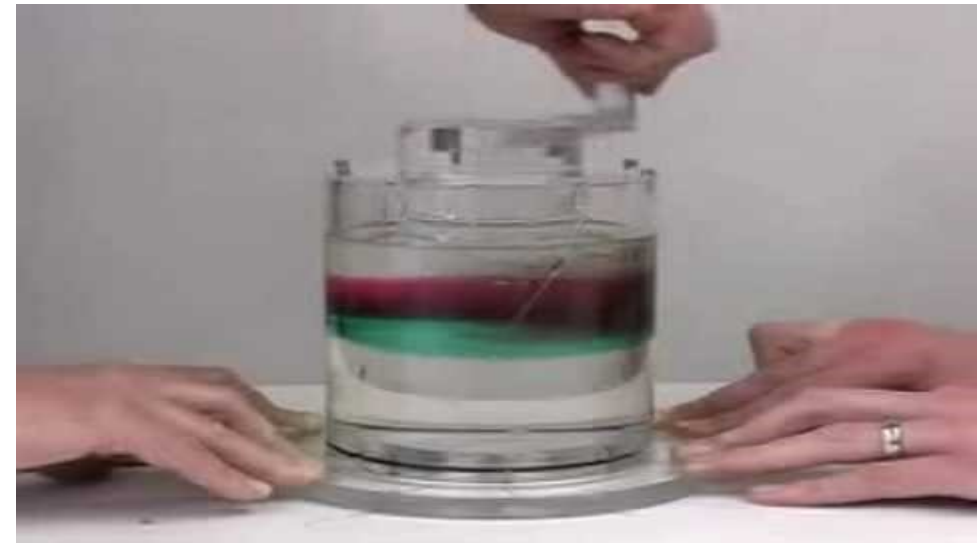
TABLE 1.5

Relative Importance of Diffusion and Convection				
Molecule	MW (g mol ⁻¹)	D_{ij} (cm ² s ⁻¹)	Diffusion time, L^2/D_{ij} (s)	Pe = Lv/D_{ij}
Oxygen	32	2×10^{-5}	5	0.05
Glucose	180	2×10^{-6}	50	0.50
Insulin	6,000	1×10^{-6}	100	1.0
Antibody	150,000	6×10^{-7}	167	1.67
Particle	Diameter	D_{ij} (cm ² s ⁻¹)	Diffusion time (s)	Pe
Virus	0.1 μm	5×10^{-8}	2,000	20
Bacterium	1 μm	5×10^{-9}	20,000	200
Cell	10 μm	5×10^{-10}	200,000	2,000

Note: For $L = 100 \mu\text{m}$, and if $v = 1 \mu\text{m s}^{-1}$, the time for convection is always equal to $L/v = 100$ s for all molecules and particles.

Reynold's # = Re

- $Re = \frac{\textit{inertial forces}}{\textit{viscous forces}} = \frac{vL}{k.v.} = \frac{vL\rho}{\mu}$
- Units?
- v = object velocity relative to flow.
- k.v. = viscosity/density
- Why does Re exist? To predict flow patterns
 - Laminar or turbulent
 - If $Re < 2000 \Rightarrow$ laminar
 - If $Re > 4000 \Rightarrow$ turbulent
 - If Re is between 2000 and 4000
transitional flow



https://www.youtube.com/watch?v=p08_KITKP50

Examples:

viscosity	9.10E-03 Poise	g/cm/s
density	1 g/cm ³	
velocity	1 cm/s	
L	50 cm	
Re	5494.51	turbulent
Cell	10 um	
cell	1.00E-03 cm	
Re	0.11	laminar

How do you calculate Reynold's numbers and why is it useful?

Peclet # = Pe

- *Time of diffusion* = $\frac{L^2}{D_{ij}}$

- *Time of convection* = $\frac{L}{\text{velocity}}$

- $Pe = \frac{\text{diffusion time}}{\text{convection time}} = \frac{\text{mass transport by convection}}{\text{mass transport by diffusion}} = \frac{\text{vel} * L}{D_{ij}} = \left(\frac{L^2}{D_{ij}} \right) \left(\frac{v}{L} \right)$

- What is dominant – convection or diffusion?
- Over the dimensions of a cell, diffusion is sufficiently efficient (up to 100 um)
- Diffusion limited: event is limited by how many are arriving by diffusion

How do you calculate the Peclet number and why is it useful?

Biot

$B = \text{Mass Transfer Across a Cell Layer} / \text{Mass Transfer by Diffusion Through Tissue} = k * L / D$

Numerator is non-diffusive mass transfer (not specific) component

Example of k:

First order diff. eq.

$$dC/dt = kC$$

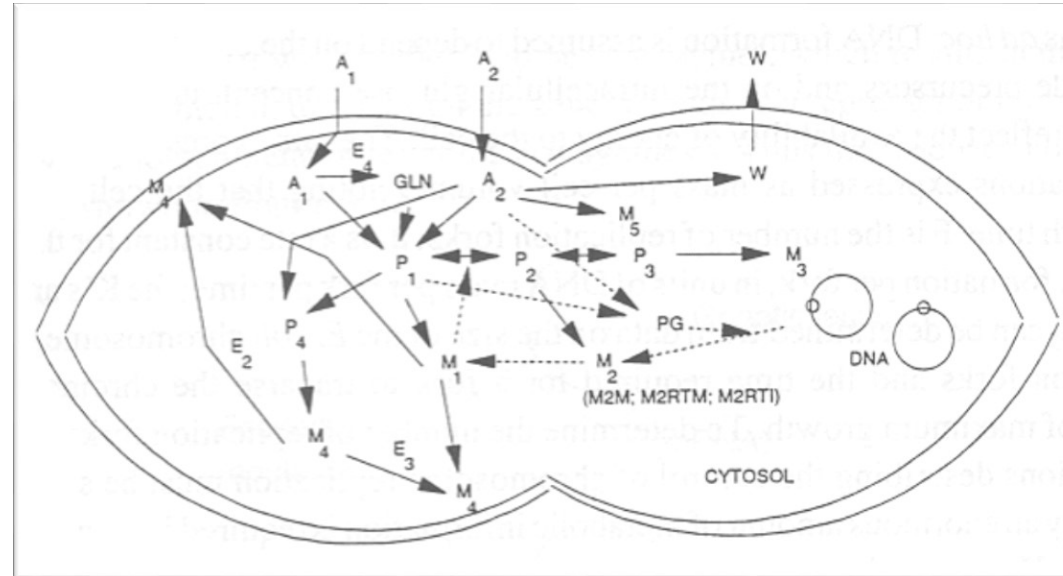
How do you calculate the Biot # and why is it useful?

Flux and Fick's 1st law

- Flux is proportional to the gradient
- What are the units of flux?
 - (#or mol)/area/time or mass/area/time...
- $J = -D \frac{dc}{dx} = -D \nabla C$; what is the upside down triangle?
 - Gradient
- what is the expansion of the equation?
 - $J = -D \left[\frac{dc}{dx} + \frac{dc}{dy} + \frac{dc}{dz} \right]$

Why are cells microscopic?

1. Diffusive transport over large distances may be inadequate.



For **Constant Flux** steady state diffusion in one direction -

Fick's First Law

$$J = -D \frac{dC}{dx}$$

D - diffusion coefficient (m²/s); **C** - kg/m³ or cm² /s and moles/l

Diffusion Across Cell Membranes and within Cells

$$J = -D \frac{dC}{dx} = -D \frac{\Delta C}{\Delta x} = -D \frac{C_A - C_B}{x_A - x_B}$$

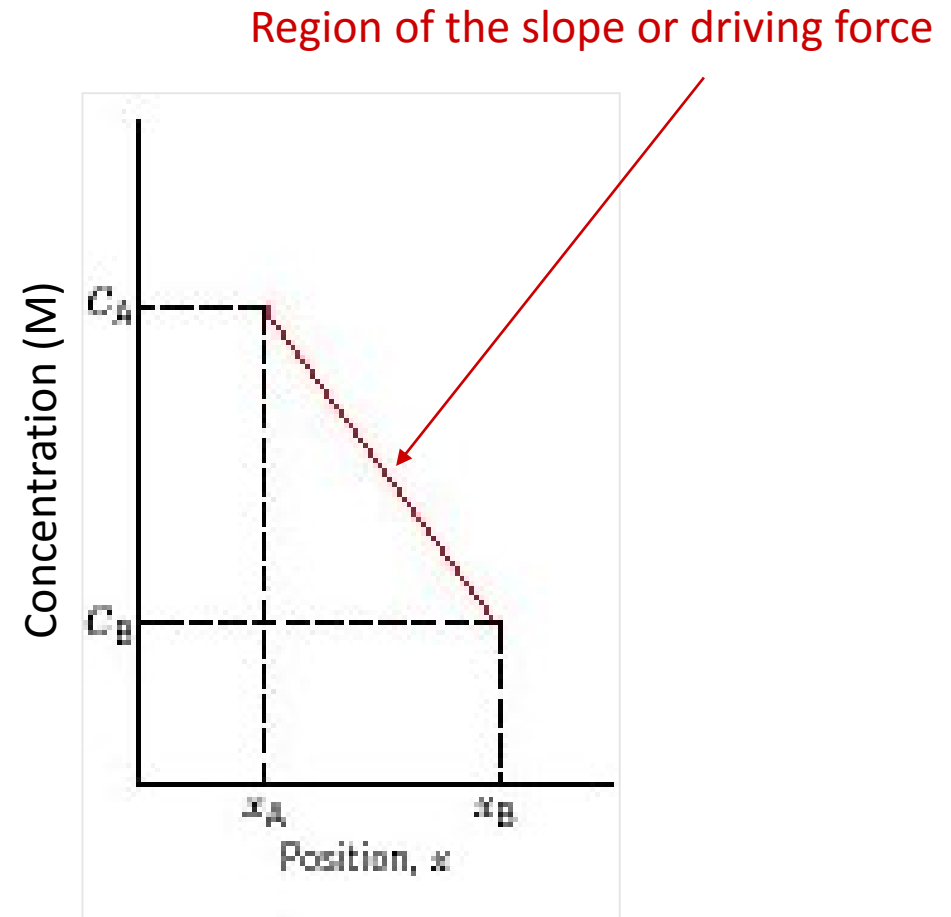
D - diffusion coefficient (m^2/s)

dc/dx - Driving force

$$J = -D \frac{C_A - C_B}{x_A - x_B}$$

$$J = -(3 \times 10^{-11} \text{ m}^2 / \text{s}) \frac{(1.2 - 0.8) \text{ kg} / \text{m}^3}{(5 \times 10^{-3} - 1 \times 10^{-2}) \text{ m}}$$

$$J = 2.4 \times 10^{-9} \text{ kg} / \text{m}^2 \cdot \text{s}$$



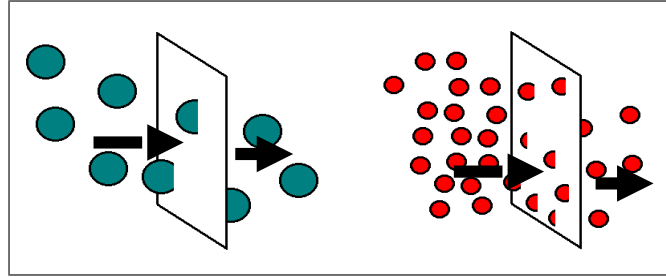
What is Fick's first law?

What is Fick's second law

- $\frac{dC}{dt} = D\Delta C$; and what is the diff between Δ and ∇ ?
- Expand this...
- $\frac{dC}{dt} = D\left[\frac{d^2C}{dx^2} + \frac{d^2C}{dy^2} + \frac{d^2C}{dz^2}\right]$

What is Fick's 2nd law?

6.4 Constitutive Relations: 6.4.1 Fick's First Law



$$J_{ix} = -D_{ij} \frac{\partial C_i}{\partial x}$$

$$J_i = -D_{ij} \nabla C_i$$

Dilute;
No reactions
Producing or
Consuming
Constituents...

J_{ix} = diffusive flux of a dissolved solute *in dilute solution*

D_{ij} = *binary* diffusion coefficient of solute i in solvent j

C = concentration of reactant

$$\mathbf{N}_i = \mathbf{J}_i + C_i \mathbf{v}_s$$

Substituting into gives when convection is present...

$$\mathbf{N}_i = -\mathbf{D}_{ij} \nabla C_i + C_i \mathbf{v}_s$$

Note, D can be a $f(C)$...

Non-Steady State Diffusion in the Solid State

- ➡ Most **real** diffusion is **non-steady state**
- ➡ The concentration of diffusing species is a function of both time and position $C = C(x,t)$
i.e., **flux** and **driving force** both change with **time**
- ➡ In this case **Fick's Second Law** is used

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

- Solution requires specified boundary conditions

On board...

6.2.1 Dilute Solution Approximation

- **Most biological solutions are dilute**
- Concentration of the solvent must be large relative to the solute: $C_{\text{solvent}} \gg C_i$ or $x_s \approx 1 \gg x_i = \text{mole fraction}$
- The molar average velocity equals the mass average velocity i.e. $v^* \approx v_{\text{solvent}}$ and $v \approx v_{\text{solvent}}$ so that $v \approx v^*$ and $J_i = J_i^*$

$$J_i^* = N_i - C_i v^* \quad \text{or} \quad N_i = J_i^* + C_i v^* \quad \text{becomes} \quad N_i = J_i + C_i v_s$$

$$N_1 = \frac{1}{(1-x_1)} (J_1^* + x_1 N_2) \quad \Rightarrow \quad N_i = J_i + C_i v_s$$

When N2 is solvent

Can study dilute solutions as if they were binary

Justification of dilute –solution problems in biological contexts

- Water is 1 g/cm^3 . 1 mole of water is 18g and is 55.56 M.
- Salt concentrations: 1 μM to 300 mM
 - $1.8\text{e-}8$ to 0.0054 mole fractions
- Protein: 1 nM to 1 mM
 - $1.8\text{e-}11$ and $1.8\text{e-}5$ mole fractions.
- Exceptions: gas diffusion in the lung, purification of biological molecules in high salt concentrations (1-5M), fermentation processes

Give 2 justifications of why biological fluids are able to be considered dilute and give an example of a biological solution that is not dilute.

6.3.2 Boundary Conditions

Useful for investigating conservation relations...

Concentrations are not necessarily constant or continuous across a fluid-fluid **interface**

At the gas (1) solution (2) interface, at equilibrium:

$$C_i|_1 = H_i C_i|_2$$

Where H_i is the *Henry's Law Constant*

At the liquid (1) immiscible liquid (2) interface, at equilibrium:

$$C_i|_1 = \Phi_i C_i|_2$$

Where Φ_i is the *Partition Coefficient*

Since the discontinuity cannot be abrupt it establishes an **interphase**

While concentrations may not be equal, fluxes across a fluid-fluid or liquid-liquid **interphase are always equal, thus:**

$$N_{ix}|_1 = N_{ix}|_2$$

$$N_{ix}|_1 = \pm R_{ix}|_2$$

Where R is the reaction rate

“+” if i is produced

“-” if i is consumed

Boundary Conditions

$$\Phi_i = a_i|_2 / a_i|_1 = \gamma_i C_i|_2 / \gamma_i C_i|_1 \quad a = \text{solute activity coefficients}$$

$$\gamma_i \approx 1$$

Dilute Solution Approximation

$$\Phi_i = C_i|_2 / C_i|_1$$

If the surface , e.g. solid-liquid interface, is impermeable there is no flux across its surface

Then:

$$N_{ix}|_2 = 0$$

If the surface , e.g. solid-liquid interface, is permeable then the flux across its surface

$$N_{ix}|_1 = k(\Phi_i C_i|_2 - C_i|_1)$$

Where

k is the *permeability*

Φ_i is the *Partition Coefficient*

What is Henry's law and why is it useful?

What is a partition coefficient and why is it useful?

Random Walk

- $\langle x \rangle^2 = 2 * \text{dimensions} * Dt$; i.e., = $4Dt$ in 2-D...

Imagine taking a vector with various values for random steps an entity can take in 1-D...

RandomNums = [-1 0 1]; the value of kronecker for this is $\text{mean}(\text{RandomNums}.^2)$

The average distance the entity will go is directly proportional to the $\text{sqrt}(\text{number of steps taken})$...

Theoretical distance = $(\text{kroncker}=\text{mean}(\text{RandomNums}.^2)) * \text{sqrt}(\text{steps})$ (true for 1-D)

Also, the same kinetic energy will result in smaller displacement as the entity becomes larger...

How does time come into play? $n = \text{steps} = t/\tau$ where τ is the time to take a single step.

Show how to calculate what the kroneckers are if random values are able to be chosen of $[-1 \ 1]$ & $[-1 \ 0 \ 1]$?

How do you calculate the theoretical distance to be traveled using kronecker values?



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Random walk

The mean-square displacement in one direction:

$$\langle x^2 \rangle = \delta^2 t / \tau$$

If we define the one-dimensional binary diffusion coefficient as $D_{ij} = \delta^2 / \tau$; then...

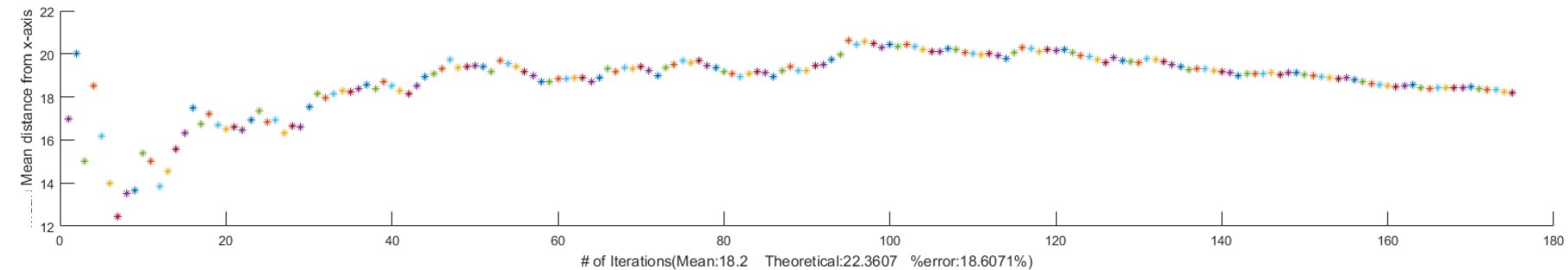
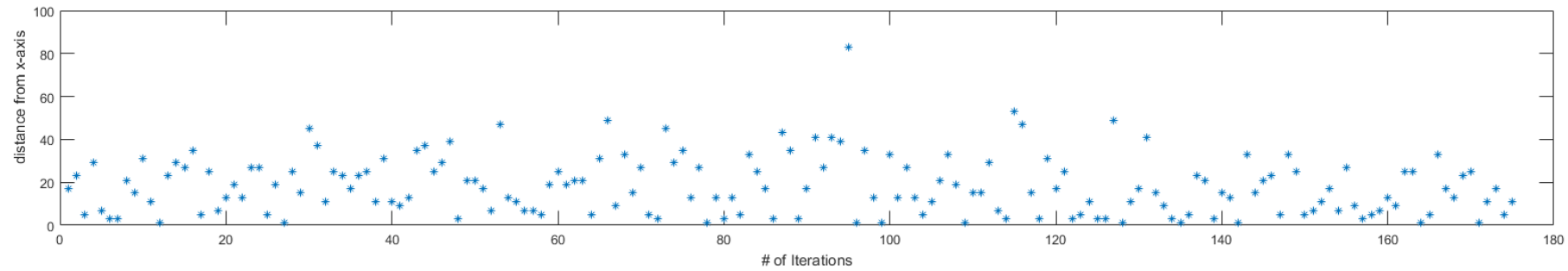
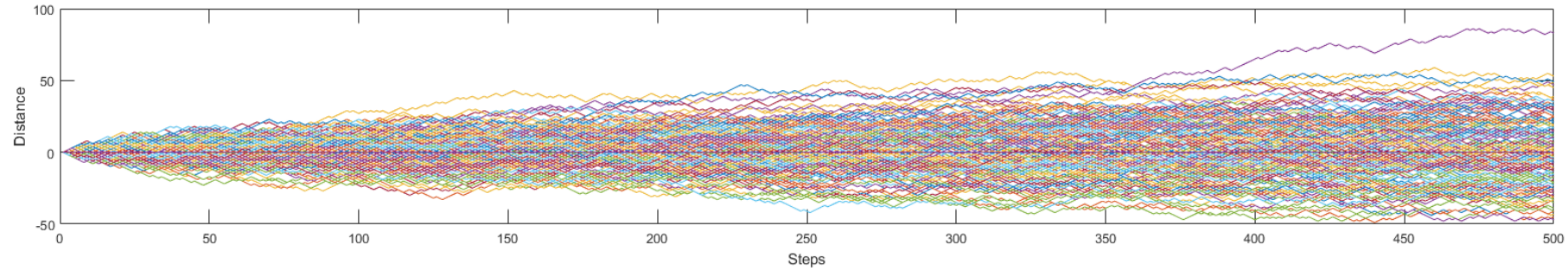
$$\langle x^2 \rangle = 2D_{ij} t$$

The mean-square distance sampled by a molecule increases linearly with the \sqrt{t}

For three dimensional random walk:

$$\langle r^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle = 3(2D_{ij} t) = 6D_{ij} t$$

-1 and 1 (replicating = problem 6.3)



Problem 1: Objectives (1-D)

- In MatLab,
 - Sub-figure 1: Observe in 1-D the distance traveled from the x-axis after a certain number of steps. Have the distance chosen to step be a vector of choices [-1 -1 0 1], [-1, 1], [-1, 0, 1], etc.
 - Sub-figure 2: Calculate the distance traveled from the x-axis after a certain number of steps; repeating this process.
 - Sub-figure 3: Calculate the running average of figure 2 and watch the answer converge to the theoretical answer.
- Quantify the % error as it steps through this process.

