Fick's first law relates the diffusive flux to the concentration gradient in steady state. It postulates that the flux goes from regions of high concentration to regions of low concentration, with a magnitude that is proportional to the concentration gradient (spatial derivative), or in simplistic terms the concept that a solute will move from a region of high concentration to a region of low concentration across a concentration gradient. In one dimension, the law is:

$$J = -D\frac{d\varphi}{dx}$$

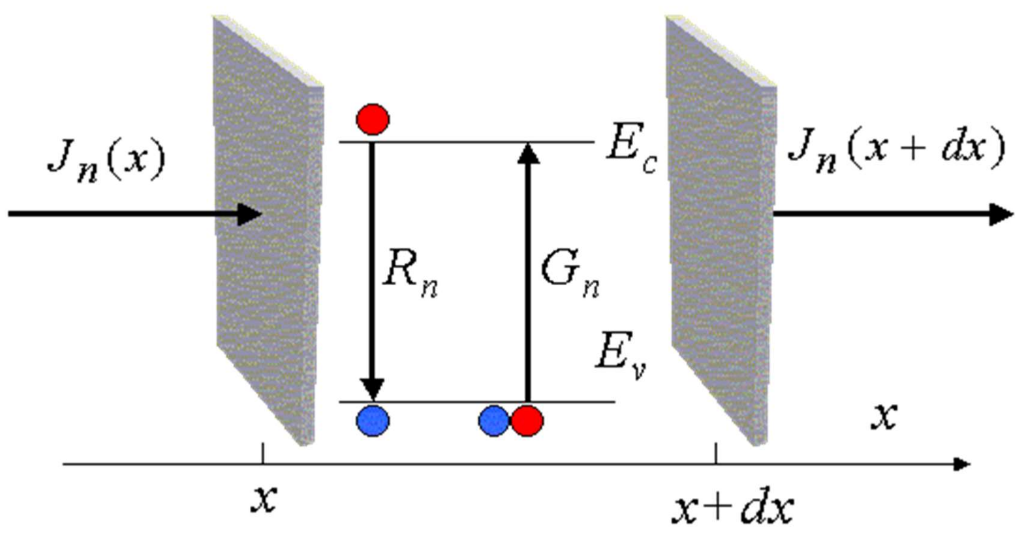
Where, J is the flux in number of particles per unit area per unit time. D is called as diffusion constant or diffusivity which is having the unit of area per unit time. And $\frac{d\varphi}{dx}$ is the particle concentration gradient. In 3 dimensional systems, the law can be written as:

$$J = -D\nabla\varphi$$

Fick’s Second law follows from the first law which predicts how diffusion causes the concentration to change with time

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

The continuity equation describes a basic concept, namely that a change in carrier density over time is due to the difference between the incoming and outgoing flux of carriers plus the generation and minus the recombination. The flow of carriers and recombination and generation rates are illustrated in fig given below



Continuity equation model

The rate of change of the carriers between x and x+dx equals the difference between the incoming flux and the outgoing flux plus the generation and minus the recombination:

$$\frac{\partial n(x,t)}{\partial t}Adx = \frac{1}{-q}[J_n(x) - J_n(x+dx)] + [G_n(x,t) - R_n(x,t)]Adx$$

where $n(x,t)$ is the carrier density, A is the area, $G_n(x,t)$is the generation rate and Rn(x,t) is the recombination rate. Using a Taylor series expansion

$$J_n(x+dx) = J_n(x) + \frac{\partial J_n(x)}{\partial x} dx$$

The equation can now be simplified as

$$\frac{\partial n(x,t)}{\partial t} = \frac{1}{q}\frac{\partial J_n(x,t)}{\partial x} + G_n(x,t) - R_n(x,t)$$

Similarly for Holes:

$$\frac{\partial p(x,t)}{\partial t} = \frac{1}{-q}\frac{\partial J_p(x,t)}{\partial x} + G_p(x,t) - R_p(x,t)$$

A solution of this equation can be obtained from the expression of total current of electron and hole as:

$$\frac{\partial n(x,t)}{\partial t} = \mu_n n \frac{\partial E(x,t)}{\partial x} + \mu_n E \frac{\partial n(x,t)}{\partial x} + D_n \frac{\partial^2 n(x,t)}{\partial x^2} + G_n(x,t) - R_n(x,t)$$

A simple model for the recombination-generation mechanisms states that the recombination-generation rate is proportional to the excess carrier density. It acknowledges the fact that no net recombination takes place if the carrier density equals the thermal equilibrium value. The resulting expression for the recombination of electrons in a p-type semiconductor is given by:

Excess Recombination rate U_n =Recombination rate (R_n)-Generation rate (G_n)

$$U_n = R_n - G_n = \frac{n_p - n_{p_0}}{\tau_n}$$

Expression for the recombination of holes in a n-type semiconductor is given by:

$$U_p = R_p - G_p = \frac{p_n - p_{p_0}}{\tau_p}$$

From the above equations it is clear that Recombination rate depends on excess minority carrier concentration from its equilibrium values and the minority carrier lifetime.

