Topics covered
- Transient state diffusion
  - $\Rightarrow$ Error function solution
  - $\Rightarrow$ Point source solution

Can you think of any real or hypothetical physical example?

Error function solution: Unlimited supply on one boundary in a semi-infinite domain
Point source solution: Depleting supply from a point source in an infinite domain
Fourier series solution: General solution for finite domain

One-dimensional step function initial condition (Error function solution)
Example

$$c(x,t=0) = \begin{cases} c_L & -\infty < x < 0 \\ c_R & 0 < x < \infty \end{cases}$$

$$c(-\infty,t) = c_L$$

$$c(\infty,t) = c_R$$

We want to know the concentration profile at any time t;
i.e., we have to solve the diffusion equation

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

Change of variable: let $\eta = \dfrac{x}{\sqrt{4Dt}}$ (note: η is a dimensionless variable)

Applying the chain rule

$$\frac{\partial c}{\partial t} = \frac{\partial \eta}{\partial t}\frac{\partial c}{\partial \eta} = \frac{-\eta}{2t}\frac{\partial}{\partial \eta}, \text{ and}$$

$$\frac{\partial c}{\partial x} = \frac{\partial \eta}{\partial x}\frac{\partial c}{\partial \eta}$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial c}{\partial x}\right) = \frac{\partial \eta}{\partial x}\frac{\partial}{\partial \eta}\left(\frac{\partial \eta}{\partial x}\frac{\partial c}{\partial \eta}\right)$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{\partial \eta}{\partial x}\frac{\partial}{\partial \eta}\left(\frac{\partial \eta}{\partial x}\frac{\partial c}{\partial \eta}\right) = \left(\frac{\partial \eta}{\partial x}\right)^2\frac{\partial^2 c}{\partial \eta^2}$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{1}{4Dt}\frac{\partial^2 c}{\partial \eta^2}$$

Substituting back to the diffusion equation

$$-2\eta \frac{dc}{d\eta} = \frac{d^2c}{d\eta^2}$$

Notice that c now depends only on η; therefore, the diffusion equation has transformed from a partial differential equation into an ordinary differential equation, which can be solved by another change of variable, for example

$$q = \frac{\partial c}{\partial \eta}$$

After two integrations, we get the concentration profile in terms of η as

$$c(\eta) - c(\eta = \eta_o) = a_1 \int_{\eta_o}^{\eta} e^{-\zeta^2} d\zeta$$

Applying boundary conditions

$$c(\eta = -\infty) = c_L$$

$$c(\eta) - c(-\infty) = a_1 \int_{-\infty}^{\eta} e^{-\zeta^2} d\zeta$$

$$c(\eta) = c_L + a_2 \left(\frac{2}{\sqrt{\pi}} \int_{-\infty}^{0} e^{-\zeta^2} d\zeta + \frac{2}{\sqrt{\pi}} \int_{0}^{\eta} e^{-\zeta^2} d\zeta \right)$$

$$c(\eta) = c_L + a_2 \left(erf(\infty) + erf(\eta) \right)$$

Using the second boundary conditions

$$c(\eta = \infty) = c_R$$

$$c(\eta = \infty) = c_R = c_L + a_2 \left(1 + erf(\infty) \right)$$

$$a_2 = \frac{c_R - c_L}{2}$$

The concentration profile for the 1-D step function initial condition is

$$c(x,t) = \frac{c_L + c_R}{2} + \frac{c_R - c_L}{2} erf\left(\frac{x}{\sqrt{4Dt}} \right)$$

Note:

- Since the concentration is a function of the dimensionless variable $\eta = \frac{x}{\sqrt{4Dt}}$, the concentration profile is identical if the parameters and the initial & boundary conditions are scaled by

$$x' = \lambda x \text{ and } t' = \lambda^2 t$$

- The diffusion depth or penetration distance for the error function solution is roughly estimated to be at a location where $c(x,t) - c_{\pm\infty} = \left| \frac{\Delta c}{8} \right|$. This gives a penetration distance at any time t to be $x \approx 1.6\sqrt{Dt}$, approximately $x \approx 2\sqrt{Dt}$. The time to reach steady state can be estimated by setting the penetration distance to be larger than the largest characteristic length (L) over which the diffusion takes place. Hence, steady state might be achieved when $t \gg \frac{L^2}{D}$. Steady-state conditions cannot be achieved when the boundary conditions are time-dependent

or the system is infinite or semi-infinite. However, under certain circumstances, a transient system can be assumed to be at a quasi steady-state

Point source solution

Several error function solutions can be "superpositioned" together to obtain some "funny-looking" concentration profiles (a.k.a. superposition method).
For example, if we merge the two following step functions

$$c(x,t=0) = \begin{cases} 0 & -\infty < x < 0 \\ c_o & 0 < x < \infty \end{cases}$$

$$c(x,t=0) = \begin{cases} 0 & -\infty < x < \Delta x \\ -c_o & \Delta x < x < \infty \end{cases}$$

we get a point source of width $\underline{\Delta x}$ (somewhat similar to a delta function).
The solution for each step function is

$$c(x,t) = \frac{c_o}{2} + \frac{c_o}{2} erf\left(\frac{x}{\sqrt{4Dt}}\right)$$

$$c(x,t) = -\frac{c_o}{2} - \frac{c_o}{2} erf\left(\frac{x-\Delta x}{\sqrt{4Dt}}\right)$$

Combining the two solutions give

$$c(x,t) = \frac{c_o}{2} + \frac{c_o}{2}\frac{2}{\sqrt{\pi}}\int_0^{\frac{x}{\sqrt{4Dt}}} e^{-\zeta^2} d\zeta - \frac{c_o}{2} - \frac{c_o}{2}\frac{2}{\sqrt{\pi}}\int_0^{\frac{x-\Delta x}{\sqrt{4Dt}}} e^{-\zeta^2} d\zeta$$

$$c(x,t) = \frac{c_o}{\sqrt{\pi}}\int_{\frac{x-\Delta x}{\sqrt{4Dt}}}^{\frac{x}{\sqrt{4Dt}}} e^{-\zeta^2} d\zeta$$

For $\Delta x << x$, the solution for the transient state concentration profile of a point source is

$$c(x,t) = \frac{c_o \Delta x}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

Note:
- The penetration depth for diffusion from a point source is also roughly equals to
  $x \approx 2\sqrt{Dt}$. Similarly, steady-state may be expected when $t >> \dfrac{L^2}{D}$.
- The solution is symmetric about $x = 0$.
- The concentration gradient is zero at $x = 0$, i.e. no flux @ $x = 0$, hence the two sides of the solution are independent
- In semi-infinite case, the solution has the same general form but concentration is
  twice as large, $c(x,t) = \dfrac{N}{\sqrt{\pi Dt}} e^{-\frac{x^2}{4Dt}}$
- The solution is identical for point source diffusion in a line, line source diffusion into a plane and planar source diffusion into a volume.

- The solution is similar for 1-D, 2-D and 3-D diffusion of a point source

Point source in 1-D	$c(x,t) = \dfrac{N}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$
Point source in 2-D	$c(x,t) = \dfrac{N}{4\pi Dt} e^{-\frac{r^2}{4Dt}}$
Point source in 3-D	$c(x,t) = \dfrac{N}{8(\pi Dt)^{3/2}} e^{-\frac{r^2}{4Dt}}$

- The point source solution can be used to find the concentration profile from complicated initial conditions by the Green's function method. The point source solution is integrated over the domain of the initial condition:

$$c(x,t) = \int_a^b \frac{c_o \, d\xi}{\sqrt{4\pi Dt}} e^{-\frac{(\xi-x)^2}{4Dt}}$$