FYI: (not going to be tested on this but)

Extrapolation of principles:

https://en.wikipedia.org/wiki/Rotational_diffusion

Diffusivity or Diffusion Coefficient and Temperature

Temperature influences manifest in the diffusion coefficient.
Hence, diffusion coefficient, D , increases with increasing T .

$$D = D_o \exp\left(-\frac{Q_d}{RT}\right)$$

D = diffusion coefficient [m^2/s]

D_o = temperature dependent pre-exponential [m^2/s]

Q_d = the activation energy for diffusion [J/mol or eV/atom]

R = the molar gas constant [8.314 J/mol-K]

T = absolute temperature, Kelvin [K]

	Temperature	D
	500°C (773K)	3.0×10^{-21}
	900°C (1173K)	1.8×10^{-15}

Diffusivity or Diffusion Coefficient and Activation Energy

$$D = D_o \exp\left(-\frac{Q_d}{RT}\right)$$

Taking logarithms:

$$\ln D = \ln D_o - \frac{Q_d}{R} \left(\frac{1}{T}\right) \quad \log D = \log D_o - \frac{Q_d}{2.303R} \left(\frac{1}{T}\right)$$

$$y = mx + c$$

Where

$$\mathbf{Slope} = -Q_d / 2.303R$$

$$\mathbf{Intercept} = \log D_o$$

Diffusivity or Diffusion Coefficient and Activation

Energy

$$\log D = \log D_o - \frac{Q_d}{2.303R} \left(\frac{1}{T} \right)$$

Where

$$\text{Slope} = -Q_d / 2.303R$$

$$\text{Intercept} = \log D_o$$

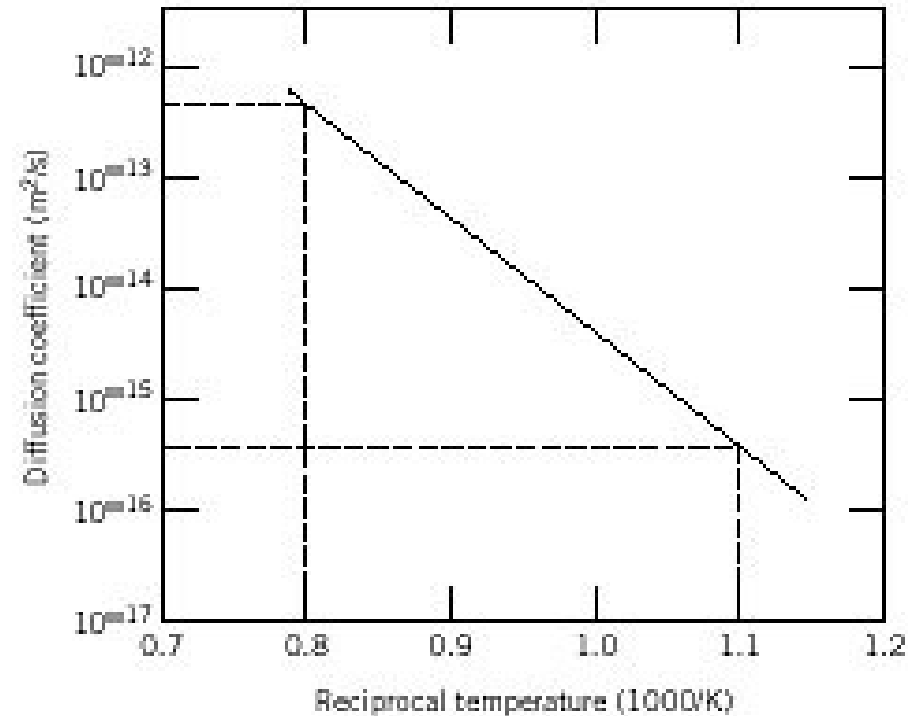
Solve for Activation Energy:

$$Q_d = -2.303R \left(\frac{\Delta(\log D_o)}{\Delta\left(\frac{1}{T}\right)} \right)$$

$$Q_d = -2.303R \left(\frac{\log D_1 - \log D_2}{\frac{1}{T_1} - \frac{1}{T_2}} \right)$$

Solve for D_o

$$\log D_o = \log D + \frac{Q_d}{2.303R} \left(\frac{1}{T} \right)$$

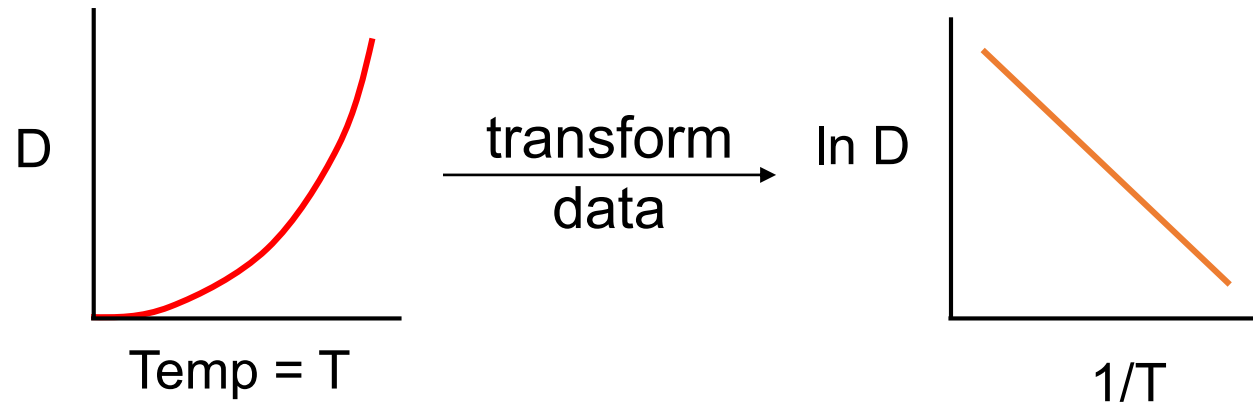


Example: At 300°C the diffusion coefficient and activation energy for Cu in Si are

$$D(300^\circ\text{C}) = 7.8 \times 10^{-11} \text{ m}^2/\text{s}$$

$$Q_d = 41.5 \text{ kJ/mol}$$

What is the diffusion coefficient at 350°C?



$$\ln D_2 = \ln D_0 - \frac{Q_d}{R} \left(\frac{1}{T_2} \right) \quad \text{and} \quad \ln D_1 = \ln D_0 - \frac{Q_d}{R} \left(\frac{1}{T_1} \right)$$

$$\therefore \ln D_2 - \ln D_1 = \ln \frac{D_2}{D_1} = -\frac{Q_d}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right)$$

Example (cont.)

$$D_2 = D_1 \exp \left[-\frac{Q_d}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) \right]$$

$$T_1 = 273 + 300 = 573 \text{ K}$$

$$T_2 = 273 + 350 = 623 \text{ K}$$

$$D_2 = (7.8 \times 10^{-11} \text{ m}^2/\text{s}) \exp \left[\frac{-41,500 \text{ J/mol}}{8.314 \text{ J/mol} \cdot \text{K}} \left(\frac{1}{623 \text{ K}} - \frac{1}{573 \text{ K}} \right) \right]$$

$$D_2 = 15.7 \times 10^{-11} \text{ m}^2/\text{s}$$

Estimation of diffusion coefficients

- Protein diffusivity in plasma is about $1e-7$ cm²/s.
- From edge of cell to center: 2.5 seconds
- Through tissue that is 0.02 mm thick: 27.7 hours
- What is a binary diffusion coefficient?
 - Characterizes diffusion of one molecule in a solvent
- What is Deffective?
 - Incorporates: drag forces exerted by ECM and cells

1-D, 2-D, 3-D differences?

A protein molecules with a D of $1e-7 \text{ cm}^2/\text{s}$ will diffuse from the edge to the center of a 20 μm diameter cell in how many seconds?

Diffusivity, D , is commonly written as D_{ij} . What is the i and what is the j ?

Given you know diffusivity, $D = D_1$ and you know temperature, T_1 and T_2 , how do you calculate D_2 which is at T_2 ? Write out an equation for each of 2 methods to do so and state what each of the variables are.

6.6.5: The Wilkie-Chang

- See problem 6.1.

$$D = 7.4e - 10 \frac{T(\varphi M)^{0.5}}{\mu V_o^{0.6}} ; \varphi_{water} = 2.26$$

What is the name of the equation that you can calculate diffusivity based on molecular weight?

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 Text **COREYBISHOP271** to **22333** once to join, then text your message

Stoke's-Einstein Equation:

$$D = \frac{kT}{6\pi\eta R}$$

- Regarding calculating D_2 at T_2 , knowing either D_1 and T_1 , is there another way we can do this using the SE equation?

$f_{\text{bar}} = \text{denominator}$
 TABLE 6.3

Values of the Mean Frictional Drag Coefficient for Different Shapes [9,10]

Shape	Frictional drag coefficient
Sphere of radius R	$f = 6\pi\mu R$
Prolate ellipsoid, $p = a/b > 1$, where a is a major axis, b is a minor axis	$\bar{f} = \frac{6\pi\mu b(p^2 - 1)^{1/2}}{p^{1/3} \ln[p + (p^2 - 1)^{1/2}]}$
Oblate ellipsoid, $p = a/b < 1$	$\bar{f} = \frac{6\pi\mu b(1 - p^2)^{1/2}}{p^{1/3} \tan^{-1}[(1 - p^2)^{1/2} p^{-1}]}$
Thin circular disk of radius a	$\bar{f} = 16\mu a$
Cylinder of radius a and length L	$\bar{f} \approx \frac{4\pi\mu L}{\ln(L/a) + 0.193}$

Source: From Refs [9,10].

Estimation of frictional drag coefficients

- For low Reynold's #s, the drag force is (K is translation tensor; \mathbf{v} = velocity): K is a symmetric tensor and the components thereof are friction coefficients f_{ij}

$$F_D = K * v \quad (\text{or } v = K^{-1} * FD) = \frac{1}{2} * \rho * velocity^2 * Dc * A; Dc = \text{drag coefficient}$$

assume $f_{11} = f_{22} = f_{33} = f_1 = f_2 = f_3$

By solving for the f s when $\text{Det}(K - fI) = 0$ ($f_1 = f_2 = f_3$ etc for an isotropic body) we obtain the non-zero values. The f s are eigenvalues.

f_{bar} = average = the harmonic mean:

$$1/f_{\text{bar}} = 1/3(1/f_1 + 1/f_2 + 1/f_3 + \dots)$$

Note that for a sphere $f = 6\mu R$... sound familiar?

Eigenvectors are scalable and translatable... $\mathbf{v}(A - \lambda I) = 0$... $\mathbf{v}(A - \lambda I) = 0$ (these vectors (\mathbf{v}) are not velocity vectors)

These are the eigenvalues and are the friction coefficients. The only non-zero solutions are calc. via the det.

$$\det(A) = \begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix}$$
$$= a(ei - hf) - d(bi - hc) + g(bf - ec)$$

- Π vs Σ ?
- Harmonic mean = $1/A$
- Geometric mean $G = \sqrt{AH}$
- Arithmetic mean = $1/H$

Skip this for this semester for the sake of time.

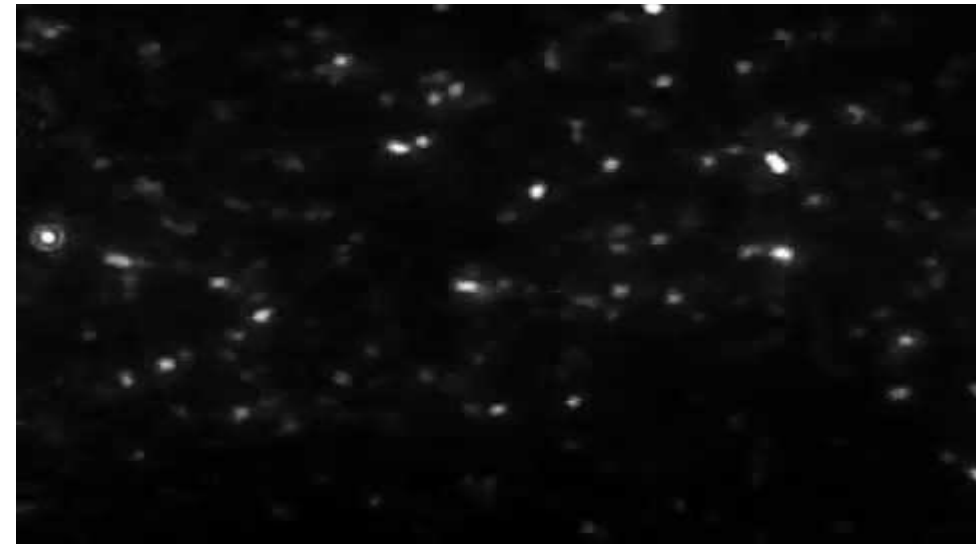
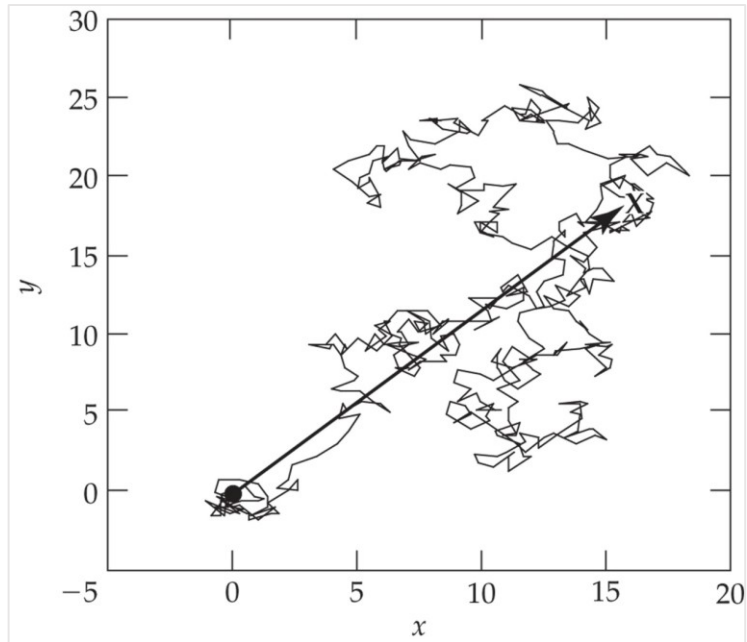
What does the \bar{f} assume for the Stoke's-Einstein equation?

Instrumentation using diffusion principles

- Nanoparticle Tracking Analysis (NTA)
- Dynamic Light Scattering (DLS)

NTA

What happens if the paths cross during the video?

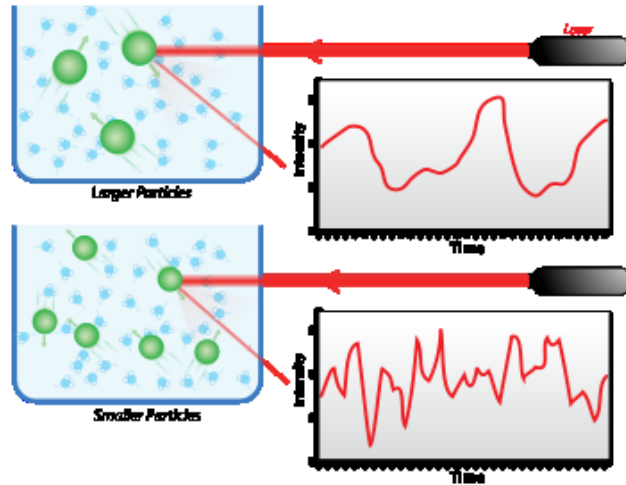


<https://www.youtube.com/watch?v=65k3fX2X7pQ>

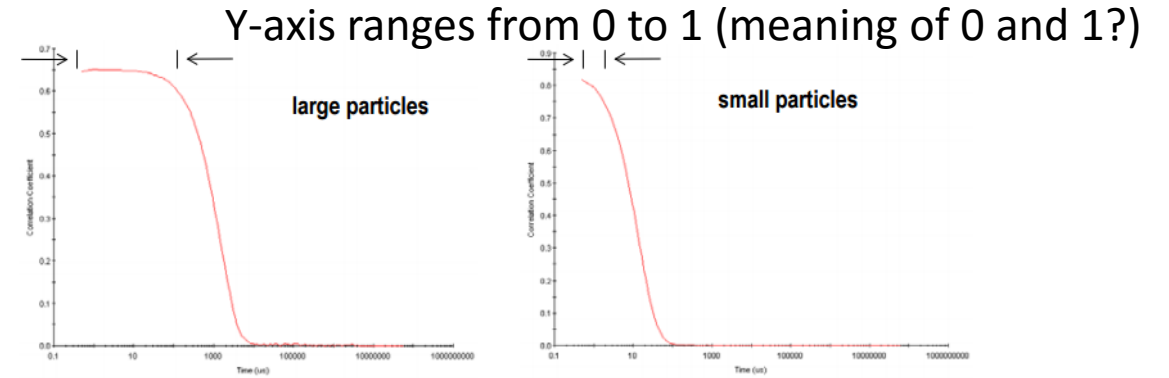
500-step random walk.

The walk begins at coordinates $x = 0, y = 0$ denoted by the “●” and ends in the upper right hand quadrant denoted by “X”. The arrow represents the **net** displacement.

