Q5

NUMERICAL SIMULATIONS OF POISSON'S EQUATION

a) Linearization of Poisson equation

We start with Poisson equation

$$\frac{d^2V}{dx^2} = -\frac{q}{\epsilon}(p-n+N_D-N_A) \quad (1) \quad \text{[Assuming complete ionization]}.$$

Here, $p = n_i e^{-\frac{qV}{KT}}$ and $n = n_i e^{qV/KT}$

We take $\frac{KT}{q} = V_T$. Also, $V = \frac{E_F - E_i}{KT}$.

$$\therefore (1) \Rightarrow \frac{d^2V}{dx^2} = -\frac{qn_i}{\epsilon}\left[e^{-V/V_T} - e^{V/V_T} + \frac{C}{n_i}\right], \text{ where } C = N_D - N_A.$$

To linearise, let us now assume $\boxed{V_{new} = V_{old} + \delta}$

$$\Rightarrow \frac{d^2V_{new}}{dx^2} = -\frac{qn_i}{\epsilon}\left[e^{-\frac{(V_{old}+\delta)}{V_T}} - e^{\frac{V_{old}+\delta}{V_T}} + \frac{C}{n_i}\right]$$

$$\Rightarrow \frac{d^2V_{new}}{dx^2} = -\frac{qn_i}{\epsilon}\left[e^{-\frac{V_{old}}{V_T}}\left(e^{-\delta/V_T}\right) - e^{\frac{V_{old}}{V_T}}\left(e^{\delta/V_T}\right) + \frac{C}{n_i}\right]$$

[For $\frac{\delta}{V_T} << 1$, we have $e^{-\delta/V_T} \approx 1 - \frac{\delta}{V_T}$ and so on]

$$\Rightarrow \frac{d^2V_{new}}{dx^2} = -\frac{qn_i}{\epsilon}\left[e^{-\frac{V_{old}}{V_T}}\left(1-\frac{\delta}{V_T}\right) - e^{\frac{V_{old}}{V_T}}\left(1+\frac{\delta}{V_T}\right) + \frac{C}{n_i}\right]$$

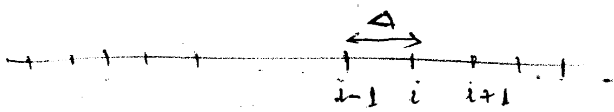
$$\Rightarrow \frac{d^2V_{new}}{dx^2} = -\frac{qn_i}{\epsilon}\left[e^{-\frac{V_{old}}{V_T}} - e^{V_{old}/V_T} + \frac{C}{n_i}\right] + \frac{q}{n_i}\left[e^{-\frac{V_{old}}{V_T}} + e^{\frac{V_{old}}{V_T}}\right]\frac{\delta}{V_T}.$$

Again, as $\delta = V_{new} - V_{old}$,

$$\Rightarrow \frac{d^2V_{new}}{dx^2} = -\frac{qn_i}{\epsilon}\left[e^{-\frac{V_{old}}{V_T}} - e^{\frac{V_{old}}{V_T}} + \frac{C}{n_i}\right] + \frac{q}{n_i}\left[e^{-\frac{V_{old}}{V_T}} + e^{\frac{V_{old}}{V_T}}\right] \cdot \left(\frac{V_{new}-V_{old}}{V_T}\right)$$

$$\Rightarrow \boxed{\frac{d^2V_{new}}{dx^2} - \frac{qn_i}{\epsilon V_T}\left(e^{-\frac{V_{old}}{V_T}} + e^{\frac{V_{old}}{V_T}}\right)V_{new} = -\frac{qn_i}{\epsilon}\left[e^{-\frac{V_{old}}{V_T}} - e^{\frac{V_{old}}{V_T}} + \frac{C}{n_i}\right] - \frac{qn_i}{\epsilon V_T}\left(e^{-\frac{V_{old}}{V_T}} + e^{\frac{V_{old}}{V_T}}\right)V_{old}.} \qquad (2)$$