The Diffusion Equation: In the quasi-neutral region where the electric field is small and the current is due to diffusion only, we can use the simple recombination model for the net recombination rate since the recombination rates depend only on the minority carrier density. This leads to the time-dependent diffusion equations for electrons in p-type material and for holes in n-type material:

$$\frac{\partial n(x,t)}{\partial t} = D_n \frac{\partial^2 n_p(x,t)}{\partial x^2} - \frac{n_p(x,t) - n_{p_0}}{\tau_n}$$
$$\frac{\partial p(x,t)}{\partial t} = D_p \frac{\partial^2 p_n(x,t)}{\partial x^2} - \frac{p_n(x,t) - p_{n_0}}{\tau_p}$$

At steady state where the rate of change of carrier is zero we can rewrite the diffusion equation and find the time independent solution:

$$0 = D_n \frac{\partial^2 n_p(x)}{\partial x^2} - \frac{n_p(x) - n_{p_0}}{\tau_n}$$

$$0 = D_p \frac{\partial^2 p_n(x)}{\partial x^2} - \frac{p_n(x) - p_{n_0}}{\tau_p}$$

So the equation can be written as:

$$\frac{\partial^2 \left(n_p(x) - n_{p_0}\right)}{\partial x^2} = \frac{n_p(x) - n_{p_0}}{L_n^2}$$

$$\frac{\partial^2 \left(p_n(x) - p_{n_0}\right)}{\partial x^2} = \frac{p_n(x) - p_{n_0}}{L_p^2}$$

Where $L_n = \sqrt{D_n \tau_n}$ and $L_p = \sqrt{D_p \tau_p}$ are called the Diffusion Lengths of electrons and holes respectively. Now the general solution to these equations are:

$$n_p(x_p) - n_{p_0} = Ae^{\frac{-x_p}{L_n}} + Be^{\frac{x_p}{L_n}}$$

$$p_n(x_n) - p_{n_0} = Ae^{\frac{-x_n}{L_p}} + Be^{\frac{x_n}{L_p}}$$

By using boundary conditions we can find the value of these constants. The boundary conditions are:

$$n_p(x_p) = n_p(0) \quad at \;\; x_p = 0$$

$$n_p(x_p) = n_{p_0} \qquad at \;\; x_p = \infty$$

$$p_n(x_n) = p_n(0) \quad at \;\; x_n = 0$$

$$p_n(x_n) = p_{n_0} \qquad at \;\; x_n = \infty$$

So the final solutions become:

$$\delta p(x_n) = p_n(x_n) - p_{n_0} = \left(p_n(0) - p_{n_0}\right)e^{\frac{-x_n}{L_p}}$$

$$\delta n(x_p) = n_p(x_p) - n_{p_0} = \left(n_p(0) - n_{p_0}\right)e^{\frac{-x_p}{L_n}}$$

Formalism of time dependent diffusion equation using backward Euler scheme:
The time dependent diffusion equation is:

$$\frac{\partial n(x)}{\partial t} = D\frac{\partial^2 n(x)}{\partial x^2}$$

In backward Euler scheme the above equation can be written as:

$$\frac{n_i(t) - n_i(t-\Delta t)}{\Delta t} = D\frac{n_{i+1}(t-\Delta t) - 2n_i(t-\Delta t) + n_{i-1}(t-\Delta t)}{\Delta x^2}$$

$$n_i(t) = \frac{D\Delta t}{\Delta x^2}n_{i-1}(t-\Delta t) + \left(1 - \frac{2D\Delta t}{\Delta x^2}\right)n_i(t-\Delta t) + \frac{D\Delta t}{\Delta x^2}n_{i-1}(t-\Delta t)$$

So for the matrix formalism at a time instance and at ith position will look like:

$$n_i(t) = \left[\frac{D\Delta t}{\Delta x^2} + \left(1 - \frac{2D\Delta t}{\Delta x^2}\right) + \frac{D\Delta t}{\Delta x^2}\right]\begin{bmatrix} n_{i-1}(t-\Delta t) \\ n_i(t-\Delta t) \\ n_{i-1}(t-\Delta t) \end{bmatrix}$$

Here i is the position instant and t is the time instant. If we discretise the distance into nx division then for each time instant we will get a spars matrix of (nx X nx).