Dynamic Light Scattering: Skipping DLS this semester



Wikipedia.org



- Larger particles in which the correlation of the signal takes a long time to decay.
- Small particles move more rapidly so correlation decreases more quickly



NNIN
NANO SCIENCE
ENGINEERING & TECHNOLOGY



NANO RESEARCH FACILITY

Washington University in St. Louis
SCHOOL OF ENGINEERING & APPLIED SCIENCE

Correlation Function

- Correlation function:

$$G(\tau) = \langle I(t) \cdot I(t+\tau) \rangle$$

- Monodisperse particles: cumulants analysis

$$G(\tau) = A[1 + B \exp(-2\Gamma\tau)]$$

$$\Gamma = Dq^2 \quad \text{refractive index of dispersant}$$

$$q = (4 \pi n / \lambda_0) \sin(\theta/2)$$

How do you get size out of this Information?

What is this size based on?

What limitations are there when calculating diameters from intensities?

<http://www.nano.wustl.edu/>

What does the slope mean of a plot of the correlation function versus time, with respect to dynamic light scattering? Will the correlation value start to become more dissimilar first for larger or smaller particles?



Respond at **PollEv.com/coreybishop271**



Text **COREYBISHOP271** to **22333** once to join, then text your message

How to calculate diameter of particles using data obtained from a video

Stokes-Einstein Equation

Raleigh Scattering

Root Mean Square? $x_{rms} = \sqrt{\frac{1}{n}(x_1^2 + x_2^2 + x_3^2 + x_4^2 + \dots + x_n^2)}$

Geometric mean? $x_{GM} = \sqrt[n]{x_1 x_2 x_3 \dots x_n}$ What happens to the outliers?

Important rhetorical questions:

If the size of the particle were much smaller than the wavelength of the light being used to see it, what happens?

What is this phenomenon called? How can you estimate the diameter of it? What does this size mean?

What if the particle being measured were actually a rod?

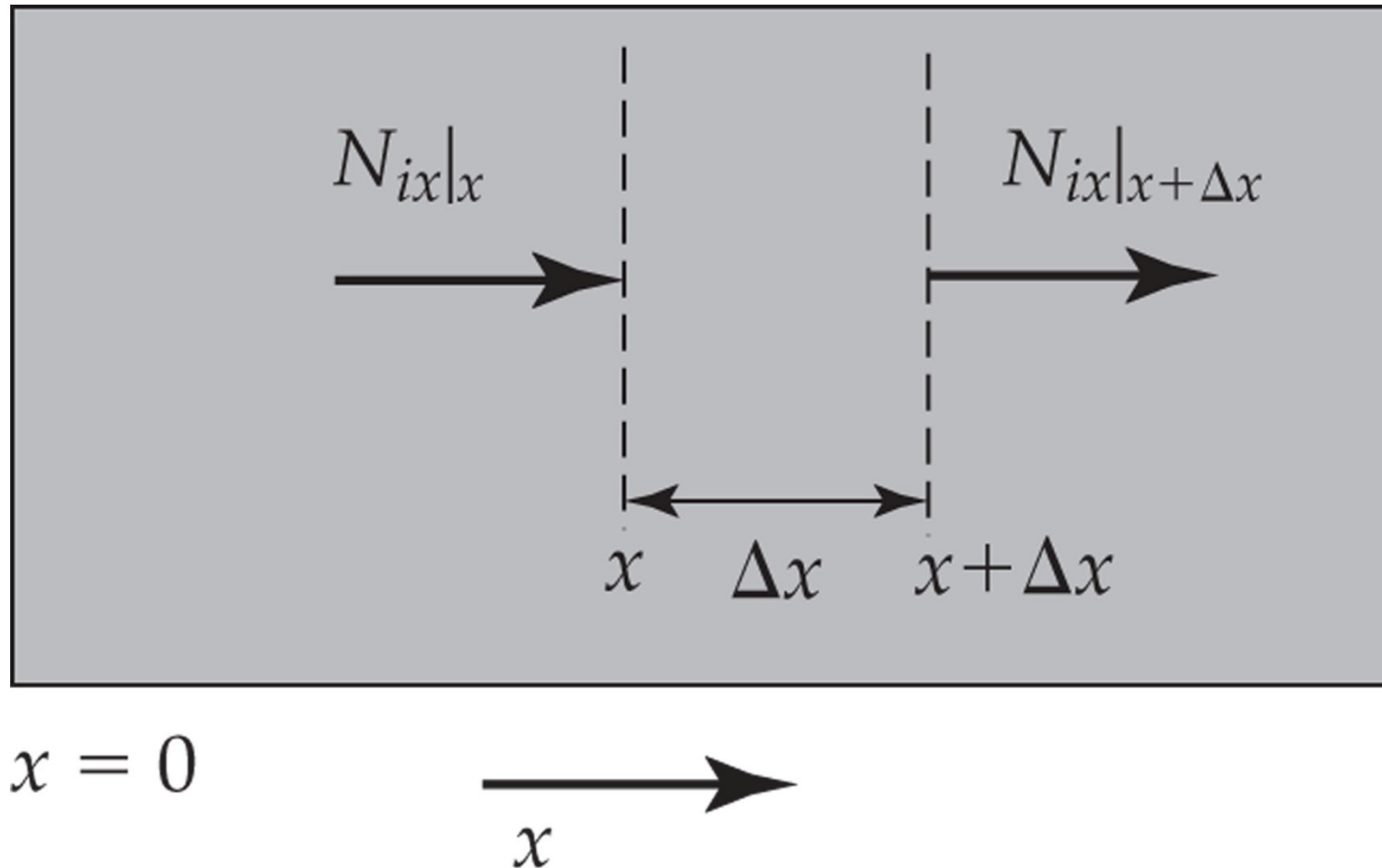
What if the distribution of sizes were heterogeneous (i.e., limitations?) in the context of NTA vs DLS

How do you calculate the root mean square versus the geometric mean? What happens to outliers in each case?

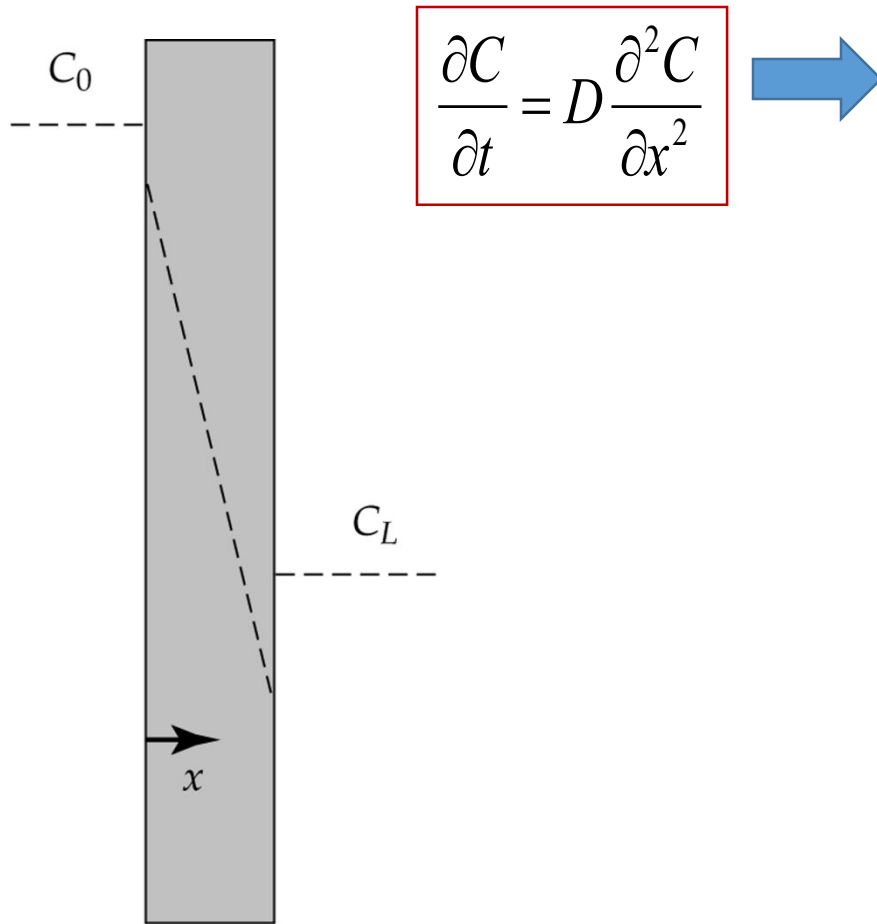
Examples in book with more clarity

- FYI: examples given in slides that are not “Problems” at the back of the chapter are also fair game for exams.

Figure 6.6 Diffusion through a small rectangular volume of area A and thickness Δx .

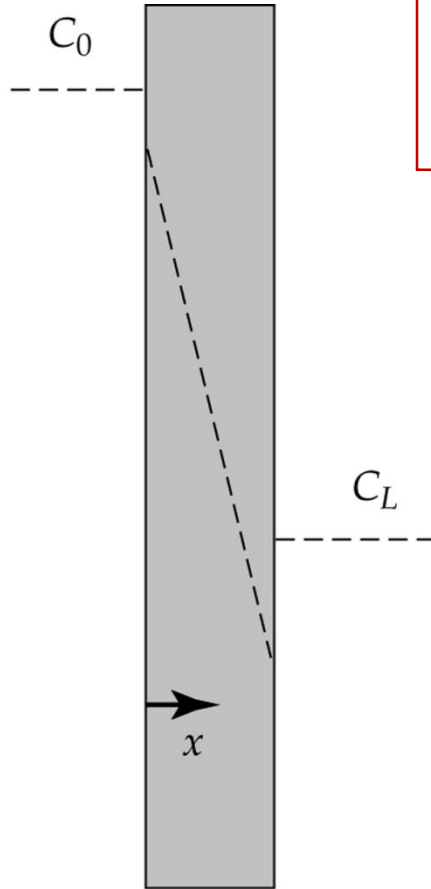


Schematic of steady diffusion across a membrane of thickness L that separates two well-mixed solutions. For this situation $\Phi < 1$.



Membrane of thickness L

Schematic of steady diffusion across a membrane of thickness L that separates two well-mixed solutions. For this situation $\Phi < 1$.



Membrane of thickness L

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



Handwritten solution on a piece of paper:

$$0 = D \frac{d^2 C_m}{dx^2}$$

$$\frac{0}{D} dx^2 = d^2 C_m$$

$$\iint 0 dx^2 = \iint d^2 C_m = C_m$$

$$C_m = \int C_1 dx = C_1 x + C_2$$

B.C. #1 @ $x=0$ $C_m = \Phi C_0$
 B.C. #2 @ $x=L$ $C_m = \Phi C_L$

apply B.C.#1 $C_m = C_1(x=0) + C_2 = \Phi C_0$
 B.C.#2 $C_m = C_1(x=L) + C_2 = \Phi C_L$
 $C_1 = \frac{\Phi C_L - \Phi C_0}{L}$

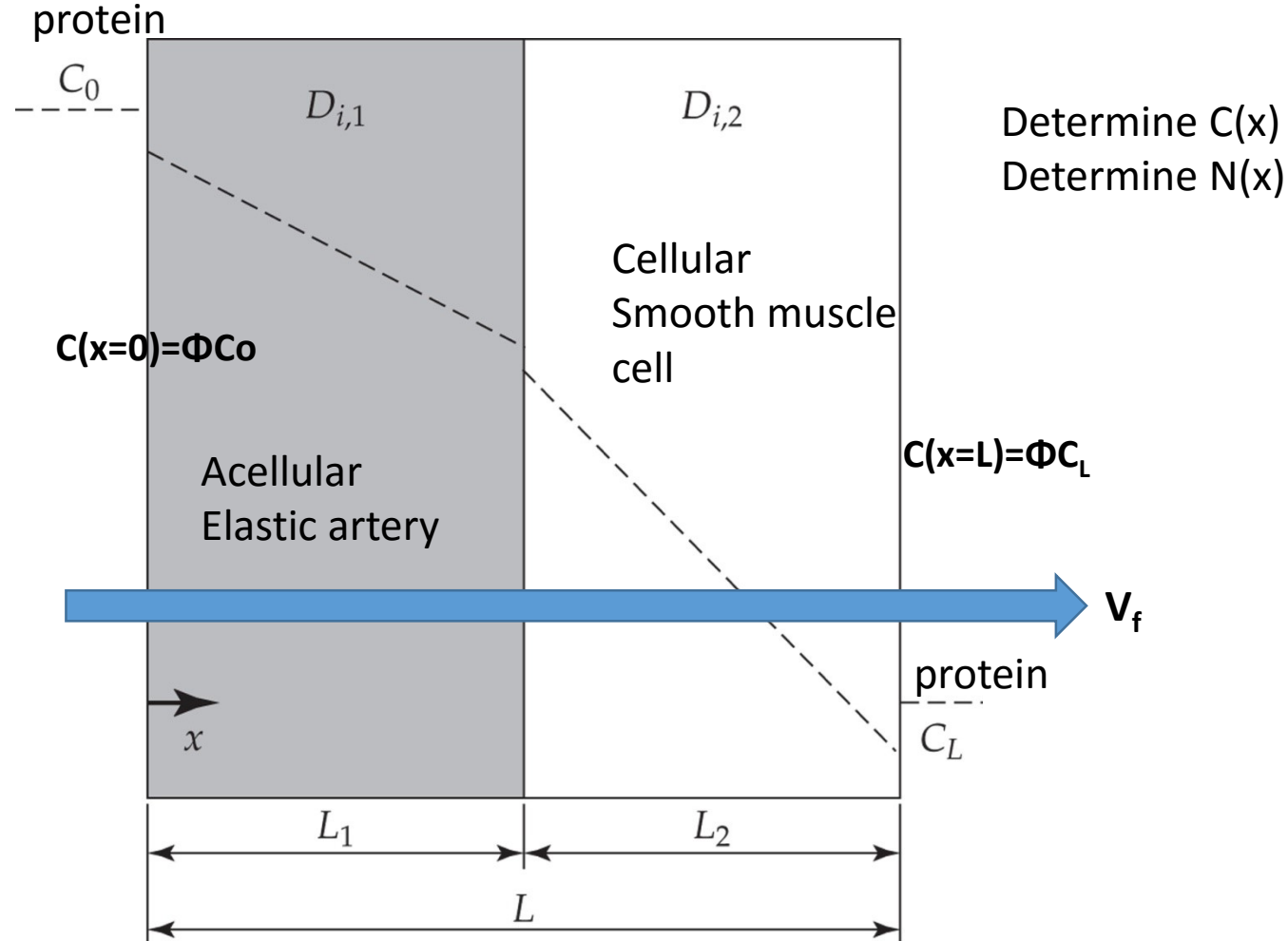
so $C_m = \left(\frac{\Phi C_L - \Phi C_0}{L} \right) x + \Phi C_0$

$$J = -D \frac{dC_m}{dx} = -D \frac{d \left[\frac{(\Phi C_L - \Phi C_0)}{L} x + \Phi C_0 \right]}{dx}$$

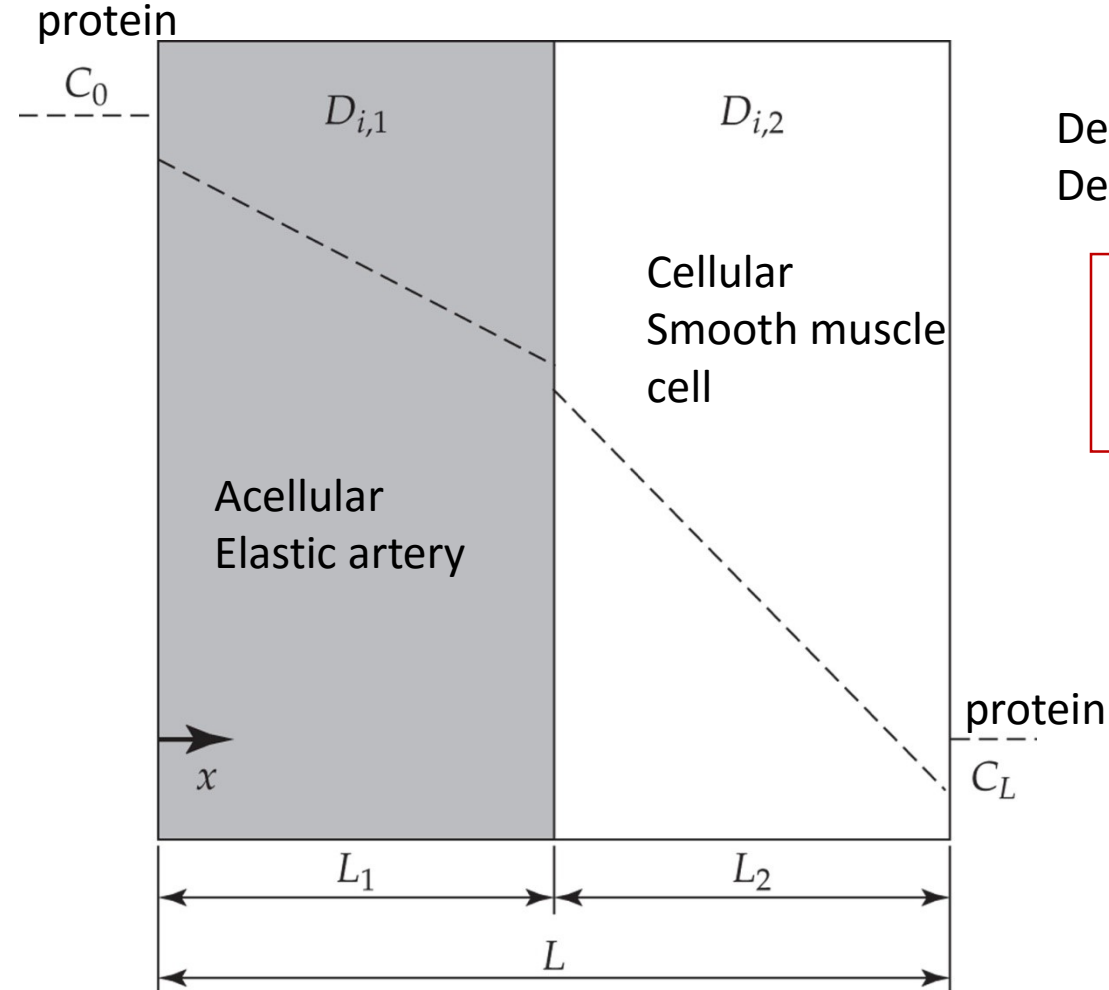
$$= -D \left(\frac{\Phi C_L - \Phi C_0}{L} \right) = -\frac{D \Phi}{L} (C_L - C_0)$$

Example 6.5

Diffusion through a two-layer laminate. Each layer is described by a separate diffusion coefficient.



Diffusion through a two-layer laminate. Each layer is described by a separate diffusion coefficient.



