Diffusion

Derivation of micro-scale diffusion

Fick’s First Law.

Fick’s Seconds Law.

We are going to introduce a form of differential equation the partial derivative, this is a differential equation with two derivatives, for example space and time.

We are going to swap between using heat and concentration as examples to investigate diffusion. In general they are going to be very similar phenomena. For clarities sake I am going to define a few terms now so that you don’t get lost.

Q (heat)	Heat note temperature =Q/ heat capacity
Q (chemical)	Q is moles
T	Temperature
A	Area
t	Time
K’	Thermal Conductivity

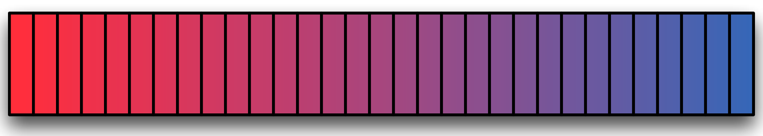
Lets take a bar and heat it at one end

We could look at the temperature change across the bar at a time t or we could look at the temperature of a small section of the bar as a function of time. Experimentally we know that the rate of change in the heat at a specific point on the bar depends of the temperature gradient, the size of the bar and the thermal conductivity, such that we can write.

$$\frac{dQ}{dt} = \frac{K'A}{D}(T_1 - T_2)$$

Where K is the thermal conductivity, A is the area D the thickness and T the temperatures.

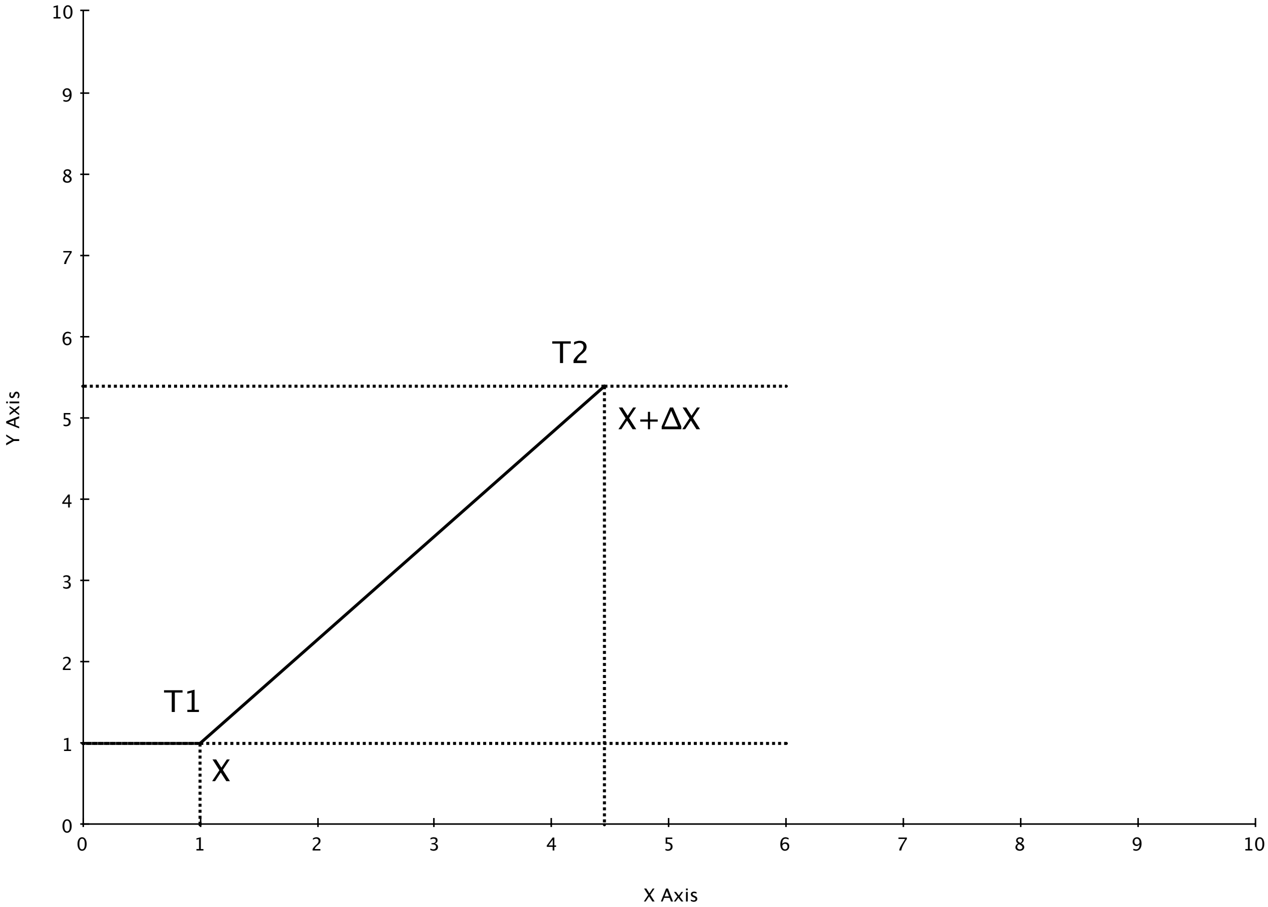
Now we cut up, in our head the bar in to small sections of length Dx