To proceed further, if



If Δ be the seperation between two mesh points, then

$$\frac{dV^{i}_{new}}{dx} = \frac{V^{i+1}_{new} - V^{i}_{new}}{\Delta}$$

$$\Rightarrow \frac{d^2 V^{i+1}_{new}}{dx^2} = \frac{d}{dx}\left(\frac{dV^{i+1}_{new}}{dx}\right) = \frac{d}{dx}\left(\frac{V^{i+1}_{new} - V^{i}_{new}}{\Delta}\right)$$

$$= \frac{\frac{V^{i+1}_{new} - V^{i}_{new}}{\Delta} - \frac{V^{i}_{new} - V^{i-1}_{new}}{\Delta}}{\Delta}$$

$$= \frac{V^{i+1}_{new} - 2V^{i}_{new} + V^{i-1}_{new}}{\Delta^2}$$

$$\frac{d}{dx}\left(\frac{dV_{new}}{dx}\right)_{at\ i} = \frac{\left(\frac{dV_{new}}{dx}\right)_{i+1/2} - \left(\frac{dV_{new}}{dx}\right)_{i-1/2}}{\Delta}$$

$$= \frac{V^{i+1}_{new} - 2V^{i}_{new} + V^{i-1}_{new}}{\Delta^2}$$

FINITE DIFFERENCE DISCRETIZATION (of 1D Poisson)

Now using (2) further to take out the matrix elements, we have -

$$\boxed{\frac{V^{i+1}_{new} - 2V^{i}_{new} + V^{i-1}_{new}}{\Delta^2} - \frac{qn_i}{V_T}\left(e^{-\frac{V^{i}_{old}}{V_T}} + e^{\frac{V^{i}_{old}}{V_T}}\right)V^{i}_{new} = -\frac{qn_i}{\epsilon}\left[e^{-\frac{V^{i}_{old}}{V_T}} - e^{\frac{V^{i}_{old}}{V_T}} + \frac{C}{n_i}\right] - \frac{qn_i}{\epsilon V_T}\left[e^{-\frac{V^{i}_{old}}{V_T}} + e^{\frac{V^{i}_{old}}{V_T}}\right]V^{i}_{old}.} \qquad (3)$$

b) LU decomposition:-

We know, in a lower-upper (LU) decomposition, we can write a matrix as a product of a lower triangular and an upper triangular matrix.

If LU decomposition exists, then we can write -

$$\begin{bmatrix} a_1 & c_1 & & & \\ b_2 & a_2 & c_2 & & \\ & \cdots & & & \\ & & b_{n-1} & a_{n-1} & c_{n-1} \\ & & & b_n & a_n \end{bmatrix} = \begin{bmatrix} 1 & & & & \\ \beta_2 & 1 & & & \\ & \beta_3 & & & \\ & & \cdots & & \\ & & & \beta_n & 1 \end{bmatrix} \begin{bmatrix} \alpha_1 & c_1 & & & \\ & \alpha_2 & c_2 & & \\ & & \cdots & & \\ & & & \cdots & c_{n-1} \\ & & & & \alpha_n \end{bmatrix}$$

Where, $\boxed{a_1 = \alpha_1}$, $\boxed{a_2 = \beta_2 c_1 + \alpha_2}$ $\boxed{b_2 = \alpha_1 \beta_2}$

$\therefore \beta_2 = \frac{b_2}{\alpha_1} = \frac{b_2}{a_1}$ and $a_2 = \beta_2 c_1 + \alpha_2$

$$\Rightarrow a_2 = \frac{b_2}{a_1} c_1 + \alpha_2$$

$$\Rightarrow \alpha_2 = a_2 - \frac{b_2}{a_1} c_1 .$$

In general,

$$\boxed{\beta_K = \frac{b_k}{\alpha_{K-1}}} \quad \text{and} \quad \boxed{\alpha_K = a_K - \frac{b_k}{\alpha_{K-1}} c_k} \quad \frac{(K \in N)}{(K \neq 1)}$$

For linearised Poisson equation,

We rewrite equation (3) as

$b_i V_{i+1} + a_i V_i + c_i V_{i-1} = F$ [b_i, a_i and c_i are constants

F = left side function].

In matrix form, we have

$$[A][V] = [F]$$

More specifically, using notations of "new" and "old", we have -

$$[A][V_{new}] = [F_{old}]$$

As, A can be expressed in LU decomposition,

$[A] = [L][U]$ $\quad$ L = lower triangular matrix

U = Upper Triangular matrix.

$$\therefore \quad [L][U][V_{new}] = [F_{old}] \qquad \{[V_{new}] = [V] \text{ also}\}$$

(We represent F_{old} as F)

