

Q1.

Forward difference method

Minority carrier diffusion equation is given by

$$\frac{\partial C(i, t)}{\partial t} = D \frac{\partial^2 C(i, t)}{\partial x^2} \quad (1)$$

Using the forward finite difference method for time derivative and central difference method for space derivative we get

$$\frac{C(i, t+1) - C(i, t)}{\Delta t} = D \frac{C(i+1, t) - 2C(i, t) + C(i-1, t)}{\Delta x^2} \quad (2)$$

Rearranging terms in Eq. 2 we get

$$C(i, t+1) = K(C(i-1, t) + C(i+1, t)) + C(i, t)(1 - 2K) \text{ where } K = \frac{D\Delta t}{\Delta x^2} \quad (3)$$

The above equation can be written in the matrix form

$$[C]_i^{t+1} = [A][C]_i^t \quad (4)$$

where $[C]_i^t$ is the spatial concentration matrix at time t and A is a tri-diagonal matrix given by

$$A = \begin{bmatrix} 1-2K & K & \dots & \dots & 0 \\ K & 1-2K & K & \dots & 0 \\ 0 & K & \ddots & \ddots & 0 \\ \dots & \dots & \ddots & \ddots & K \\ \dots & \dots & \dots & K & 1-2K \end{bmatrix} \quad (5)$$

Eq. 4 is stable and converges for $K \leq 0.5$. which imposes a restriction on the time step for which the above finite difference scheme could be evaluated

Backward Difference method

Instead of using the forward difference method for partial time derivative at time equal to t, we could use the backward difference method for partial time derivative at time equal to t+1.

$$\frac{C(i, t+1) - C(i, t)}{\Delta t} = D \frac{C(i+1, t+1) - 2C(i, t+1) + C(i-1, t+1)}{\Delta x^2} \quad (6)$$

Rearranging terms in the above equation we get

$$C(i, t) = -K(C(i-1, t+1) + C(i+1, t+1)) + C(i, t+1)(1 + 2K) \text{ where } K = \frac{D\Delta t}{\Delta x^2} \quad (7)$$

The above equation can be written in the matrix form

$$\begin{aligned} [A][C]_i^{t+1} &= [C]_i^t \\ [C]_i^{t+1} &= [A]^{-1}[C]_i^t \end{aligned} \quad (8)$$

where A is given by

$$A = \begin{bmatrix} 1+2K & -K & \dots & \dots & 0 \\ -K & 1+2K & -K & \dots & 0 \\ 0 & -K & \ddots & \ddots & 0 \\ \dots & \dots & \ddots & \ddots & -K \\ \dots & \dots & \dots & -K & 1+2K \end{bmatrix} \quad (9)$$

Applying Neumann Boundary conditions the matrix A is modified to

$$A = \begin{bmatrix} 1+2K & -2K & \dots & \dots & 0 \\ -K & 1+2K & -K & \dots & 0 \\ 0 & -K & \ddots & \ddots & 0 \\ \dots & \dots & \ddots & \ddots & -K \\ \dots & \dots & \dots & -2K & 1+2K \end{bmatrix} \quad (10)$$

Eq. 8 is unconditionally stable thereby allowing us to choose Δx and Δt independent of each other