So we can now write

$$\frac{dQ}{dt} = \frac{K'A}{D} \frac{(T_{(x)} - T_{(\Delta x)})}{\Delta x}$$

Where T1=T(x), T2=T(x+Dx) and D= Dx



The gradient is T2-T1/ (DX)
In the limit of DX=>0 we can write this in the form of a derivative and say that we now have;

Formally

$$\frac{Limit}{\Delta x \rightarrow 0} \frac{T_{(x+\Delta x)} - T_{(x)}}{\Delta x} = \frac{\delta T}{\delta x}$$

$$\frac{dT}{dx}$$

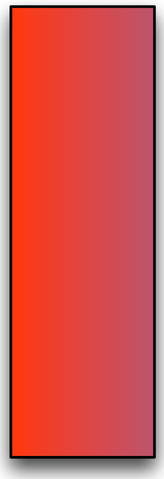
combining these two terms we get

$$\frac{dQ}{dt} = -K'A\left(\frac{dT}{dx}\right)$$

In the previous equation we had the rate of change of heat flow with respect to time (the position was fixed) now here we have the rate of change of temperature with respect to position. Note that dT/dx is the temperature gradient.

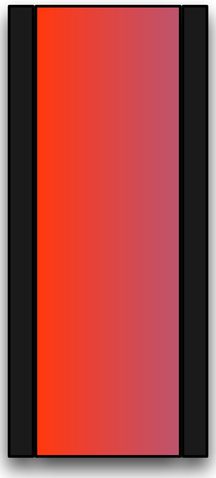
This tell us that the rate at which heat travels through an infinitesimally thin slice of a metal.

We want to know how the temperature of the metal within the slice changes, to do this we must know how the heat (Q) accumulates within a thin slice / section



ΔX

Lets take another slice of metal and we will call this slice DX, this is a thickish slice of metal, i.e we are not currently in the limits of small dx. We do however place two very thin slices at each end of our thicker slice, these are dx