We take $[U][V_{new}] = [y]$

$$\Rightarrow \quad [L][y] = [F] \quad \text{——— (4)}$$

$$\Rightarrow \begin{bmatrix} 1 & & & & \\ \beta_2 & 1 & & & \\ & \beta_3 & \ddots & & \\ & & & \beta_n & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_n \end{bmatrix}$$

$$\Rightarrow \boxed{y_1 = F_1} \qquad \beta_2 y_1 + y_2 = F_2 \Rightarrow y_2 = F_2 - \beta_2 y_1$$

$$\boxed{\Rightarrow y_2 = F_2 - \beta_2 F_1}$$

In general, $\boxed{y_n = F_n - \beta_n y_{n-1}}$ (Recursive relation) (5)

Using (4),

$$\begin{bmatrix} \alpha_1 & c_1 & & \\ & \alpha_2 & c_2 & \\ & & \ddots & c_{n-1} \\ & & & \alpha_n \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \\ \vdots \\ V_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

$$\Rightarrow \quad \alpha_n V_n = y_n \quad \boxed{V_n = y_n/\alpha_n} \Rightarrow \boxed{V_n = \frac{F_n - \beta_n y_{n-1}}{\alpha_n}} \text{ — (6)}$$

(using 5)

$$\alpha_{n-1} V_{n-1} + V_n c_{n-1} = y_{n-1}$$

$$\boxed{\Rightarrow \quad V_{n-1} = \frac{y_{n-1} - \frac{y_n}{\alpha_n} c_{n-1}}{\alpha_{n-1}}} \text{ — (7)}$$

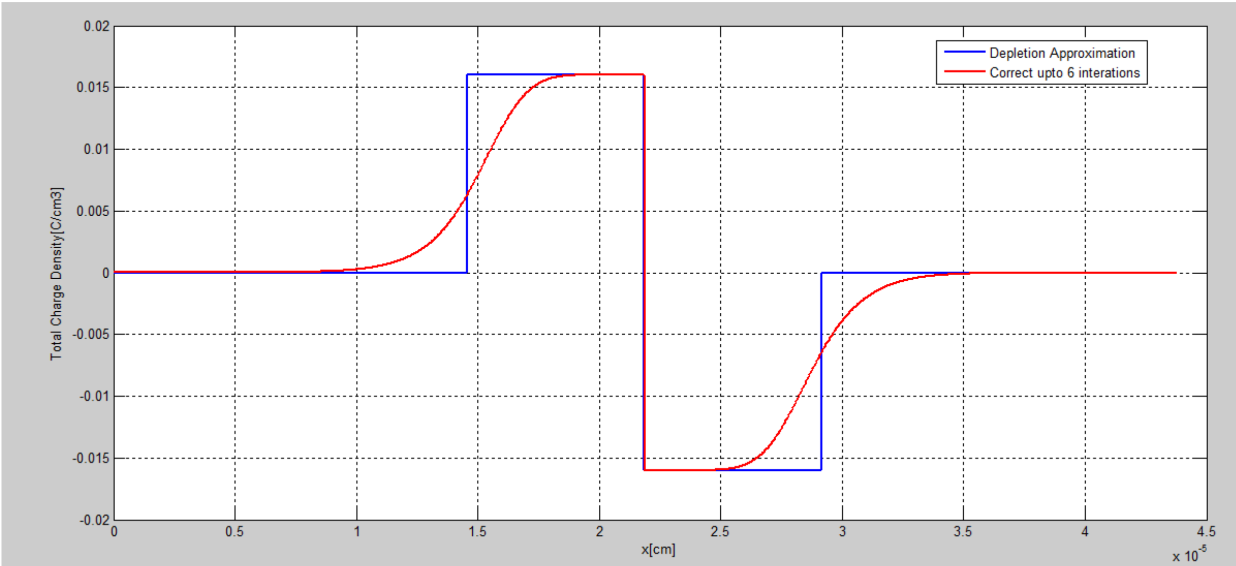
Solving (6) & (7),

$$V_{n-1} \cdot \alpha_{n-1} = \frac{F_n - V_n \alpha_n}{\beta_n} - \frac{F_n - \beta_n y_{n-1}}{\alpha_n} c_{n-1}$$