Determine $C(x)$
Determine $N(x)$

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



$$\frac{d^2 c_i}{dx^2} = 0$$

$$\int \int d^2 c_i = \int \int 0 \cdot dx^2$$

$$c_i = C_1 x + C_2 \Rightarrow c_i = A x + B \Rightarrow 2 \text{ equations}$$

$$C_1 = A_1 + B_1 x$$

$$C_2 = A_2 + B_2 x$$

$$\textcircled{1} x=0 \quad C_1 = \Phi_1 C_0$$

$$\textcircled{2} x=L=L_1+L_2 \quad C_2 = \Phi_2 C_L$$

$$\textcircled{3} x=L_1 \quad N_{1x} = N_{2x}$$

$$\textcircled{4} x=L_1 \quad \frac{C_1}{\Phi_1} = \frac{C_2}{\Phi_2}$$

$$\text{B.C. \#1: } C_1 = \Phi_1 C_0 = A_1 + B_1(x=0); A_1 = \Phi_1 C_0$$

$$\text{\#2 } C_2 = \Phi_2 C_L = A_2 + B_2(x=L)$$

$$A_2 = \Phi_2 C_L - B_2(L+L_2)$$

$$\text{\#3 } \frac{C_1}{\Phi_1} = \frac{A_1 + B_1 x}{\Phi_1} = \frac{\Phi_1 C_0 + B_1 x}{\Phi_1} = C_0 + \frac{B_1 x}{\Phi_1} = C_0 + \frac{B_1 L_1}{\Phi_1} = \frac{A_2 + B_2 x}{\Phi_2} = \frac{(\Phi_2 C_L - B_2 L) + B_2 L_1}{\Phi_2}$$

$$\text{\#4 } D_{i,1} \frac{dc_1}{dx} = D_{i,2} \frac{dc_2}{dx} = \frac{C_1 - B_2 L_2}{\Phi_2}$$

$$D_{i,1} \frac{d(A_1 + B_1 x)}{dx} = D_{i,2} \frac{d(A_2 + B_2 x)}{dx} = D_{i,1} B_1 = D_{i,2} B_2$$

solving for unknowns yields

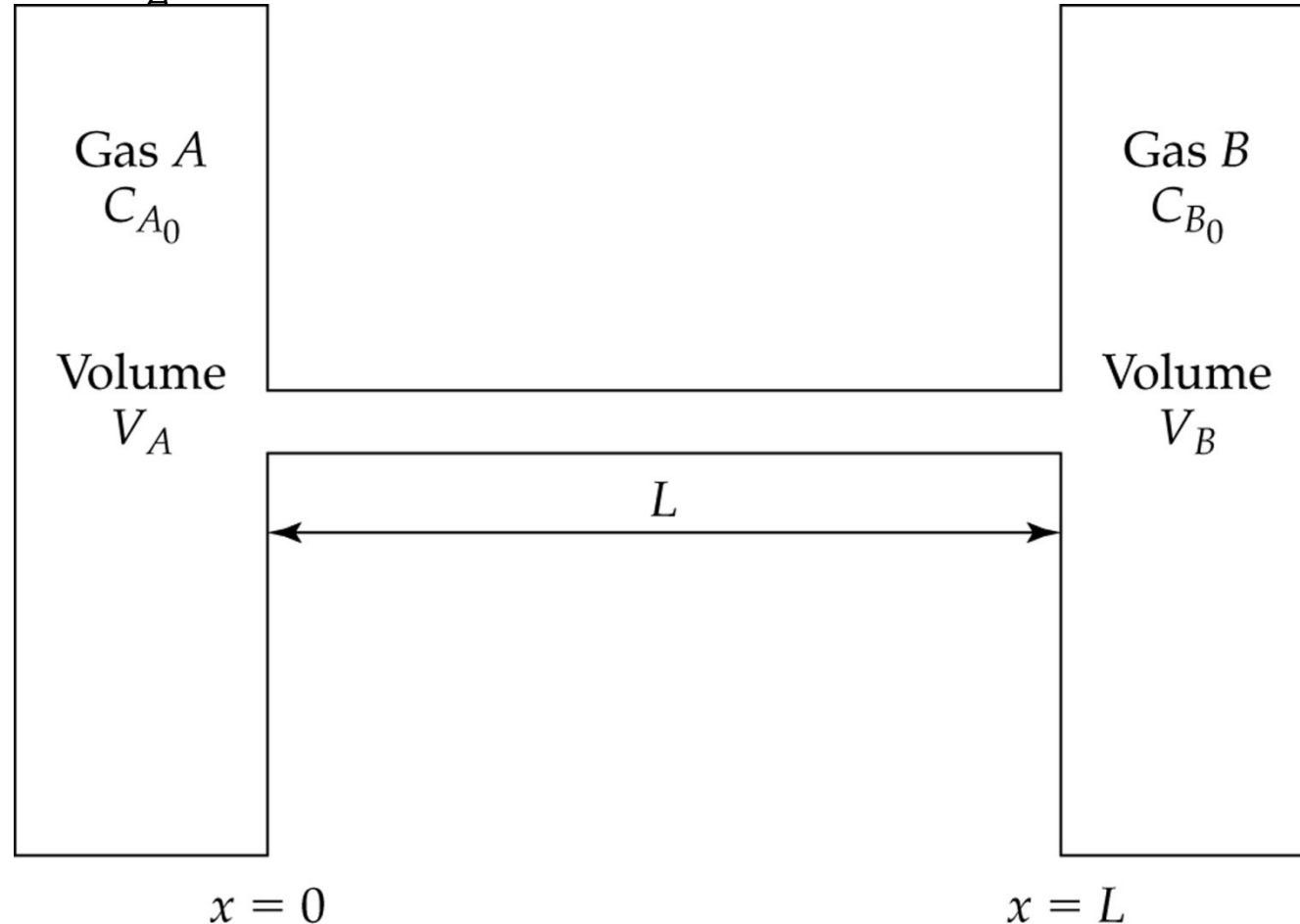
$$N_{ix} = \frac{\Phi_{\text{eff}} D_{\text{eff}}}{L} (C_0 - C_L) \quad \Phi \frac{L}{\Phi_{\text{eff}} D_{\text{eff}}} = \frac{L_1}{\Phi_1 D_{i,1}} + \frac{L_2}{\Phi_2 D_{i,2}} \quad \leftarrow \begin{array}{l} \text{diffusive} \\ \text{resistances} \\ \text{electrical} \\ \text{systems} \end{array}$$

generalizing...

$$\frac{L}{\Phi_{\text{eff}} D_{\text{eff}}} = \sum_{j=1}^N \frac{L_j}{\Phi_j D_{i,j}} \quad \left\{ \begin{array}{l} 0 < x < L_1 : C_1 = ? \\ L_1 < x < L_2 : C_2 = ? \end{array} \right.$$

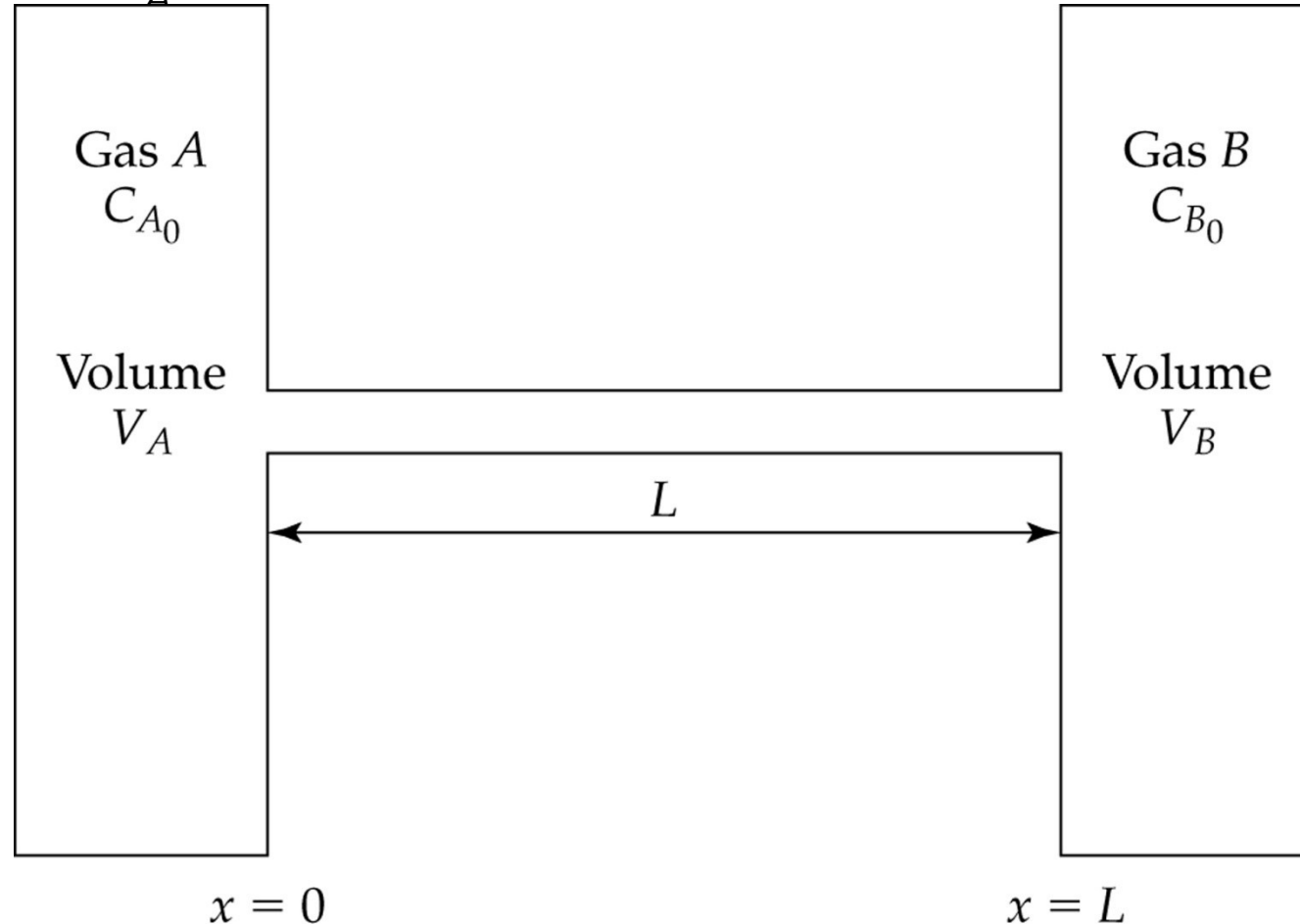
6.7.1: Diffusion in gases

Figure 6.10 Diffusion of two gases. The concentrations in each reservoir are kept constant such that at steady state, $C_A = C_{A0}$ and $C_B = C_{B0}$ at $x = 0$ and $C_A = 0$ and $C_B = 0$ at $x = L$.



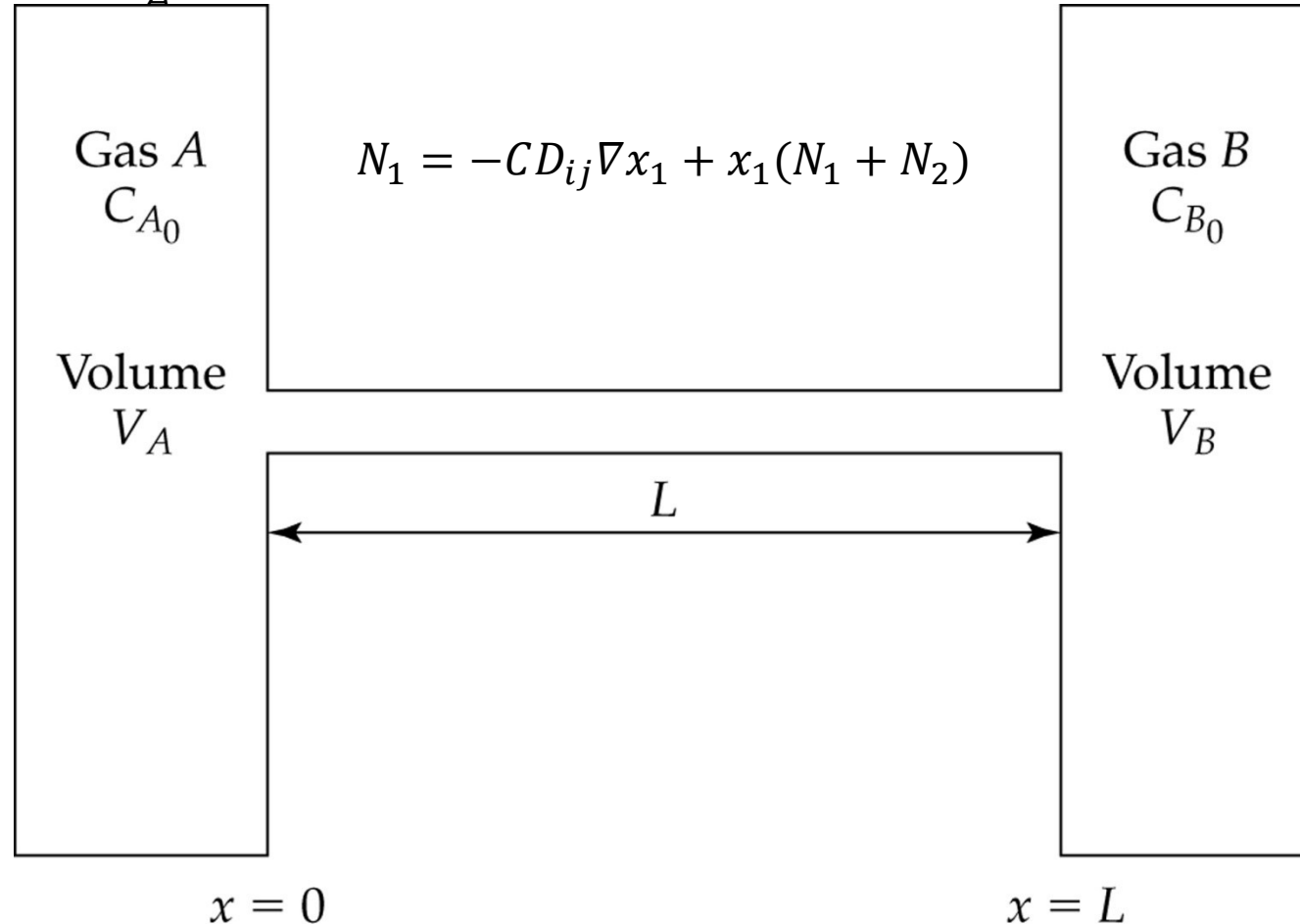
Dilute solution?

Figure 6.10 Diffusion of two gases. The concentrations in each reservoir are kept constant such that at steady state, $C_A = C_{A0}$ and $C_B = C_{B0}$ at $x = 0$ and $C_A = 0$ and $C_B = 0$ at $x = L$.



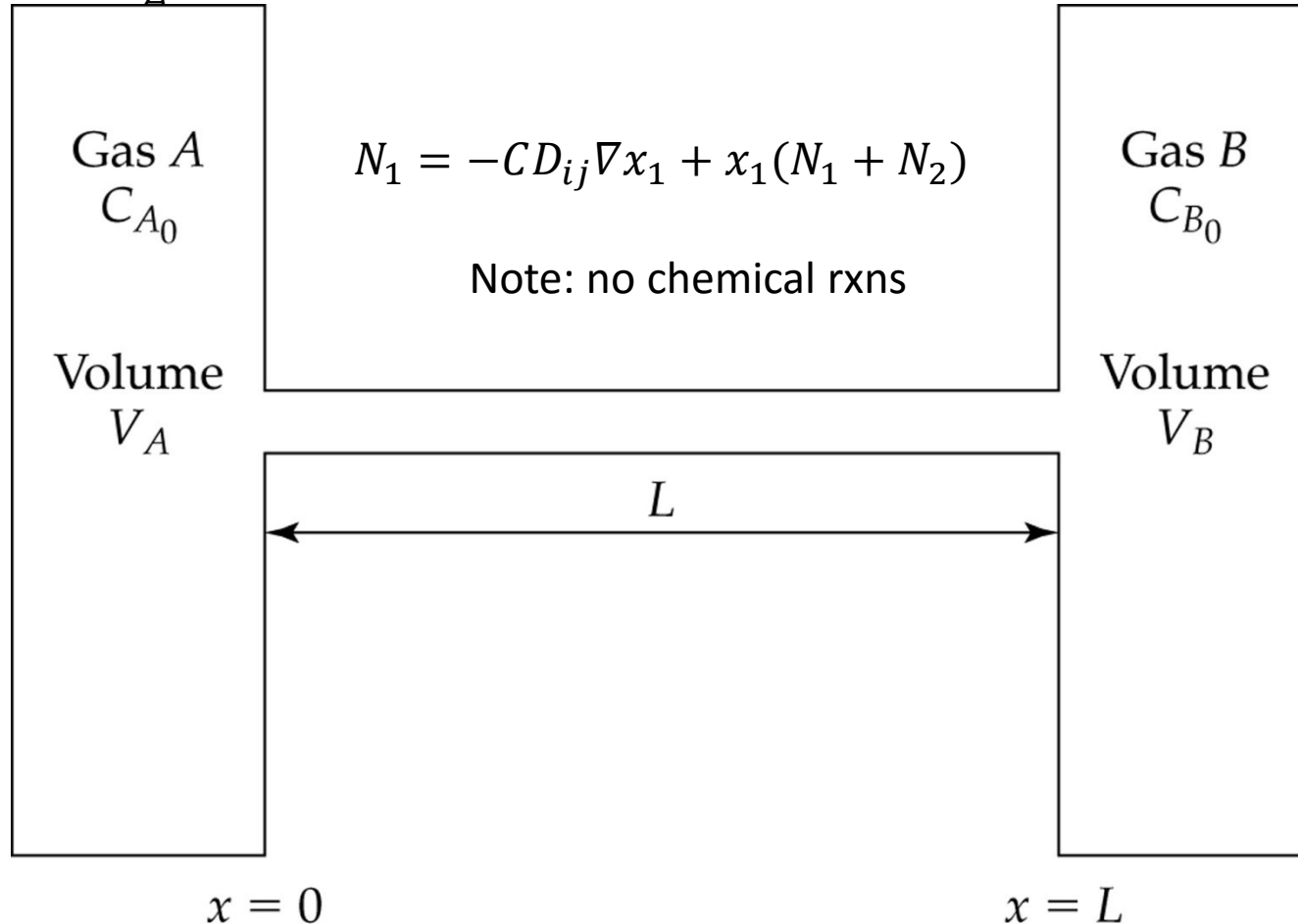
Dilute solution cannot be invoked.... Flux of one induced flux of another in the absence of bulk motion.

Figure 6.10 Diffusion of two gases. The concentrations in each reservoir are kept constant such that at steady state, $C_A = C_{A0}$ and $C_B = C_{B0}$. $C_B = 0$ at $x = 0$ and $C_A = 0$ at $x = L$.