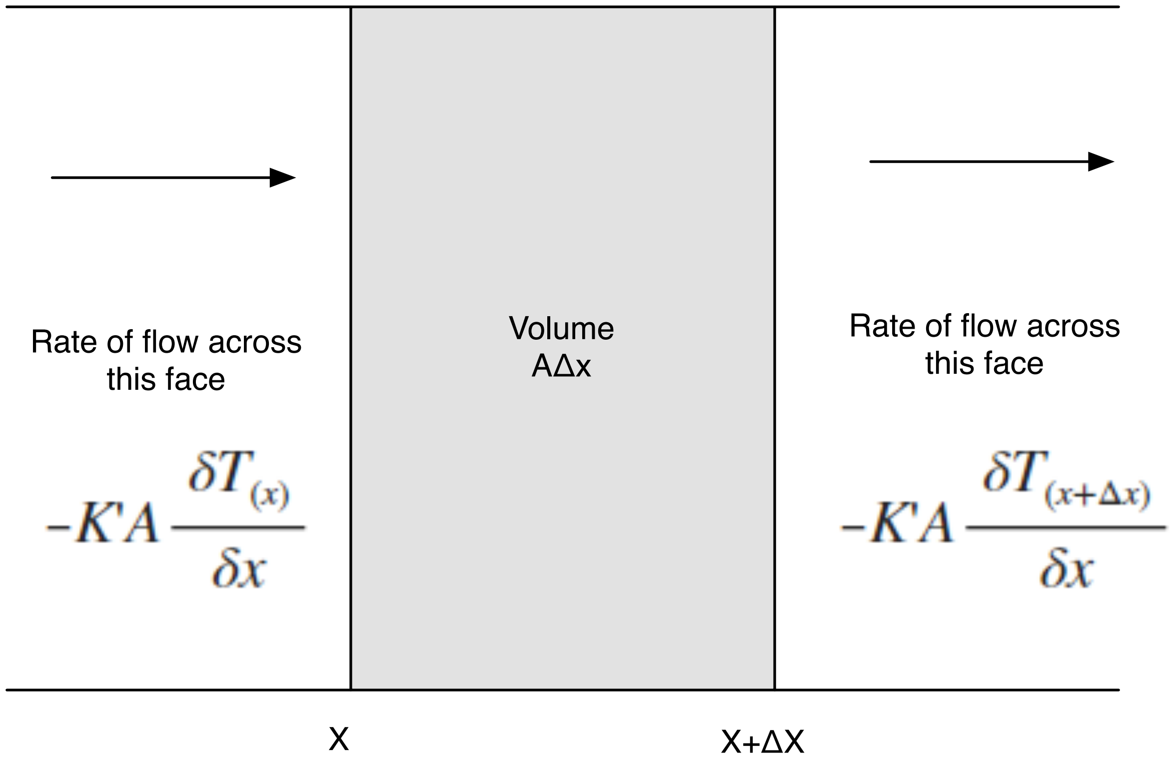
ΔX

On the left hand side we have (the small section)

$$\left.\frac{dQ}{dt}\right|_{Left} = -\frac{KA\delta T_{(x)}}{\delta x}$$

On the right hand side we have

$$\left.\frac{dQ}{dt}\right|_{Right} = -\frac{KA\delta T_{(x+\Delta x)}}{\delta x}$$



Note that these are not the same as the derivative is in a different spatial position

We know that the net change in the heat content within the volume must produce a change in temperature and we can write that down as

$$\Delta T = \frac{\Delta Q}{\Omega}$$

Where Ω is the heat capacity and is given as

Ω is the volume x density x specific heat.

$$\Delta T = \frac{\Delta Q}{\rho \sigma A \Delta x}$$

I can use this to swap between heat (Q) and temperature.

$$\frac{\Delta T}{dt} = \frac{1}{\rho \sigma A \Delta x} \left(\left. \frac{\delta Q}{\delta t} \right|_{Left} - \left. \frac{\delta Q}{\delta t} \right|_{Right} \right)$$

$$= \frac{K'A}{A\rho\sigma\Delta x}\left(\frac{\delta T_{(x+\Delta x)}}{\delta x} - \frac{\delta T_{(x)}}{\delta x}\right)$$

$$= \frac{K'A}{A\rho\sigma\Delta x}\left(\frac{\delta T_{(x+\Delta x)}}{\delta x} - \frac{\delta T_{(x)}}{\delta x}\right)$$

Using the previous trick of setting ΔX=>0 we can write

$$\frac{\delta T}{\delta t} = K\frac{\delta^2 T}{\delta x^2}$$

This is the diffusion equation note that K=K'/ps

Lets use it