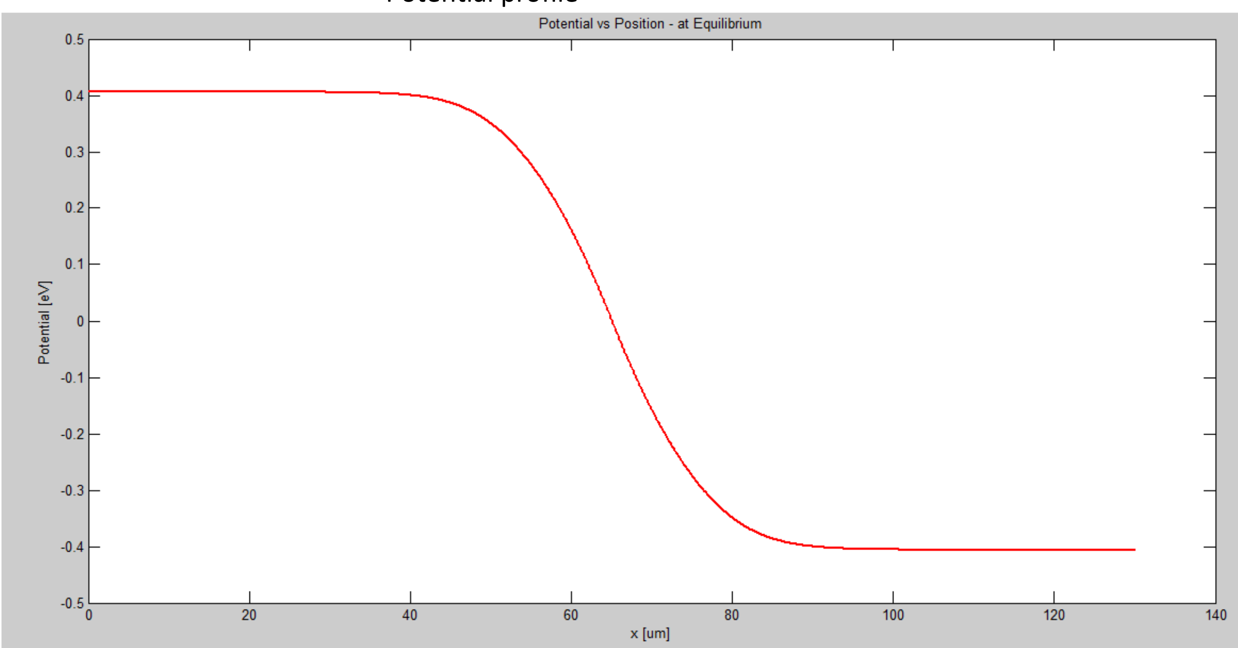
$$\Rightarrow V_{n-1} \cdot \alpha_{n-1} = \frac{F_n}{\beta_n} - \frac{F_n}{\alpha_n} - \frac{V_n \alpha_n}{\beta_n} + \frac{\cancel{\beta_n}}{\alpha_n} \frac{(-V_n \alpha_n + F_n)}{\cancel{\beta_n}} c_{n-1}$$

$$\boxed{\Rightarrow \quad V_{n-1} \cdot \alpha_{n-1} = \frac{F_n - V_n \alpha_n}{\beta_n} - \frac{F_n (1 - c_{n-1})}{\alpha_n} + c_{n-1}}$$