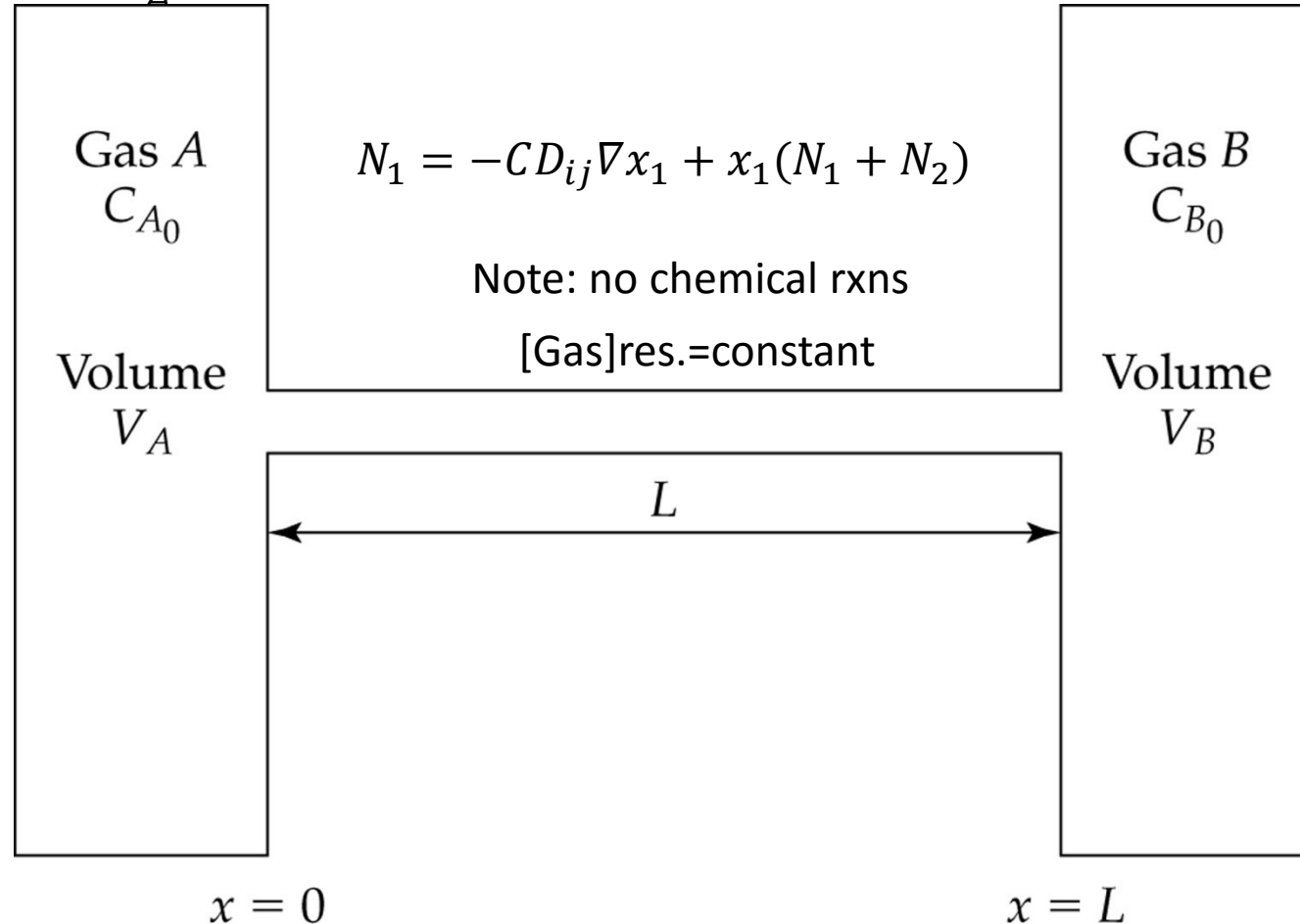
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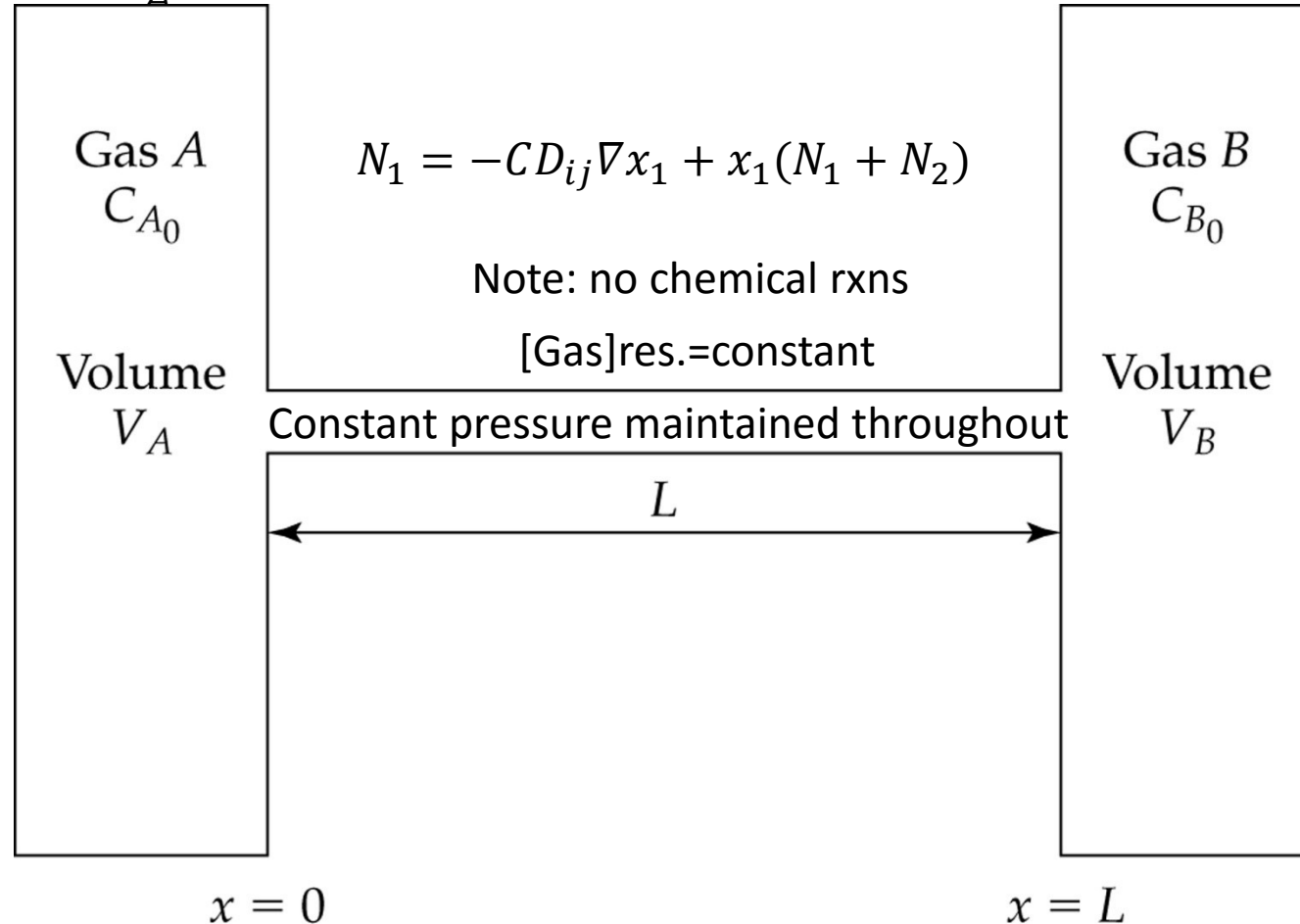
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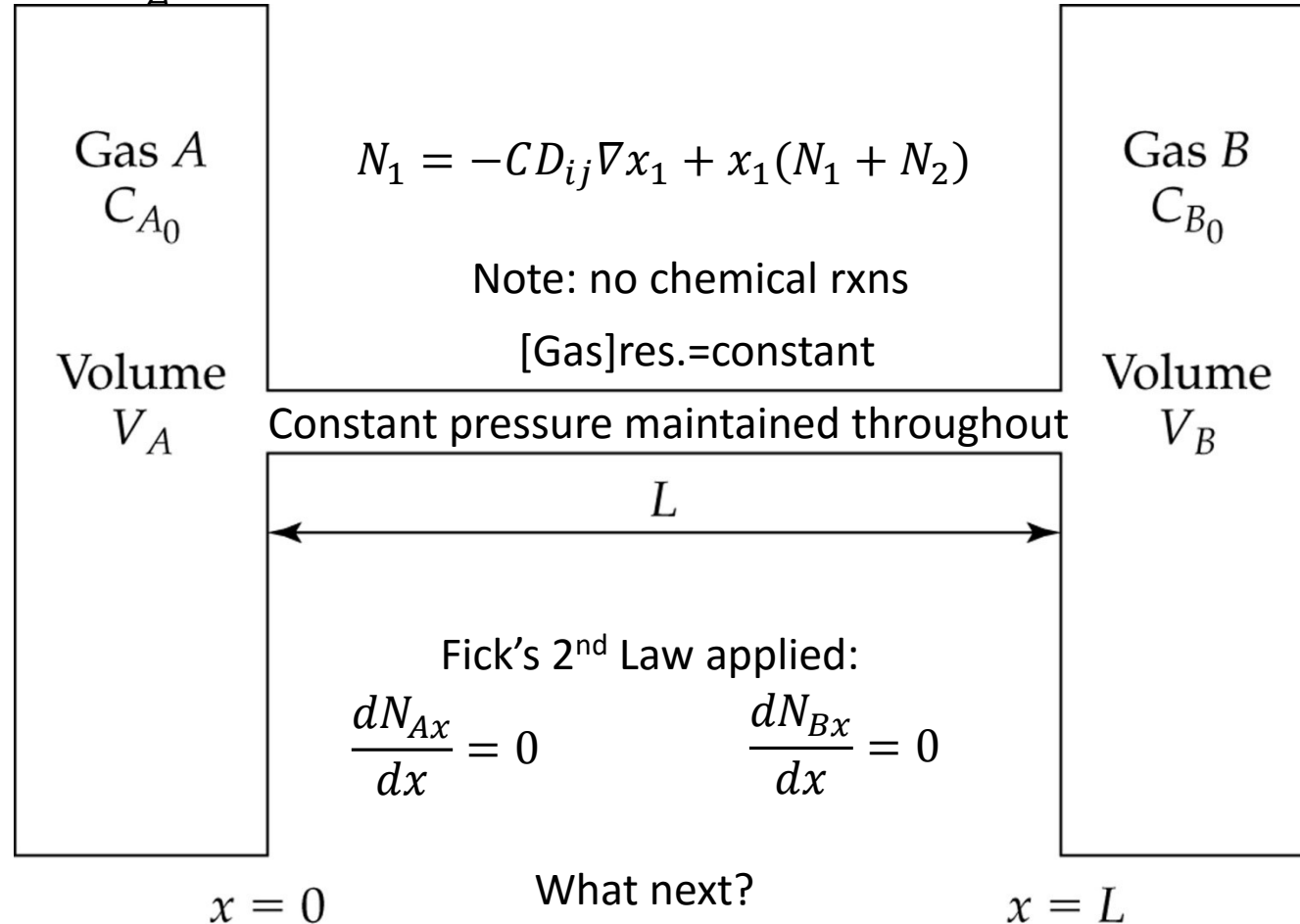
Dilute solution cannot be invoked.... Flux of one induced flux of another in the absence of bulk motion.

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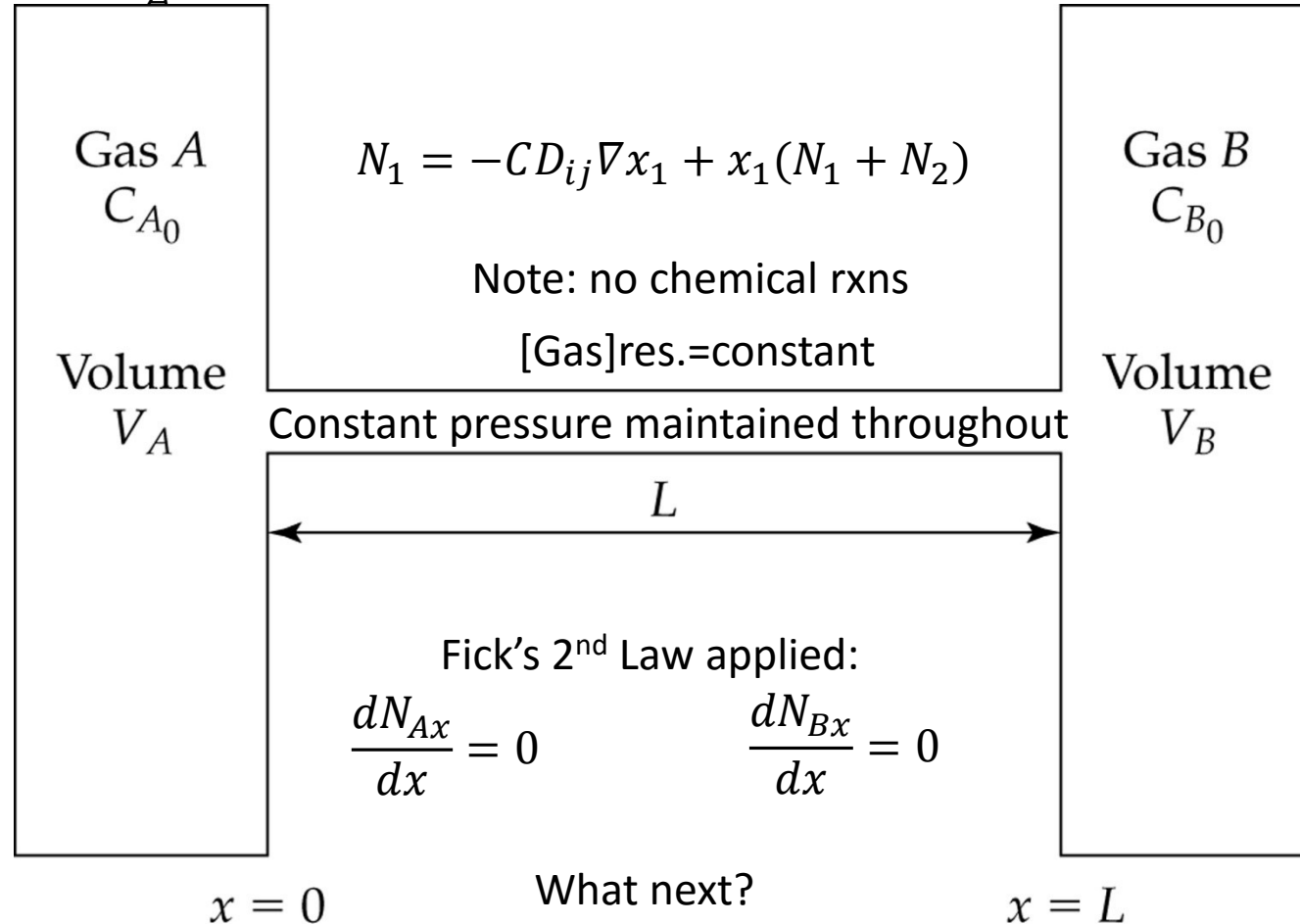
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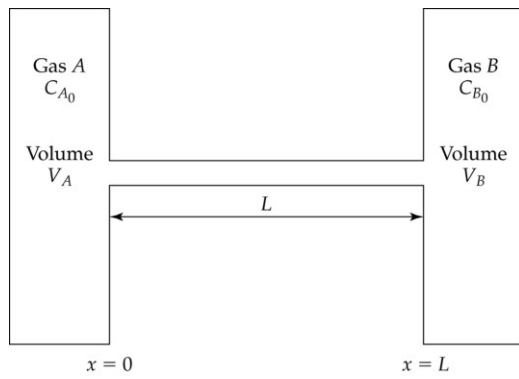


Dilute solution cannot be invoked.... Flux of one induced flux of another in the absence of bulk motion.

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Dilute solution cannot be invoked.... Flux of one induced flux of another in the absence of bulk motion.

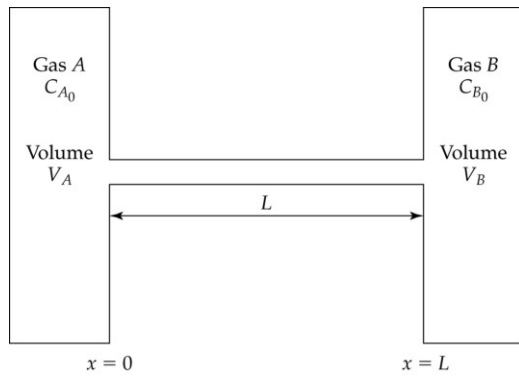


$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$

$$\frac{dN_{Ax}}{dx} = 0$$

$$\frac{dN_{Bx}}{dx} = 0$$

What next?



$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$

$$\frac{dN_{Ax}}{dx} = 0$$

$$\frac{dN_{Bx}}{dx} = 0$$

1-D

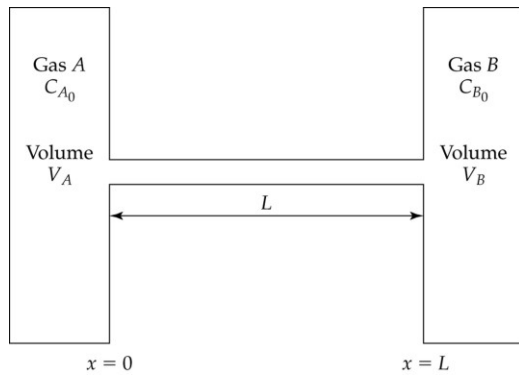
$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$



$$N_{Ax} = -CD_{AB} \frac{dx_A}{dx} + x_A(N_{Ax} + N_{Bx})$$

$$N_{Bx} = -CD_{BA} \frac{dx_B}{dx} + x_B(N_{Ax} + N_{Bx})$$

Can assume $D_{AB}=D_{BA}$



$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$

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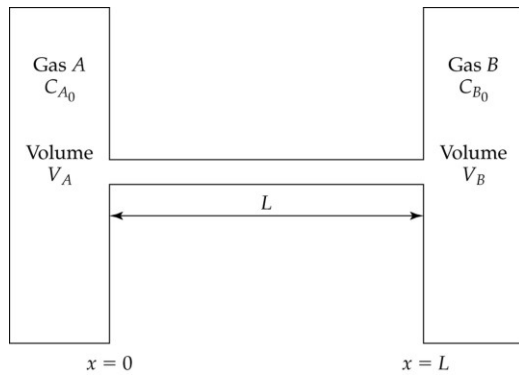
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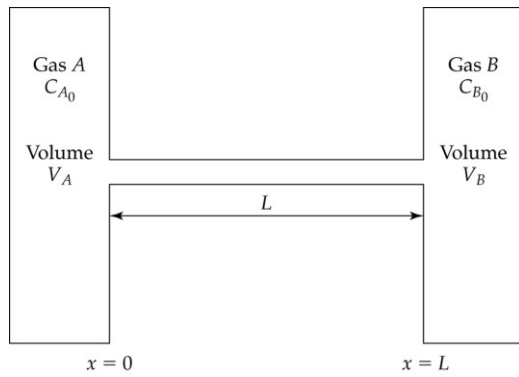
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$$N_{Bx} = -CD_{AB} \frac{dx_B}{dx} + x_B(N_{Ax} + N_{Bx})$$

Now what?



$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$

$$\frac{dN_{Ax}}{dx} = 0$$

$$\frac{dN_{Bx}}{dx} = 0$$

1-D

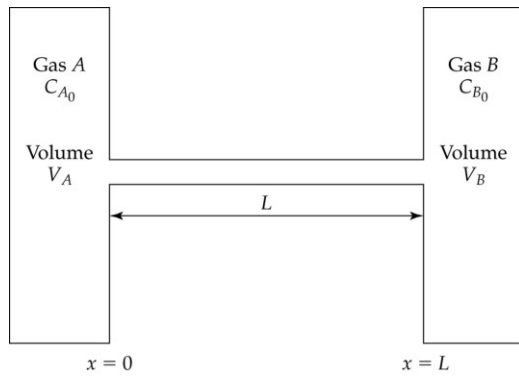
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$$N_{Bx} = -CD_{AB} \frac{dx_B}{dx} + x_B(N_{Ax} + N_{Bx})$$

Now what? Pressure is the same everywhere so...



$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$

$$\frac{dN_{Ax}}{dx} = 0$$

$$\frac{dN_{Bx}}{dx} = 0$$

1-D

$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$



$$N_{Ax} = -CD_{AB} \frac{dx_A}{dx} + x_A(N_{Ax} + N_{Bx})$$

$$N_{Bx} = -CD_{AB} \frac{dx_B}{dx} + x_B(N_{Ax} + N_{Bx})$$

$$N_{Bx} = -N_{Ax}$$

Now what? Pressure is the same everywhere so...

Equimolar counterdiffusion

Analogous to diffusion through membrane if $\phi=1$...

Example 6.6

Figure 6.11 Evaporation of liquid A and diffusion through a stagnant layer of gas B.

Is this more complex
Than the last?

