EE-735
Assignment 4

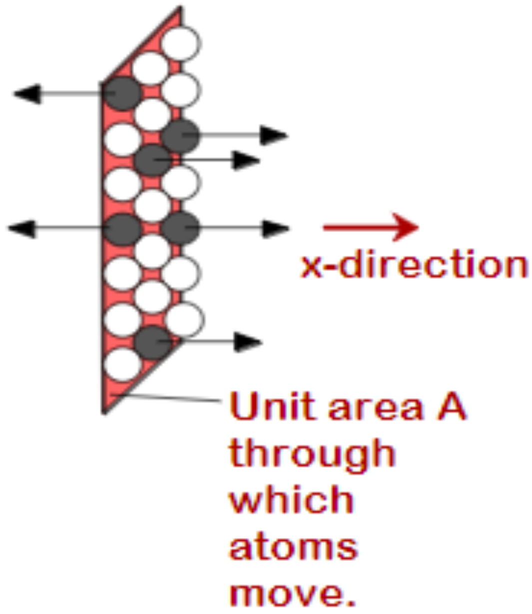
Diffusion

- What is diffusion?
- It is defined as movement of particle from a region of higher conc. to a region of lower conc.
- Diffusion is driven by concentration gradient
- Observed everywhere from atoms (in doping), electrons and holes (diffusion current) to ions in bio-molecular processes.

Flux

- The flux of diffusing particles J is used to quantify how fast the process is.
- It is defined as no of particles diffusing per unit cross-sectional area per unit time.

$$J=(1/A)dN/dt$$



Fick's First Law (steady-state diffusion)

- The diffusion along a fixed direction is proportional to the concentration gradient.

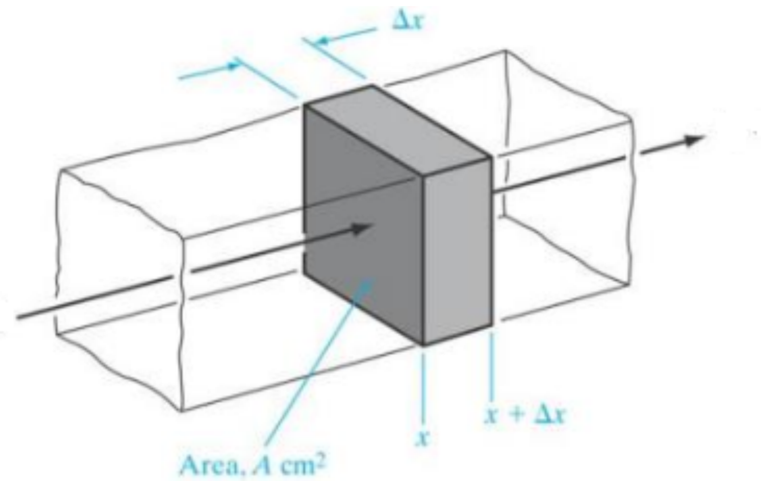
$$J = -D \frac{dC}{dx}$$

where D is the diffusion coefficient called Diffusivity.it is a material property.

- The minus sign indicates that the diffusion is in the direction of decreasing concentration.

Fick's Second Law (Non-steady state diffusion)

- If a flux of particles in entering at x at time t and leaving at x+Δx at time t+Δt



- The concentration change
- dC= (J(x+Δx)-J(x))dtA /Adx
- This reduces to

$$\frac{\partial C}{\partial t} = -\frac{\partial J}{\partial x}$$

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

The diffusion equation

- The diffusion equation is

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \qquad \nabla^2 C = \frac{1}{D}\frac{\partial C}{\partial t} \quad \text{(3-D)}$$

where D is diffusivity.

- If the concentration is time-independent the equation reduces to

$$\nabla^2 C = 0$$

- Continuity equation $$\frac{\partial n}{\partial t} = \frac{\nabla . J_n}{q} - \frac{\delta n}{\tau_n} + G_n$$

Solving the equation numerically

- The diffusion equation $$\frac{d^2n}{dx^2} - \frac{1}{D}\frac{dn}{dt} = 0$$

$$\left(\frac{d^2}{dx^2} - \frac{1}{D}\frac{d}{dt}\right)n = 0$$

- Any differential equation of the type

Of(x)=g(x)

where O is the differential operator f(x) is the response and g(x) is the source . If g(x)=0 the equation is homogeneous.

- There can be various sources of non-homogeneity

- The equation can be written numerically

$$\frac{d^2 n}{dx^2} = \frac{n_{i+1,m} - 2n_{i,m} + n_{i-1,m}}{h^2} \qquad \frac{dn}{dt} = \frac{n_{i,m} - n_{i,m-1}}{p}$$

- So diffusion equation becomes

$$\frac{n_{i+1,m} - 2n_{i,m} + n_{i-1,m}}{h^2} - \frac{n_{i,m} - n_{i,m-1}}{Dp} = 0$$

- Where i and m are indices in position domain and time domain.
- For some source the equation will become

$$\frac{n_{i+1,m} - 2n_{i,m} + n_{i-1,m}}{h^2} - \frac{n_{i,m} - n_{i,m-1}}{Dp} = S$$

Problems

- Solve the diffusion equation for the case of delta source ? Two kinds of solution exist analytical and numerical, compare both the solution.
- The analytical solution is
- Start with diffusion equation

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

- Write it in the form of Of(x)=g(x)

$$\left(\frac{d^2}{dx^2} - \frac{1}{D}\frac{d}{dt}\right)C = 0$$

Contd..