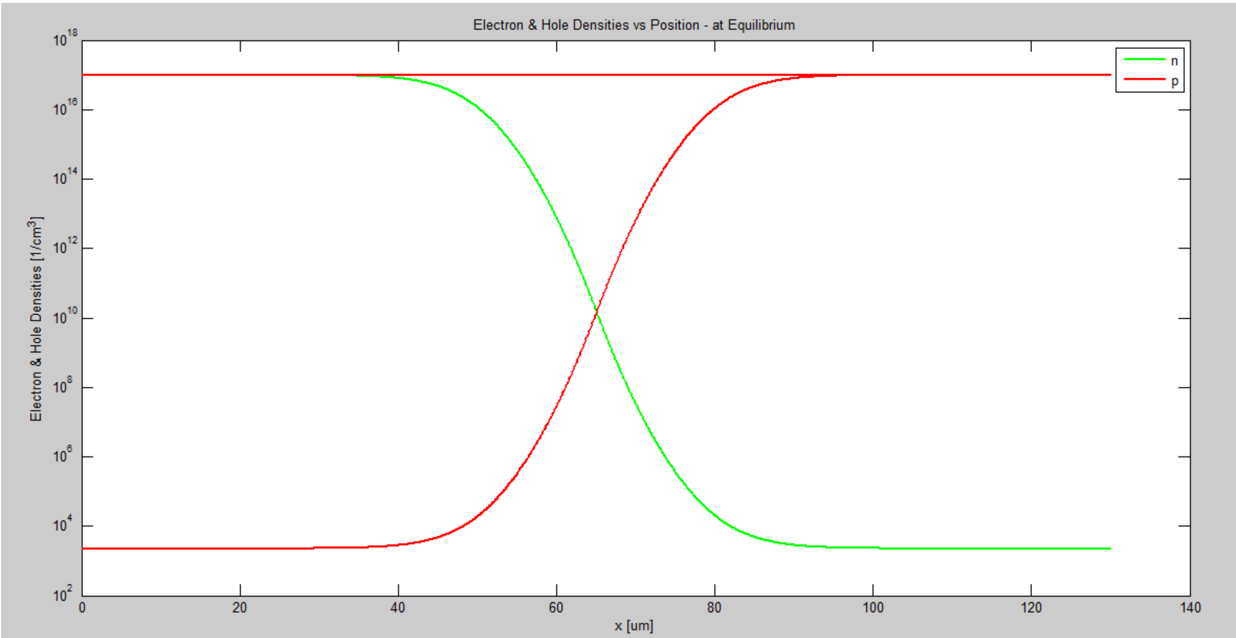
5(c.1) Charge density profile



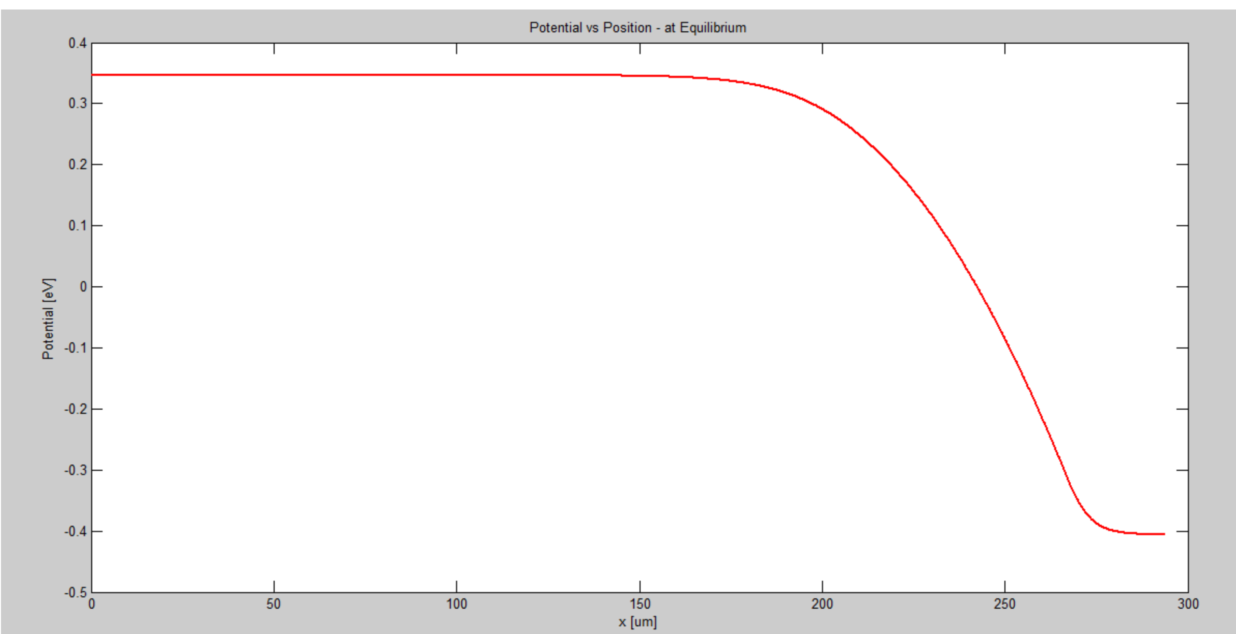
Potential profile



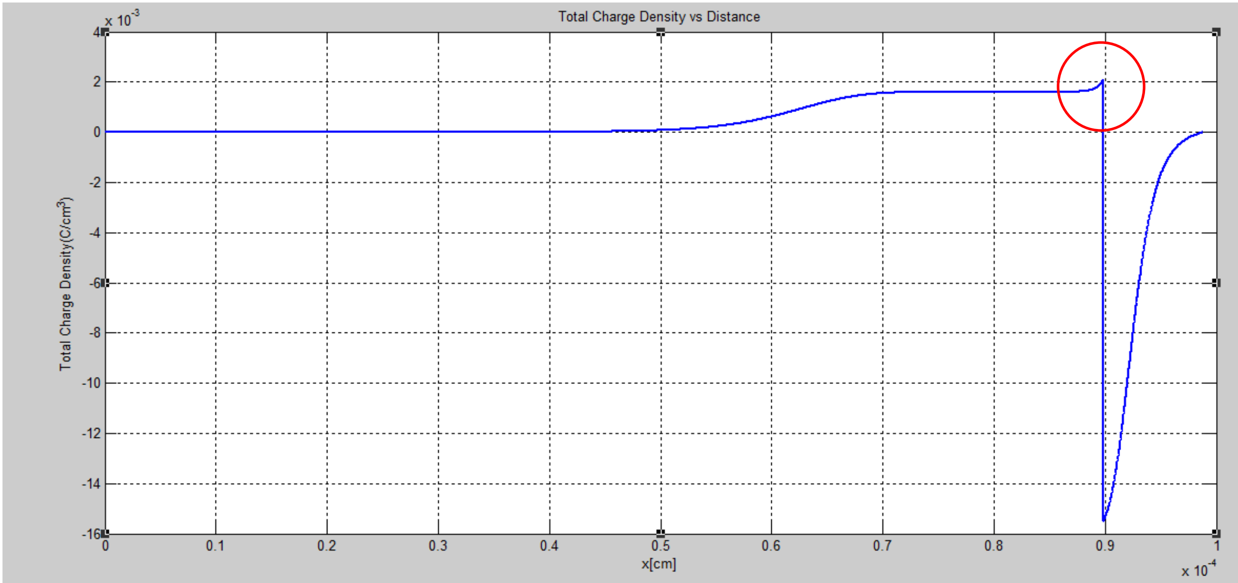
n and p profiles



5(c.2) Potential profile