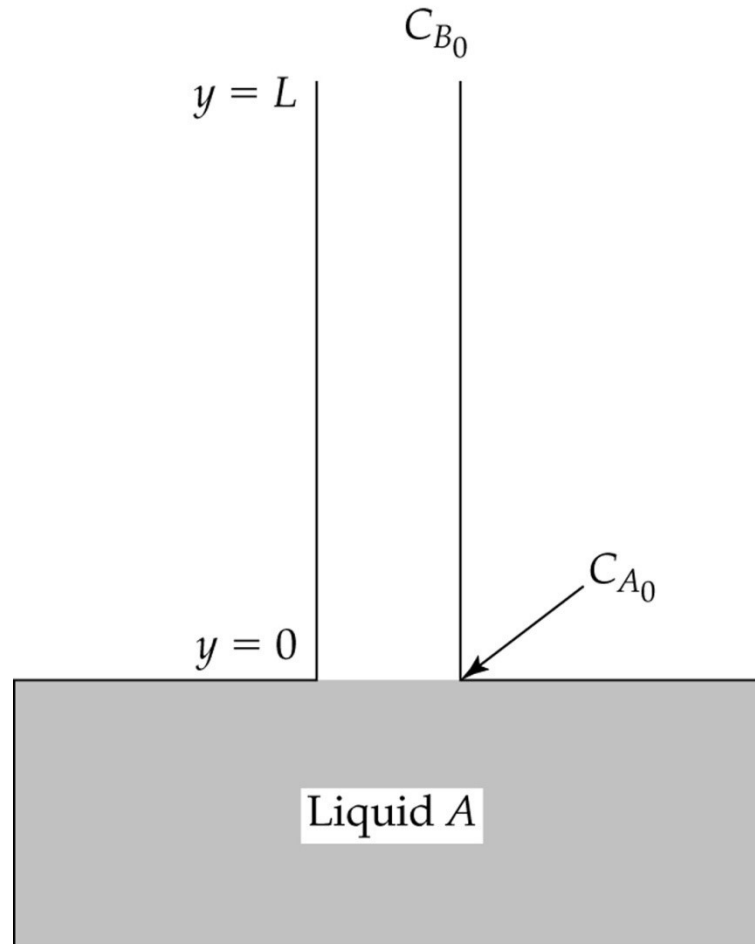


Figure 6.11 Evaporation of liquid A and diffusion through a stagnant layer of gas B.

Is this more complex

Than the last?

Yes...

Consider this to be s.s. evaporation

Of a liquid A into a stagnant layer of gas

B. If there is a stagnant layer that

Means there is no bulk flow of the gas...

Not equimolar counterdiffusion.

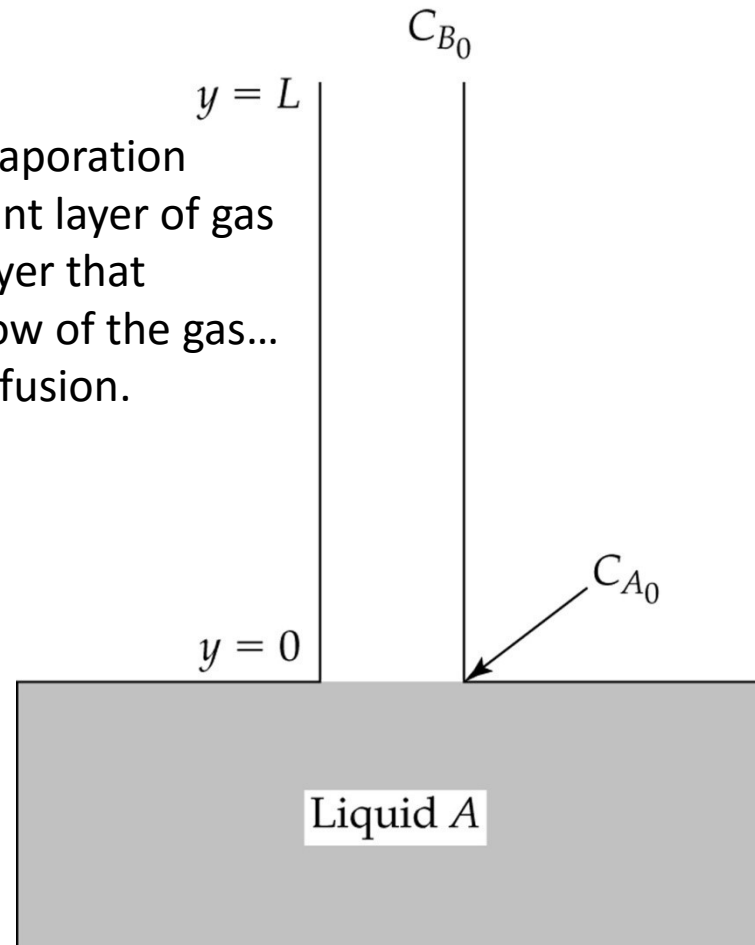


Figure 6.11 Evaporation of liquid A and diffusion through a stagnant layer of gas B.

Is this more complex

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Consider this to be s.s. evaporation

Of a liquid A into a stagnant layer of gas

B. If there is a stagnant layer that

Means there is no bulk flow of the gas...

Not equimolar counterdiffusion because

Pretend there is a large Reservoir supplying this Concentration such that It is constant.

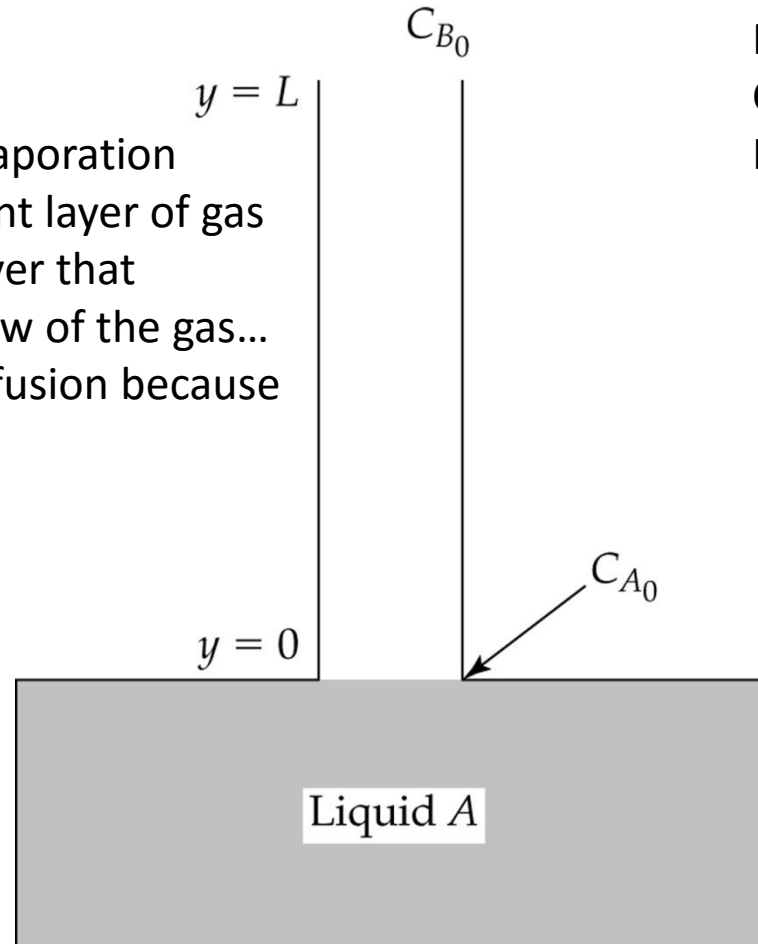


Figure 6.11 Evaporation of liquid A and diffusion through a stagnant layer of gas B.

Is this more complex

Than the last?

Yes...

Consider this to be s.s. evaporation $y = L$

Of a liquid A into a stagnant layer of gas

B. If there is a stagnant layer that

Means there is no bulk flow of the gas...

Not equimolar counterdiffusion because

B is insoluble in our fake situation...

Pressure is uniform

Pretend there is a large Reservoir supplying this Concentration such that It is constant.

What next?

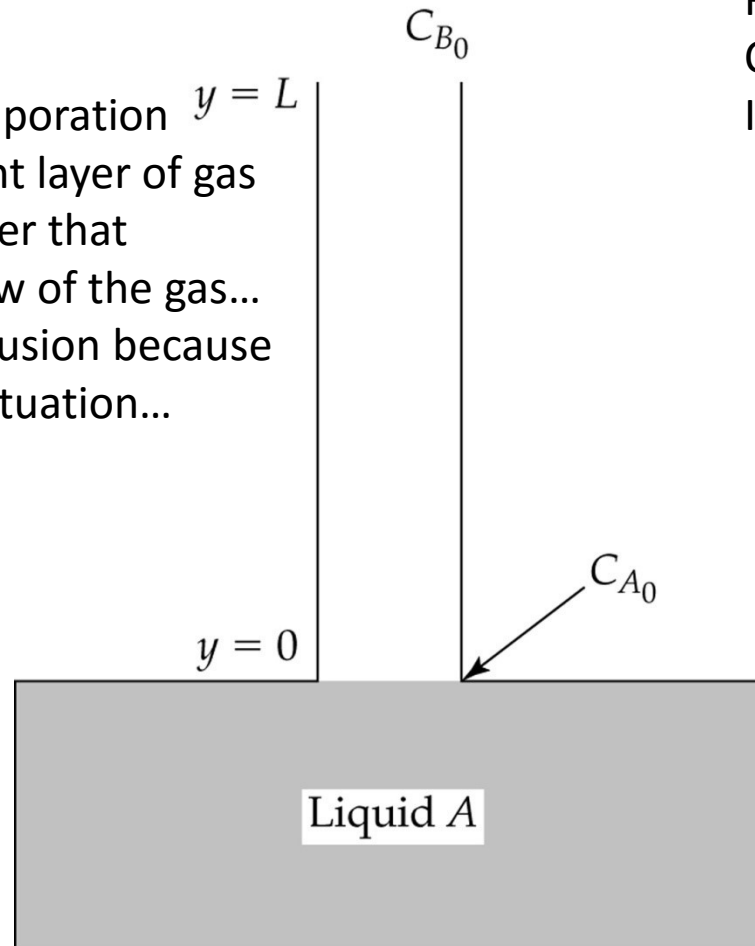


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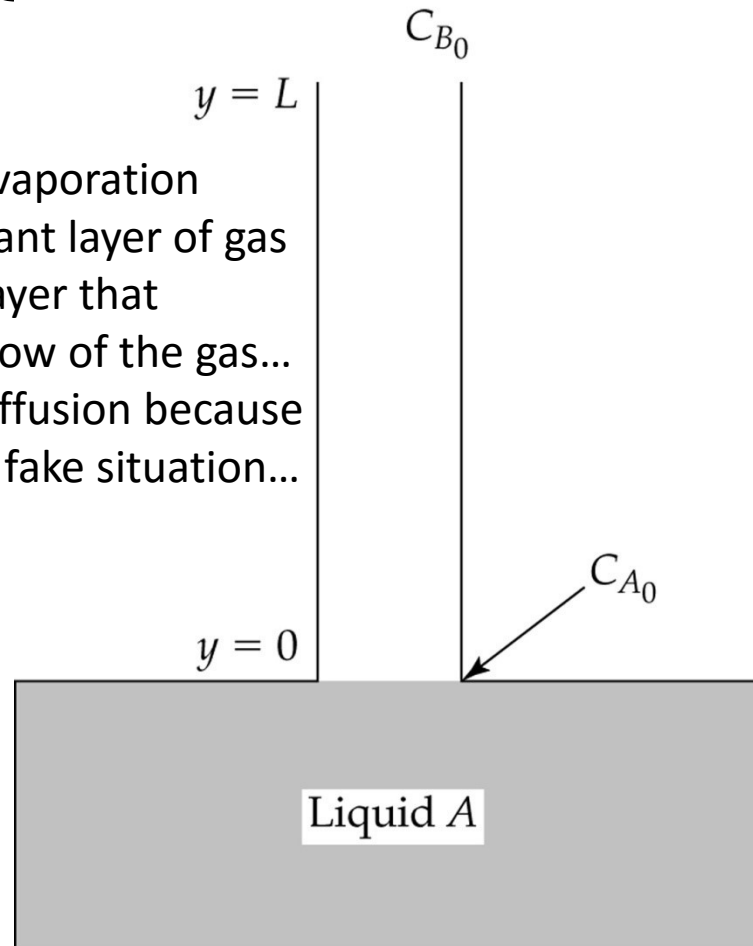
Not equimolar counterdiffusion because

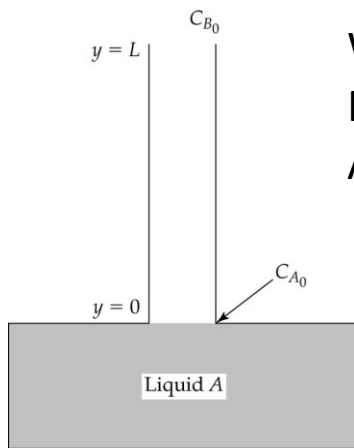
B is hardly soluble in our fake situation...

Pressure is uniform

Pretend there is a large
Reservoir supplying this
Concentration such that
It is constant.

What next?
Fick's 2nd law
At s.s.



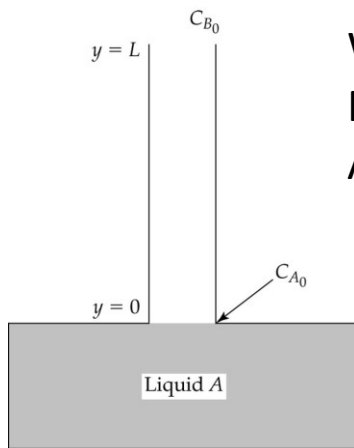


What next?
Fick's 2nd law
At s.s.

$$\frac{dN_{Ay}}{dy} = 0$$

$$\frac{dN_{By}}{dy} = 0$$

Of note, gas is very slightly soluble and is much less than the flux due to evaporation of the liquid A. so
B.C. $N_{by} \sim 0$ at $y=0$... so...



What next?
Fick's 2nd law
At s.s.

$$\frac{dN_{Ay}}{dy} = 0$$

$$\frac{dN_{By}}{dy} = 0$$

Of note, gas is very slightly soluble and is much less than the flux due to evaporation of the liquid A. so

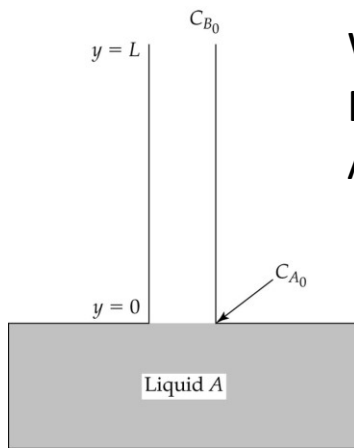
Handwritten mathematical derivation showing the integration of the boundary condition for component B:

$$\frac{dN_{By}}{dy} = 0$$

$$dN_{By} = 0 \cdot dy$$

$$\int dN_{By} = \int 0 \cdot dy$$

$$N_{By} = \text{constant.}$$



What next?
Fick's 2nd law
At s.s.

$$\frac{dN_{Ay}}{dy} = 0$$

$$\frac{dN_{By}}{dy} = 0$$

Of note, gas is very slightly soluble and is much less than the flux due to evaporation of the liquid A. so

Handwritten notes on a piece of paper:

$$\frac{dN_{By}}{dy} = 0$$

$$dN_{By} = 0 \cdot dy$$

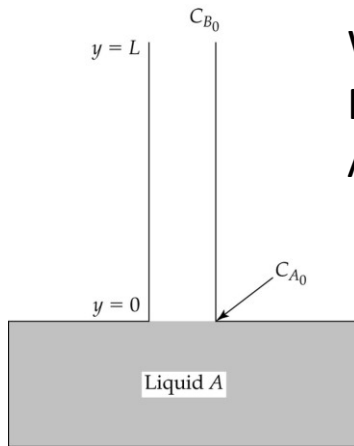
$$\int dN_{By} = \int 0 \cdot dy$$

$$N_{By} = \text{constant.}$$

B.C. given:
B is hardly soluble...

$$N_{By}(y=0) \approx 0$$

so $N_{By} = 0$
This means no flux!
but what about $[]$ (4)



What next?
Fick's 2nd law
At s.s.

$$\frac{dN_{Ay}}{dy} = 0$$

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Of note, gas is very slightly soluble and is much less than the flux due to evaporation of the liquid A. so

$$\frac{dN_{By}}{dy} = 0$$

$$dN_{By} = 0 \cdot dy$$

$$\int dN_{By} = \int 0 \cdot dy$$

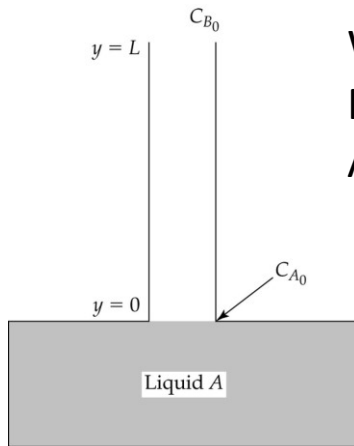
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 This means no flux!
 but what about $[]$ (4)
 There is a gradient
 because $x_A + x_B = 1$



What next?
Fick's 2nd law
At s.s.

$$\frac{dN_{Ay}}{dy} = 0$$

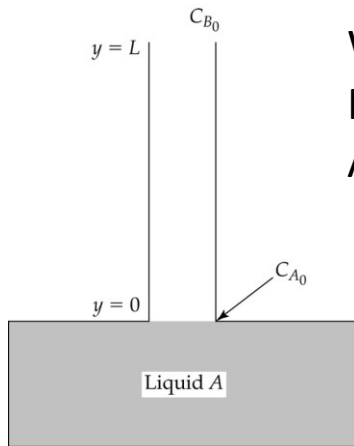
$$\frac{dN_{By}}{dy} = 0$$

Of note, gas is very slightly soluble and is much less than the flux due to evaporation of the liquid A. so

Remember:

$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$

$\frac{dN_{By}}{dy} = 0$
 $dN_{By} = 0 \cdot dy$
 $\int dN_{By} = \int 0 \cdot dy$
 $N_{By} = \text{constant}$
 B.C. given:
 B is hardly soluble...
 $N_{By}(y=0) \approx 0$
 so $N_{By} = 0$
 This means no flux!
 but what about $[]$ (B)
 There is a gradient
 because $x_A + x_B = 1$



What next?
Fick's 2nd law
At s.s.

$$\frac{dN_{Ay}}{dy} = 0$$

$$\frac{dN_{By}}{dy} = 0$$

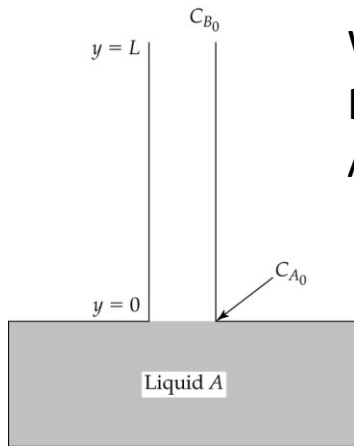
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Remember:

$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$

$$N_{Ay} = -CD_{AB} \frac{dx_A}{dy} + x_A(N_{Ay} + N_{By})$$

$\frac{dN_{By}}{dy} = 0$
 $dN_{By} = 0 \cdot dy$
 $\int dN_{By} = \int 0 \cdot dy$
 $N_{By} = \text{constant}$
 B.C. given:
 B is hardly soluble...
 $N_{By}(y=0) \approx 0$
 so $N_{By} = 0$
 This means no flux!
 but what about [] (y)
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What next?
Fick's 2nd law
At s.s.

$$\frac{dN_{Ay}}{dy} = 0$$

$$\frac{dN_{By}}{dy} = 0$$

Of note, gas is very slightly soluble and is much less than the flux due to evaporation of the liquid A. so

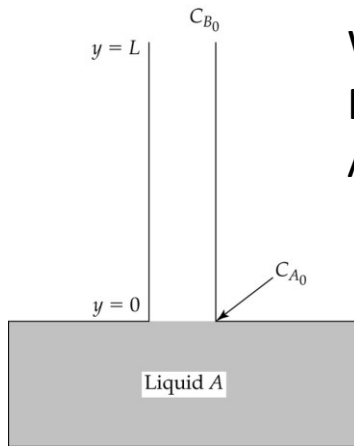
Remember:

$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$

$$N_{Ay} = -CD_{AB}\frac{dx_A}{dy} + x_A(N_{Ay} + N_{By})$$

$$N_{Ay} = -CD_{AB}\frac{dx_A}{dy} + x_A N_{Ay}$$

$\frac{dN_{By}}{dy} = 0$
 $dN_{By} = 0 \cdot dy$
 $\int dN_{By} = \int 0 \cdot dy$
 $N_{By} = \text{constant.}$
 B.C. given:
 B is hardly soluble...
 $N_{By}(y=0) \approx 0$
 so
 $N_{By} = 0$
 This means no flux!
 but what about $[]$ (B)
 There is a gradient
 because $x_A + x_B = 1$



What next?
Fick's 2nd law
At s.s.

$$\frac{dN_{Ay}}{dy} = 0$$

$$\frac{dN_{By}}{dy} = 0$$

Of note, gas is very slightly soluble and is much less than the flux due to evaporation of the liquid A. so

Remember:

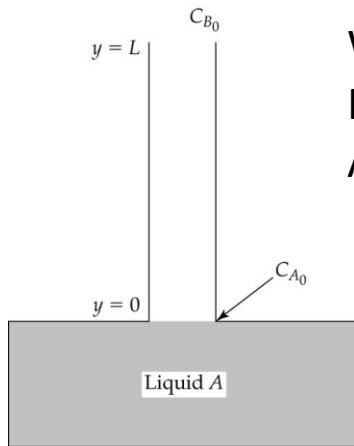
$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$

$$N_{Ay} = -CD_{AB} \frac{dx_A}{dy} + x_A(N_{Ay} + N_{By})$$

$$N_{Ay} = -CD_{AB} \frac{dx_A}{dy} + x_A N_{Ay}$$

Now what?