- Let here the source term be a delta function in space at time t=0

$$\left(\frac{d^2}{dx^2} - \frac{1}{D}\frac{d}{dt}\right)C = \delta(x - x')$$

- To find the impulse response take fourier transform of spacial co-ordinates
- The equation becomes

$$-k^2 C(k,t) - \frac{1}{D}\frac{dC(k,t)}{dt} = 0$$

- The solution is

$$C(k,t) = C(k, t = 0)exp(-k^2 Dt)$$

- Putting initial condition at t=0

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

- C(k,t=0) is nothing but the fourier transform of the point source.

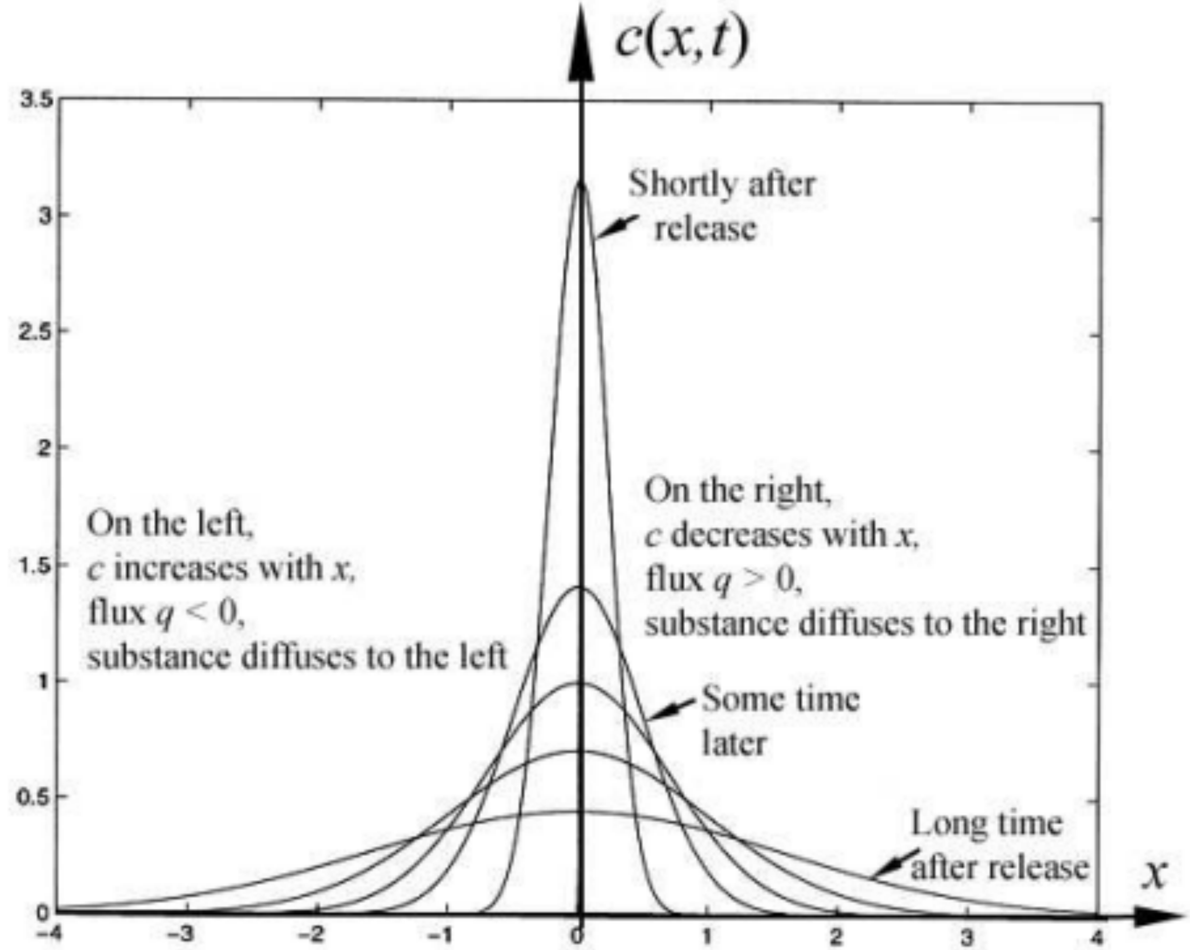
$$C(k,t=0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \delta(x-x')\exp(-ikx)\,dx$$
$$= \frac{\exp(-ikx')}{2\pi}$$

- The C(x,t) is the inverse fourier transform of C(k,t)

$$C(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp(ik(x-x'))exp(-k^2Dt)\,dk$$

- The integration gives

$$C(x,t) = \frac{1}{(4\pi Dt)^{0.5}}exp(-(x-x')^2/4Dt)$$



$c(x,t)$
Shortly after release
On the left,
c increases with x,
flux $q < 0$,
substance diffuses to the left
On the right,
c decreases with x,
flux $q > 0$,
substance diffuses to the right
Some time later
Long time after release
x
3.5
3
2.5
2
1.5
1
0.5
0
-4
-3
-2
-1
0
1
2
3
4

- If you know the impulse response we can find the solution for any source by a simple integration.
- Suppose we have an infinite source at g(0,t)=M for all t>0

$$C(x,t) = \frac{1}{(4\pi Dt)^{0.5}} \int_0^{\infty} M \exp\left(-\frac{(x-x')^2}{4Dt}\right) dx'$$

- Solve the integral, report the answer analytically and compare it with the numerical solution.
- Answer : C(x,t) will be complementary error function.