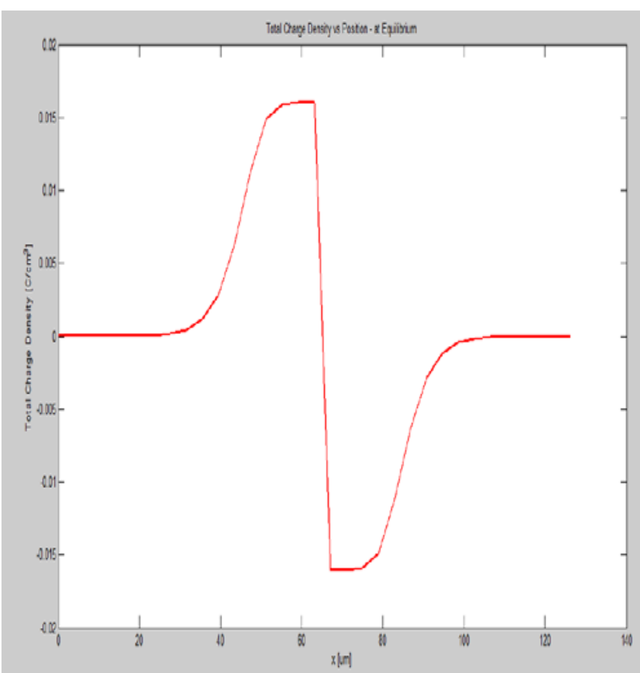
Charge density profile



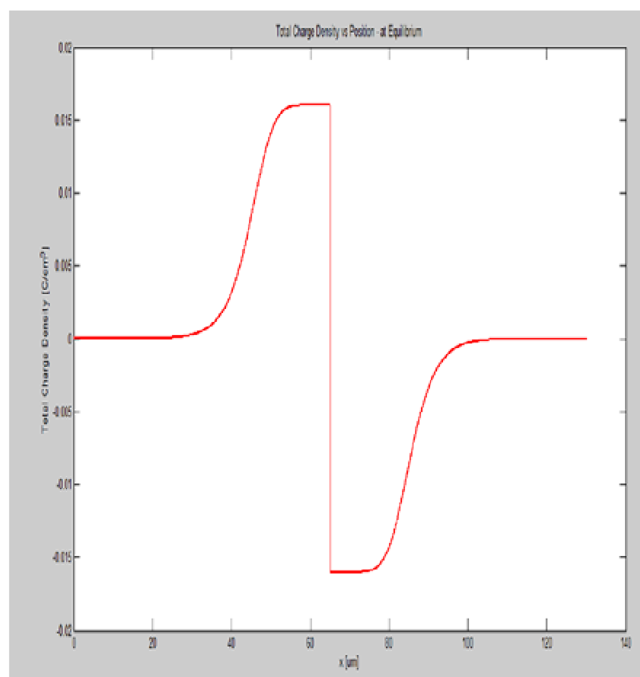
The notch is observed due to the high charge density in the p region (The free carrier concentration exceeds the depletion approximation)