$\frac{dN_{By}}{dy} = 0$
 $dN_{By} = 0 \cdot dy$
 $\int dN_{By} = \int 0 \cdot dy$
 $N_{By} = \text{constant}$
 B.C. given:
 B is hardly soluble...
 $N_{By}(y=0) \approx 0$
 so
 $N_{By} = 0$
 This means no flux!
 but what about $[]$ (B)
 There is a gradient
 because $x_A + x_B = 1$



What next?
Fick's 2nd law
At s.s.

$$\frac{dN_{Ay}}{dy} = 0$$

$$\frac{dN_{By}}{dy} = 0$$

Of note, gas is very slightly soluble and is much less than the flux due To evaporation of the liquid A. so

Remember:

$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$

$$N_{Ay} = -CD_{AB} \frac{dx_A}{dy} + x_A(N_{Ay} + N_{By})$$

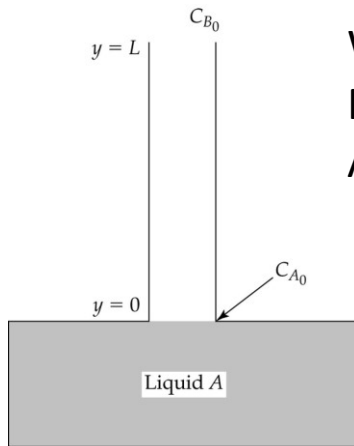
$$N_{Ay} = -CD_{AB} \frac{dx_A}{dy} + x_A N_{Ay}$$

Now what? Solve for N_{Ay}

$$N_{Ay} - x_A N_{Ay} = -CD_{AB} \frac{dx_A}{dy} = N_{Ay}(1 - x_A)$$

$$N_{Ay} = -\frac{CD_{AB} \frac{dx_A}{dy}}{1 - x_A}$$

$\frac{dN_{By}}{dy} = 0$
 $dN_{By} = 0 \cdot dy$
 $\int dN_{By} = \int 0 \cdot dy$
 $N_{By} = \text{constant.}$
 B.C. given:
 B is hardly soluble...
 $N_{By}(y=0) \approx 0$
 so $N_{By} = 0$
 This means no flux!
 but what about $[](y)$
 there is a gradient
 because $x_A + x_B = 1$



What next?
Fick's 2nd law
At s.s.

$$\frac{dN_{Ay}}{dy} = 0$$

$$\frac{dN_{By}}{dy} = 0$$

Of note, gas is very slightly soluble and is much less than the flux due To evaporation of the liquid A. so

Remember:

$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$

$$N_{Ay} = -CD_{AB} \frac{dx_A}{dy} + x_A(N_{Ay} + N_{By})$$

$$N_{Ay} = -CD_{AB} \frac{dx_A}{dy} + x_A N_{Ay}$$

Now what? Solve for N_{Ay}

$$N_{Ay} - x_A N_{Ay} = -CD_{AB} \frac{dx_A}{dy} = N_{Ay}(1 - x_A)$$

$$N_{Ay} = -\frac{CD_{AB} \frac{dx_A}{dy}}{1 - x_A}$$

Now what?

Handwritten notes on a piece of paper:

$\frac{dN_{By}}{dy} = 0$

$dN_{By} = 0 \cdot dy$

$\int dN_{By} = \int 0 \cdot dy$

$N_{By} = \text{constant}$

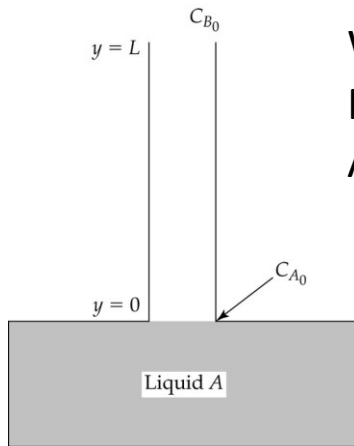
B.C. given:
B is hardly soluble...

$N_{By}(y=0) \approx 0$

so $N_{By} = 0$

This means no flux!
but what about $[]$ (4)

there is a gradient
because $x_A + x_B = 1$



What next?
Fick's 2nd law
At s.s.

$$\frac{dN_{Ay}}{dy} = 0$$

$$\frac{dN_{By}}{dy} = 0$$

Of note, gas is very slightly soluble and is much less than the flux due to evaporation of the liquid A. so

Remember:

$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$

$$N_{Ay} = -CD_{AB} \frac{dx_A}{dy} + x_A(N_{Ay} + N_{By})$$

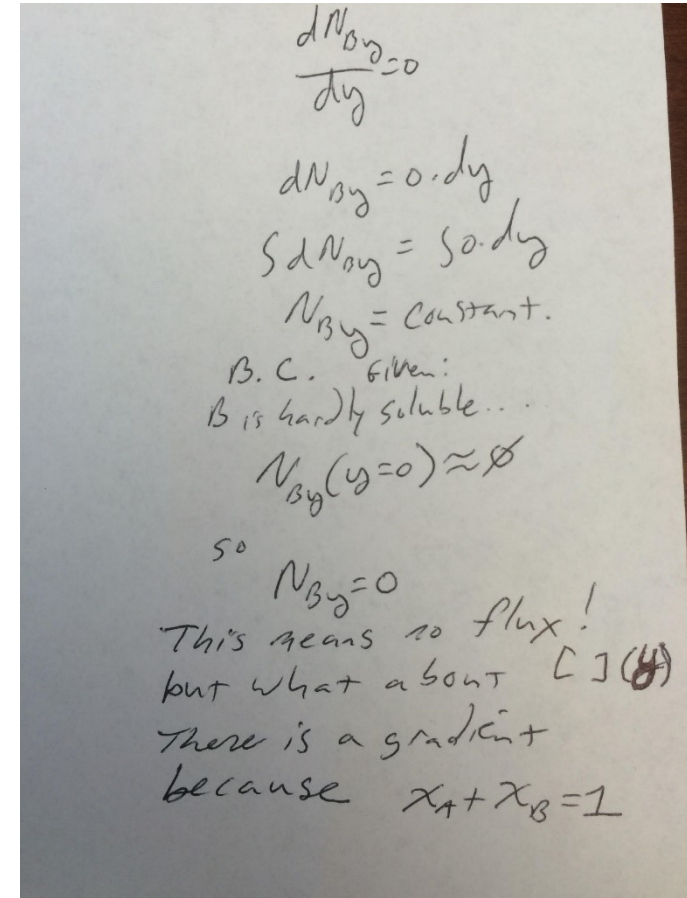
$$N_{Ay} = -CD_{AB} \frac{dx_A}{dy} + x_A N_{Ay}$$

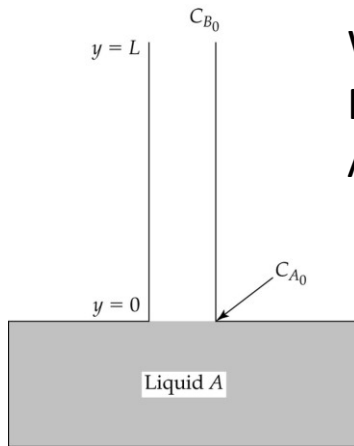
Now what? Solve for N_{Ay}

$$N_{Ay} - x_A N_{Ay} = -CD_{AB} \frac{dx_A}{dy} = N_{Ay}(1 - x_A)$$

$$N_{Ay} = -\frac{CD_{AB} \frac{dx_A}{dy}}{1 - x_A}$$

Now what?





What next?
Fick's 2nd law
At s.s.

Of note, gas is very slightly soluble and is much less than the flux due
To evaporation of the liquid A. so

$$\frac{dN_{Ay}}{dy} = 0$$

$$\frac{dN_{By}}{dy} = 0$$

Remember:

$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$

$$N_{Ay} = -CD_{AB} \frac{dx_A}{dy} + x_A(N_{Ay} + N_{By})$$

$$N_{Ay} = -CD_{AB} \frac{dx_A}{dy} + x_A N_{Ay}$$

Now what? Solve for N_{Ay}

$$N_{Ay} - x_A N_{Ay} = -CD_{AB} \frac{dx_A}{dy} = N_{Ay}(1 - x_A)$$

$$N_{Ay} = -\frac{CD_{AB} \frac{dx_A}{dy}}{1 - x_A}$$

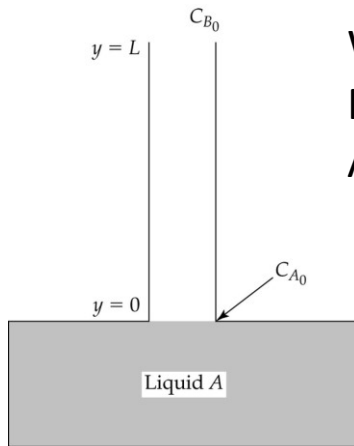
Now what?

$$\frac{dN_{Ay}}{dy} = -\frac{d\left(\frac{CD_{AB} \frac{dx_A}{dy}}{1 - x_A}\right)}{dy} = 0$$

$$\frac{dN_{Ay}}{dy} = -\frac{d\left(\frac{CD_{AB} \frac{dx_A}{dy}}{1 - x_A}\right)}{dy} = 0$$

$$\frac{d\left(\frac{CD_{AB} \frac{dx_A}{dy}}{1 - x_A}\right)}{dy} = 0$$

Now what?



What next?
Fick's 2nd law
At s.s.

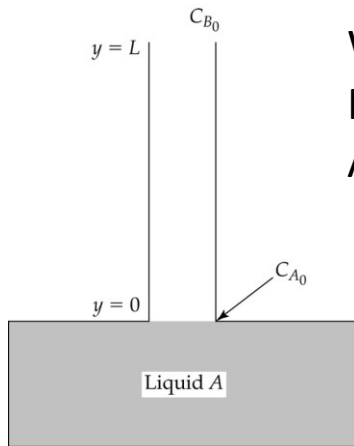
$$\frac{dN_{Ay}}{dy} = 0$$

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Of note, gas is very slightly soluble and is much less than the flux due to evaporation of the liquid A. so

$$\frac{d\left(\frac{CD_{AB} \frac{dx_A}{dy}}{1 - x_A}\right)}{dy} = 0$$

Now what?



What next?
Fick's 2nd law
At s.s.

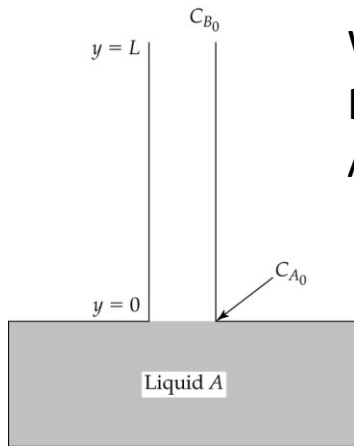
$$\frac{dN_{Ay}}{dy} = 0$$

$$\frac{dN_{By}}{dy} = 0$$

Of note, gas is very slightly soluble and is much less than the flux due to evaporation of the liquid A. so

$$\frac{d\left(\frac{CD_{AB} \frac{dx_A}{dy}}{1 - x_A}\right)}{dy} = 0$$

Now what? Apply B.C.s



What next?
Fick's 2nd law
At s.s.

$$\frac{dN_{Ay}}{dy} = 0$$

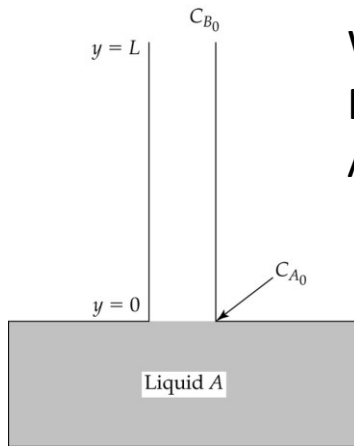
$$\frac{dN_{By}}{dy} = 0$$

Of note, gas is very slightly soluble and is much less than the flux due to evaporation of the liquid A. so

$$\frac{d\left(\frac{CD_{AB} \frac{dx_A}{dy}}{1 - x_A}\right)}{dy} = 0$$

Now what? Apply B.C.s

1) $X_A = X_{A0}$ at $y=0$ and $X_A = 0$ at $y=L$



What next?
Fick's 2nd law
At s.s.

$$\frac{dN_{Ay}}{dy} = 0$$

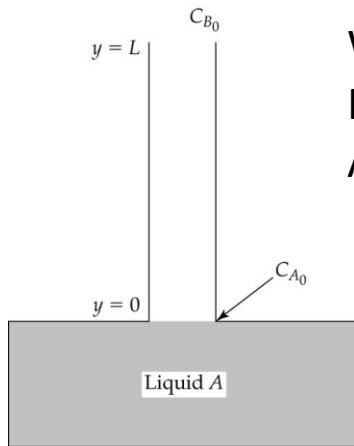
$$\frac{dN_{By}}{dy} = 0$$

Of note, gas is very slightly soluble and is much less than the flux due to evaporation of the liquid A. so

$$\frac{d\left(\frac{CD_{AB} \frac{dx_A}{dy}}{1 - x_A}\right)}{dy} = 0$$

Now what? Apply B.C.s
1) $X_A = X_{A_0}$ at $y=0$ and $X_A = 0$ at $y=L$

How?
Come to board...



What next?
Fick's 2nd law
At s.s.

$$\frac{dN_{Ay}}{dy} = 0$$

$$\frac{dN_{By}}{dy} = 0$$

Of note, gas is very slightly soluble and is much less than the flux due to evaporation of the liquid A. so

$$\frac{d\left(\frac{CD_{AB} \frac{dx_A}{dy}}{1 - x_A}\right)}{dy} = 0$$

Now what? Apply B.C.s

1) $X_A = X_{A_0}$ at $y=0$ and $X_A = 0$ at $y=L$

How?

Come to board... and try in groups...

$$\frac{d}{dy} \left(\frac{1}{1-x_A} \frac{dx_A}{dy} \right) = 0$$

$$\underbrace{d \left(\frac{1}{1-x_A} dx_A \right)}_{?} = 0 dy dy = 0 (dy)^2 = 0 dy^2$$

\Downarrow
 $\int 0 dy^2$
 $+ C_1 y + C_2$

$$\frac{d dx_A}{1-x_A} = \frac{d^2 x_A}{1-x_A}$$
$$= \frac{d^2 x_A}{u}$$

$$1-x_A = u$$

$$\frac{du}{dx_A} = -1$$

$$d \cdot du = -dx_A \cdot d$$

$$d^2 u = -d^2 x_A$$

so

$$\int \frac{d^2 x_A}{u} = - \int \frac{d^2 u}{u}$$

$$= -\ln u$$

$$= -\ln(1-x_A)$$

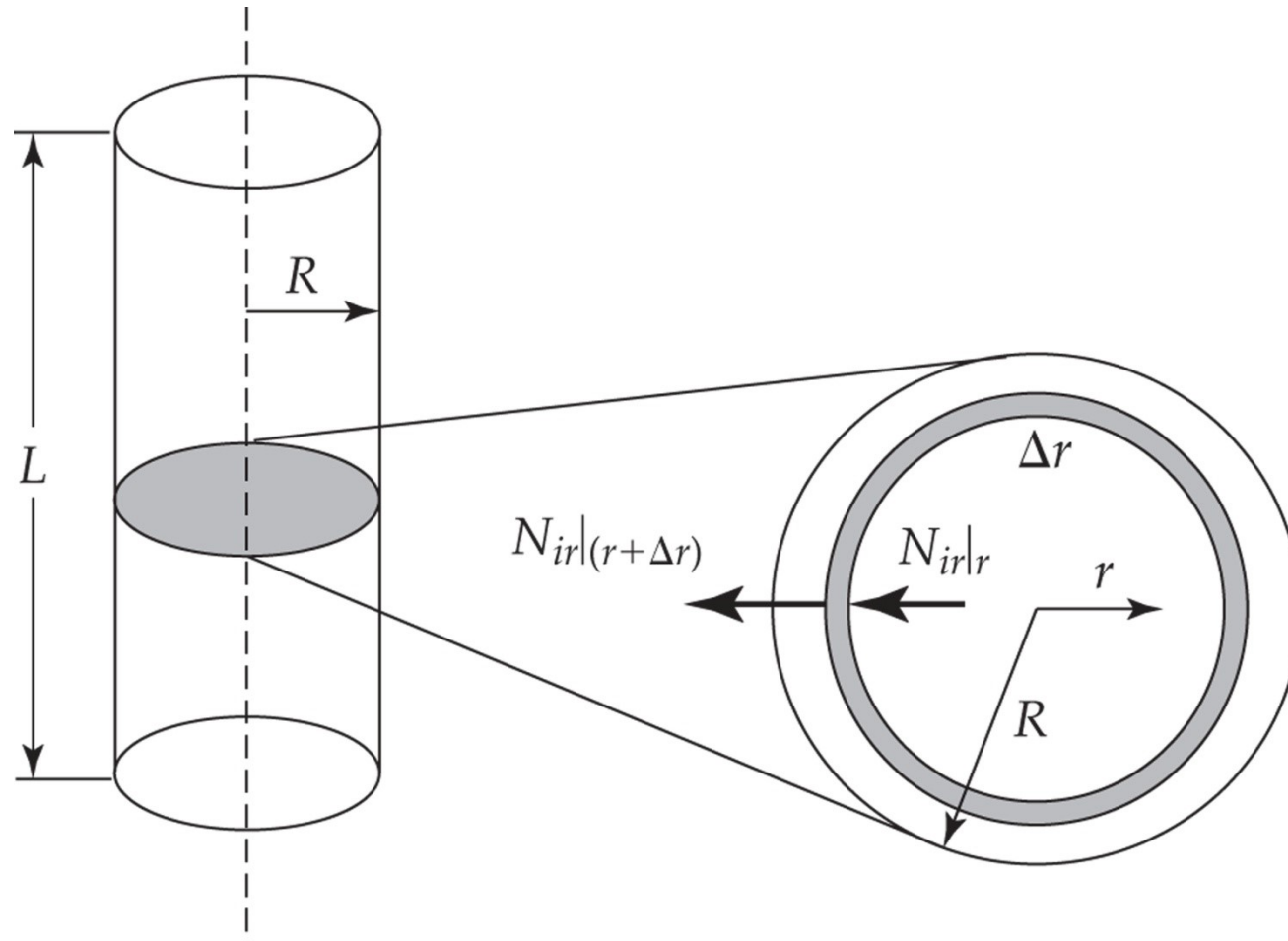
so

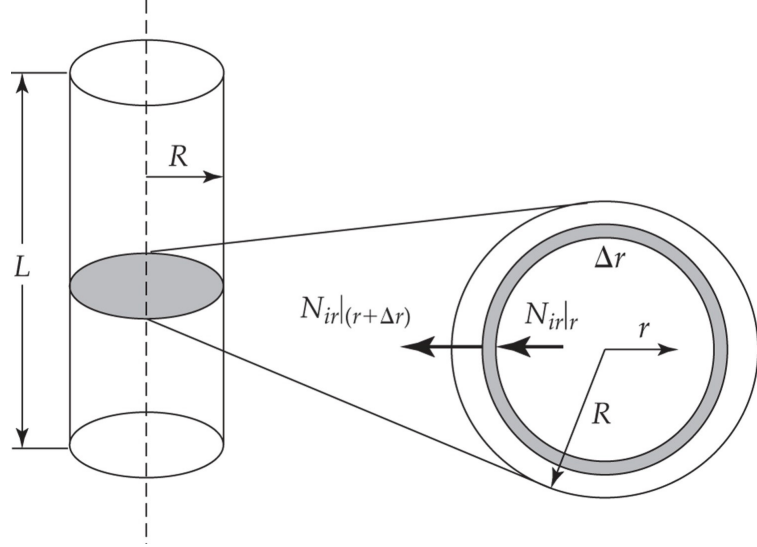
$$\ln(1-x_A) = -C_1 y + C_2$$

if you assigned equimolar counterdiffusion a partition coefficient, what would it be?