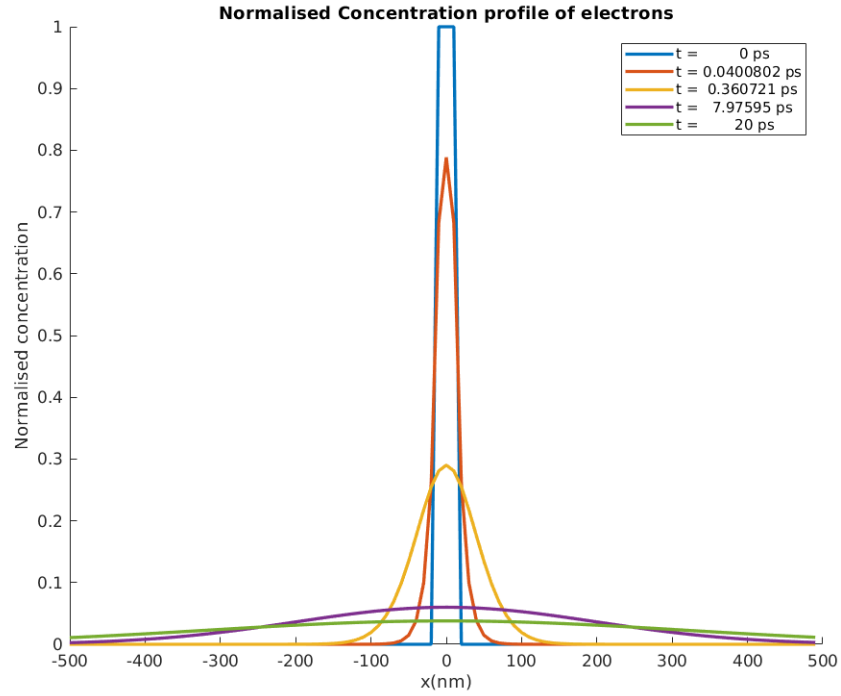


Figure 1: Simulated electron profile using Eq. 8, Normalised to initial electron dose of $N_o = 10^{19} \text{ cm}^{-3}$

Analytical diffusion profile, by assuming initial profile to be a delta function, is given by

$$C(x, t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(\frac{-x^2}{4Dt}\right) \quad (11)$$

where M is given by

$$M = \int_{-\infty}^{\infty} C(x, t) dx \quad (12)$$

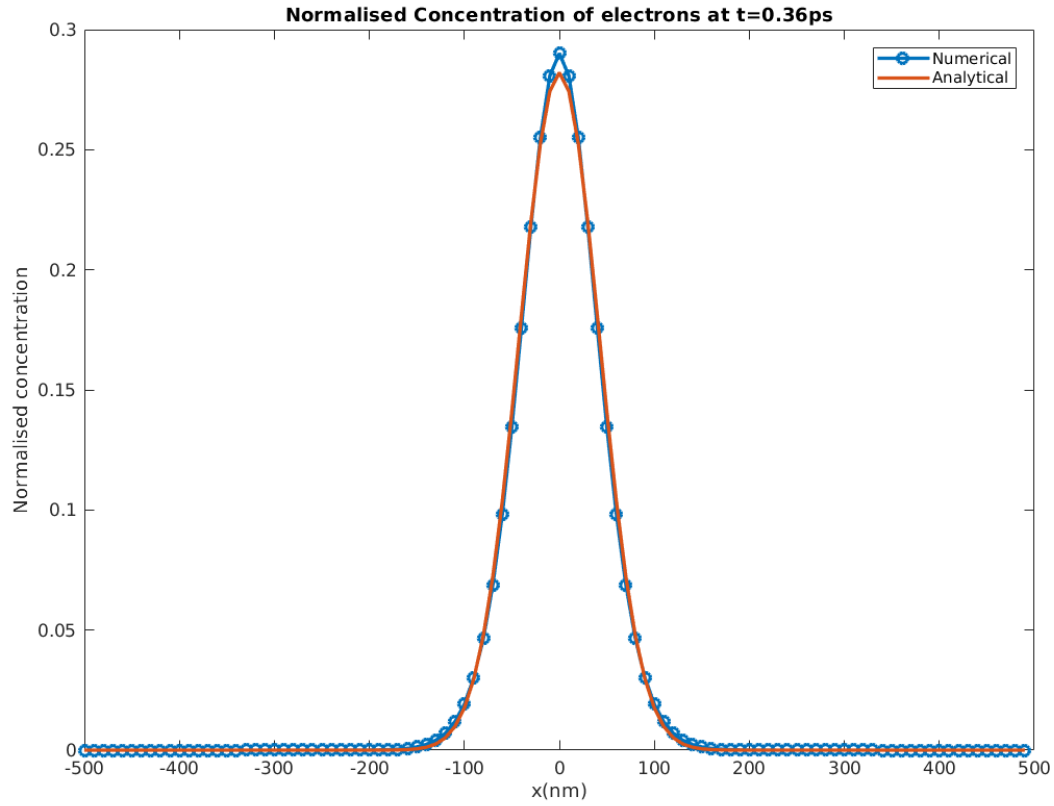


Figure 2: Comparison between analytical and simulated Diffusion profile at time $t = 0.36ps$

Form Fig. 2 it can be seen that the simulated and analytical profiles match