5 (c.4) MESHING (Uniform meshing approximation)

LOW MESHING

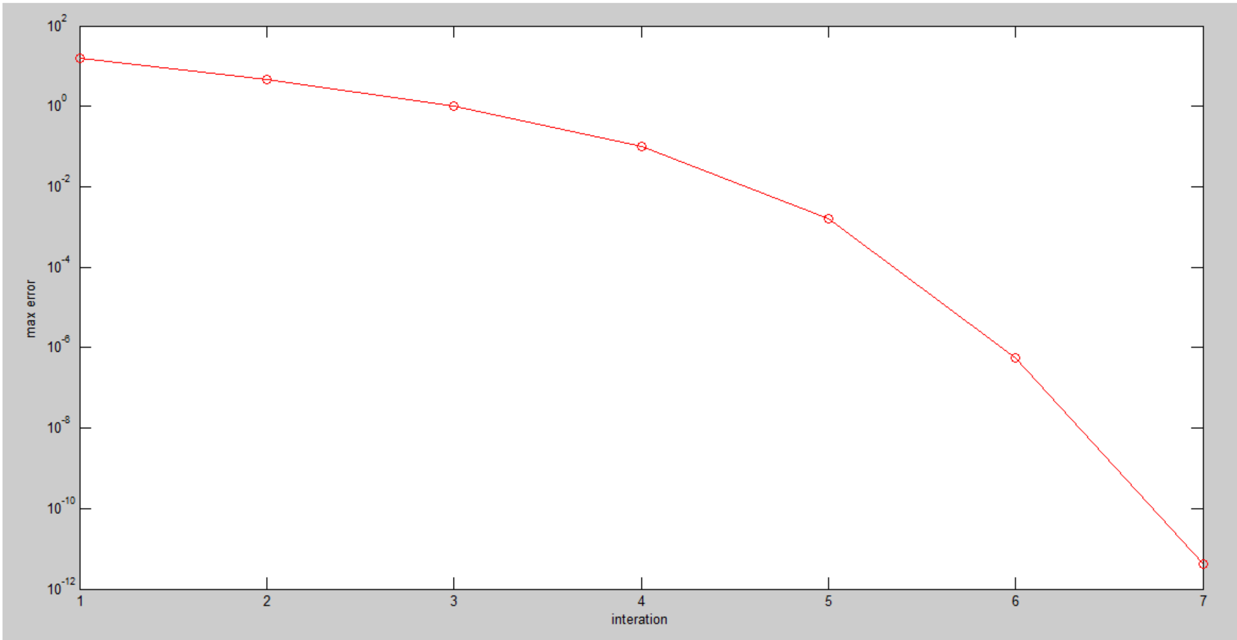


HIGH MESHING



Less meshing implies more sharp transitions. Therefore in regions such as depletion region increasing no. of meshing points should be more beneficial.

5 (c.5) Maximum error vs Meshing



5(c.6)

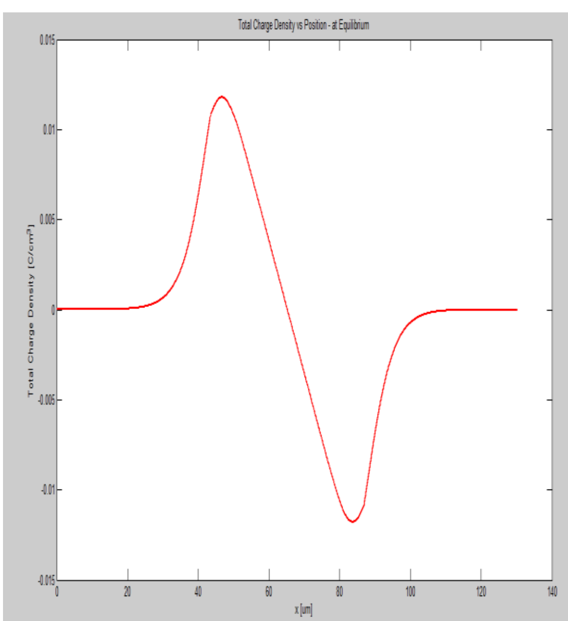
Initial guess would give an idea about the number of iterations that would be involved to arrive at the final solution. For e.g: Instead of the step function potential that we have used here, our initial guess could be a flat potential profile with steps at edges.