Example 6.7.2: Radial diffusion in cylindrical coordinates

Figure 6.13 Radial diffusion through a cylindrical shell.





- Assume no reaction
- Assume steady state

Example 6.7 Figure 6.13

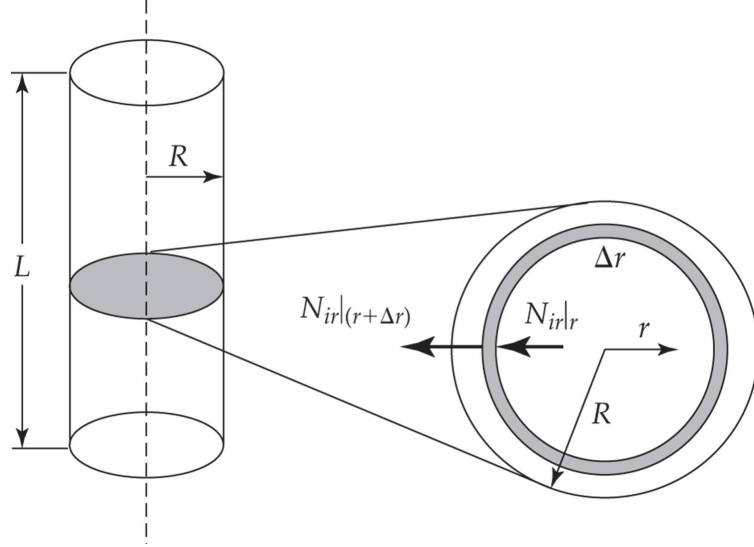
Given
$$\frac{\partial c_i}{\partial t} = -\frac{1}{r} \frac{\partial (r N_{ir})}{\partial r} + R_i$$

Fick's First:
$$N_{ir} = -D_{ij} \frac{\partial c_i}{\partial r}$$

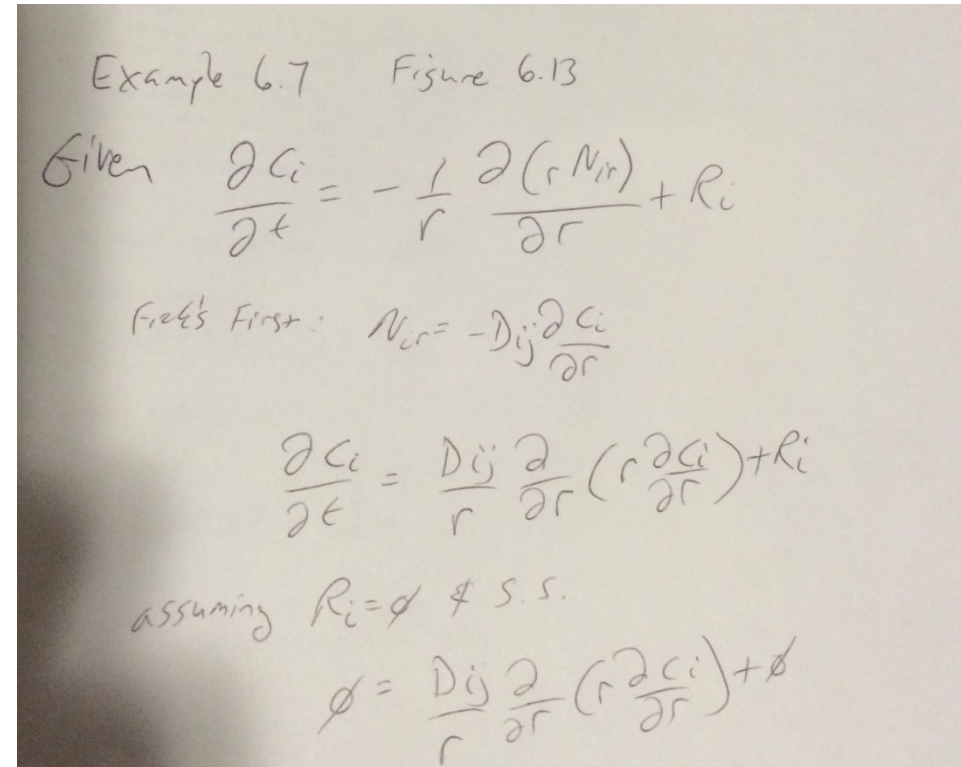
$$\frac{\partial c_i}{\partial t} = \frac{D_{ij}}{r} \frac{\partial}{\partial r} \left(r \frac{\partial c_i}{\partial r} \right) + R_i$$

assuming $R_i = \phi \neq \text{s.s.}$

$$\phi = \frac{D_{ij}}{r} \frac{\partial}{\partial r} \left(r \frac{\partial c_i}{\partial r} \right) + \phi$$



- Assume no reaction
- Assume steady state



Now what?

Come to board and solve the rest
 Without B.C.s (look in book for B.C.s;
 Assuming you can do that...)

$$\frac{0}{r} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial c_i}{\partial r} \right)$$

$$0 = \frac{1}{r} \frac{du}{dr}$$

$$0 \cdot r dr = du$$

$$0 \cdot dr = du$$

$$\int 0 \cdot dr = \int du$$

$$C_1 = u$$

$$C_1 = r \frac{dc_i}{dr}$$

$$\frac{1}{r} C_1 dr = dc_i$$

$$\int \frac{1}{r} C_1 dr = \int dc_i$$

$$C_1 \int \frac{1}{r} dr = \int dc_i = c_i$$

$$C_i = C_1 \ln r + C_2$$

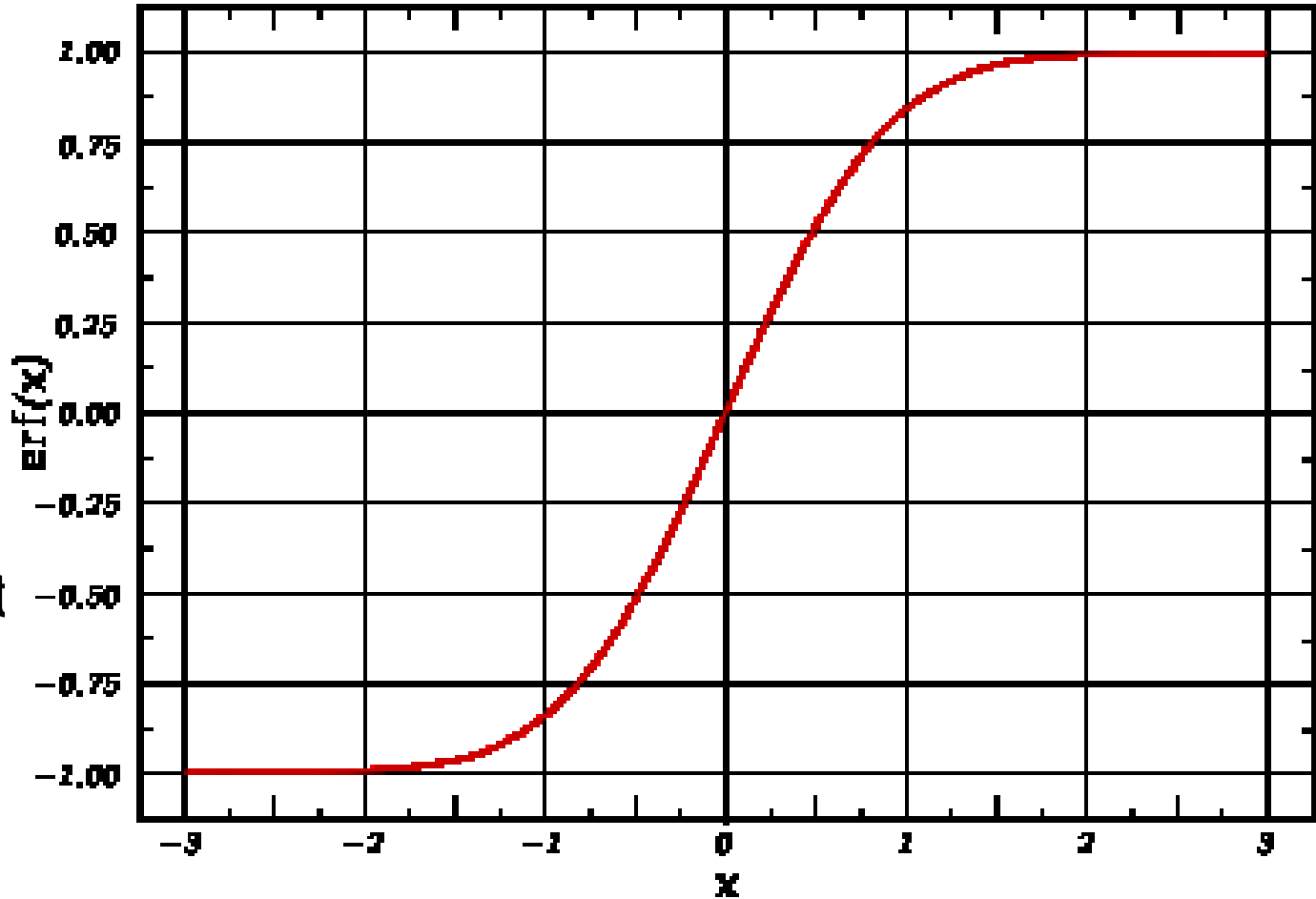
$$r \frac{dc_i}{dr} = u$$

Skipping erf this semester for the sake of time.

erf

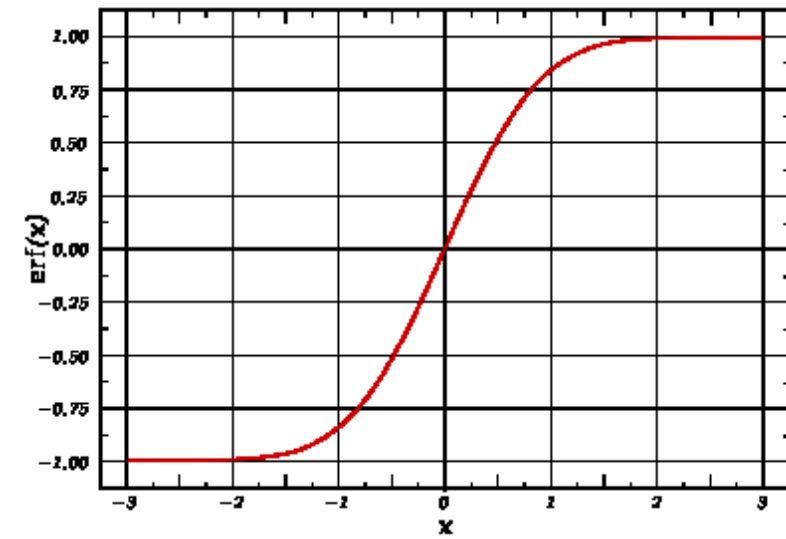
- What is it equal to?
- What is it used for?
- What does this have to do with probability density functions.

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dx$$



erf

- What is it equal to? $erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dx$
- What is it used for? Diff. Eq.s and diffusion
- What is erfc? $erfc=1-erf$



Case	Sample	Boundary conditions	Initial condition	Solution
1	Infinite	$\frac{\partial c}{\partial x}\Big _{x=-\infty,t} = 0; \frac{\partial c}{\partial x}\Big _{x=\infty,t} = 0$	$c(x, 0) = q\delta(x)$	$c(x, t) = \frac{q}{2\sqrt{\pi Dt}} e^{-x^2/4Dt}$
2	Semi-infinite	$c(0, t) = c_s; \frac{\partial c}{\partial x}\Big _{x=\infty,t} = 0$	$c(x, 0) = 0$	$c(x, t) = c_s \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$
3	Semi-infinite	$c(0, t) = 0; \frac{\partial c}{\partial x}\Big _{x=\infty,t} = 0$	$c(x, 0) = c_s$	$c(x, t) = c_s \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$
4	Infinite	$\frac{\partial c}{\partial x}\Big _{x=-\infty,t} = 0; \frac{\partial c}{\partial x}\Big _{x=\infty,t} = 0$	$c(x, 0) = \begin{cases} c_s & \text{at } x \leq 0 \\ 0 & \text{at } x > 0 \end{cases}$	$c(x, t) = \frac{c_s}{2} \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$
5	Infinite	$\frac{\partial c}{\partial x}\Big _{x=-\infty,t} = 0; \frac{\partial c}{\partial x}\Big _{x=\infty,t} = 0$	$c(x, 0) = \begin{cases} 0 & \text{at } x < 0 \\ c_s & \text{at } x \geq 0 \end{cases}$	$c(x, t) = \frac{c_s}{2} \left[1 + \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \right]$
6	Infinite	$\frac{\partial c}{\partial x}\Big _{x=-\infty,t} = 0; \frac{\partial c}{\partial x}\Big _{x=\infty,t} = 0$	$c(x, 0) = \begin{cases} 0 & \text{at } x < -a \\ c_s & \text{at } -a \leq x \leq a \\ 0 & \text{at } x > a \end{cases}$	$c(x, t) = \frac{c_s}{2} \left[\operatorname{erf}\left(\frac{a+x}{2\sqrt{Dt}}\right) + \operatorname{erf}\left(\frac{a-x}{2\sqrt{Dt}}\right) \right]$
7	Plate	$c(0, t) = c_s$ $c(L, t) = c_s$	$c(x, 0) = 0$	$c(x, t) = c_s \left\{ 1 - \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{e^{-(2n+1)^2 \pi^2 Dt/L^2}}{2n+1} \sin \frac{(2n+1)\pi x}{L} \right\}$

MatLab Code

```
close all
x = [0:0.0000001:1];

figure1 = figure;
hold on
% Create axes
axes1 = axes('Parent',figure1);
hold(axes1,'on');

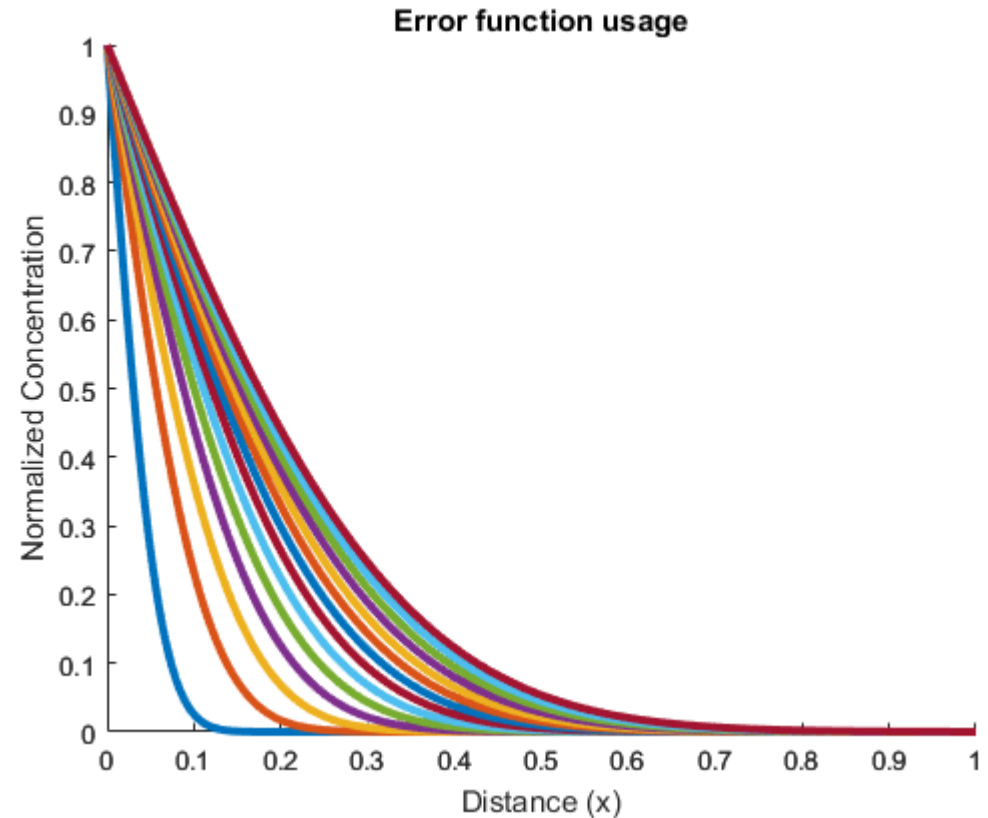
% Create multiple lines using matrix input to plot
%plot(X1,YMatrix1,'Parent',axes1);

% Create xlabel
xlabel('Distance (x)');

% Create title
title('Error function usage');

% Create ylabel
ylabel('Normalized Concentration');

% Set the remaining axes properties
%set(axes1,'FontSize',14,'FontWeight','bold');
for i = 1:2.5:35
    plot(x,1-erf(x/(2*sqrt(i*10^-3))), 'linewidth',3)
end
```



```

x = [0:0.0000001:1];
figure2 = figure;
% Create axes
axes1 = axes('Parent',figure2);
hold(axes1,'on');
% Create multiple lines using matrix input to plot
%plot(X1,YMatrix1,'Parent',axes1);

% Create xlabel
xlabel('Distance (x)');

% Create title
title('Error function usage');

% Create ylabel
ylabel('Normalized Concentration');

% Set the remaining axes properties
%set(axes1,'FontSize',14,'FontWeight','bold');
for i = 1:2.5:35
    plot(x,erfc(x/(2*sqrt(i*10^-3))), 'linewidth',3)
end

```