In such case, only the number of iterations would

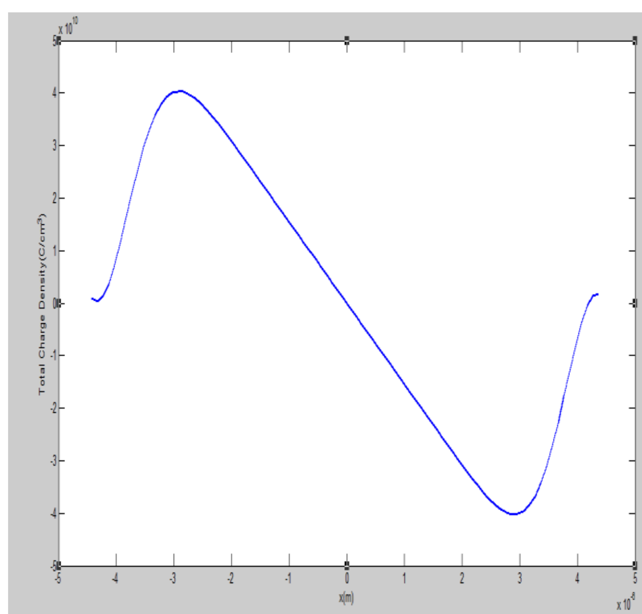
Increase but finally we will arrive at the same solution.

5(c.7) Charge density profile

Numerical simulation

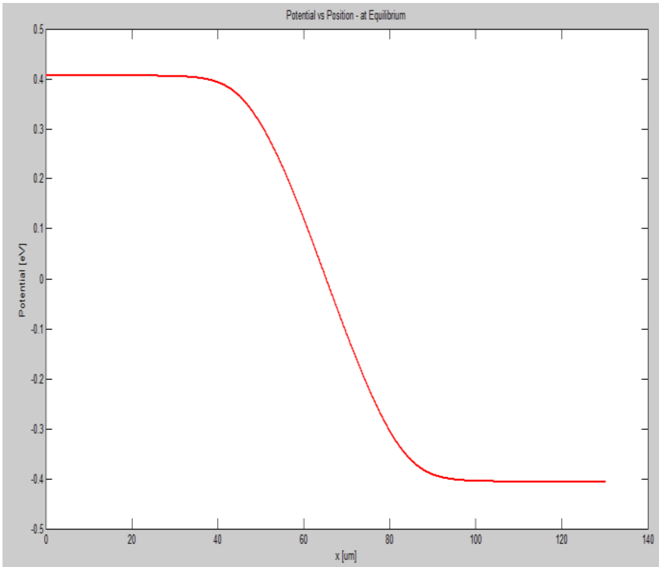


Analytical solution

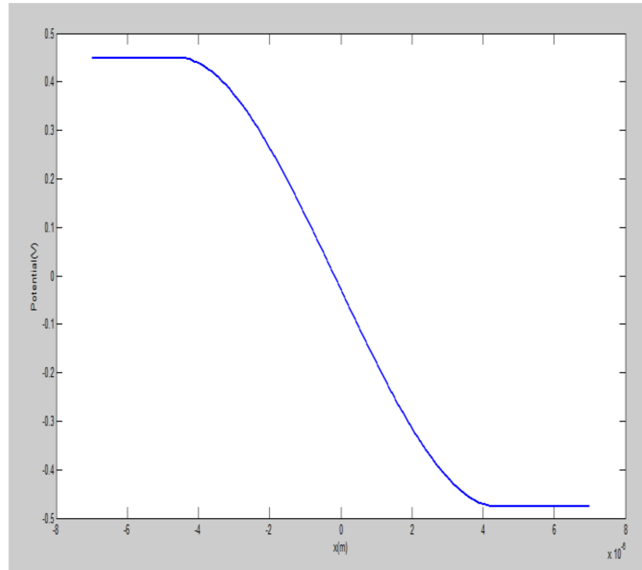


7.for a) Potential profile

Numerical



Analytical



Doping in p-region	Barrier Height
1E15	0.69
1E16	0.75
1E17	0.81
1E18	0.87
1E19	0.93
1E20	1 (approx.)

Since most of you have done this considering ques.2, so we are posting the solution considering ques.2 itself. You can also try with ques 3.a) and 3.b) as this has already been explained in class.