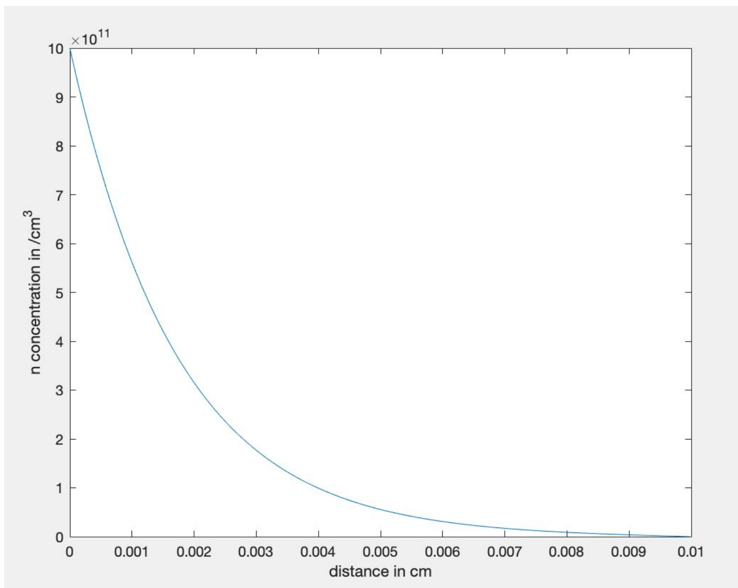
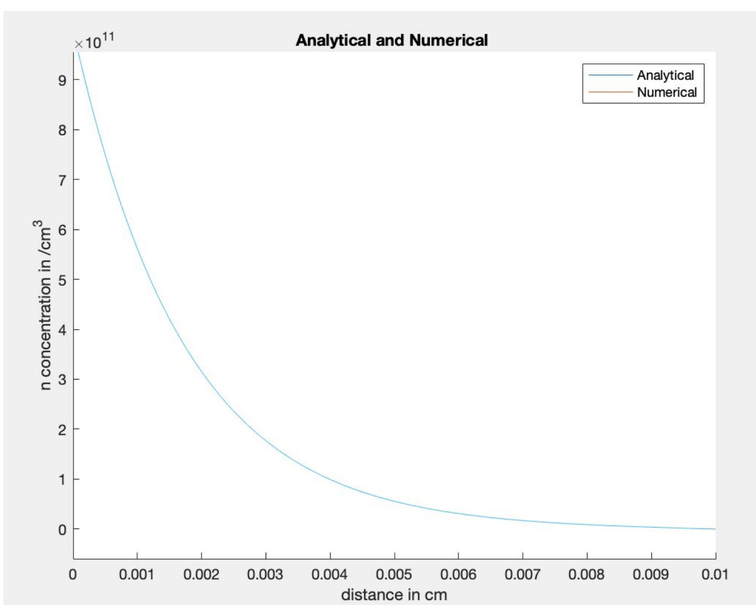
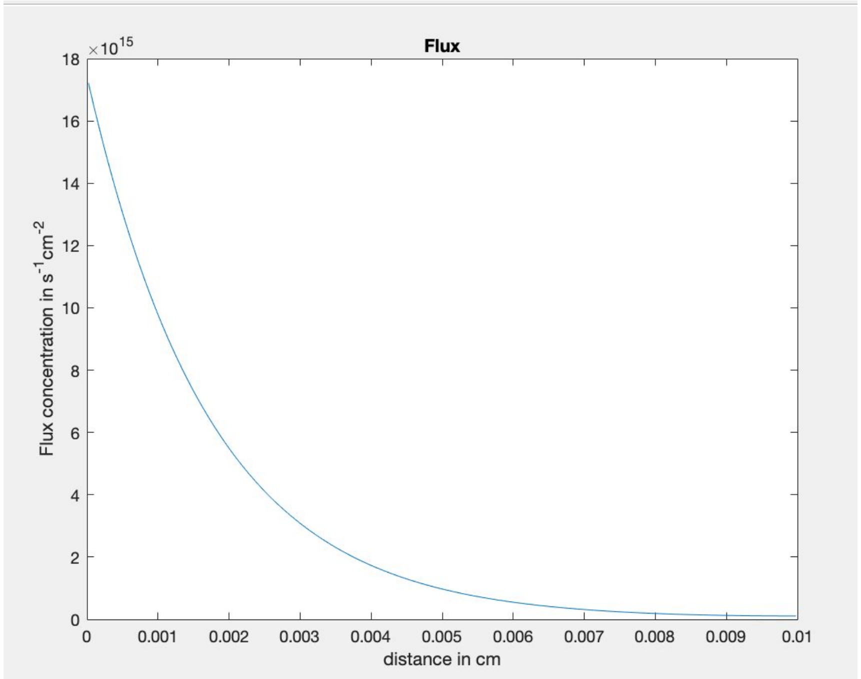
Assignment – 4

Numerical solution of steady state continuity equation: For each of the cases listed below, provide analytical solutions and compare with numerical results, if possible. Assume D=30cm2/s, unless otherwise stated. Use $D\frac{d^2n}{dx^2} = \frac{n}{\tau}$

a. Consider diffusive transport of particles from point A to point B and the separation between these points being 100μm. The concentration of particles at A is n=10+, cm-3, and at B is n=0cm-3. Assume τ=10-7 s. Find the particle profile from A to B. What is the particle flux from A to B?



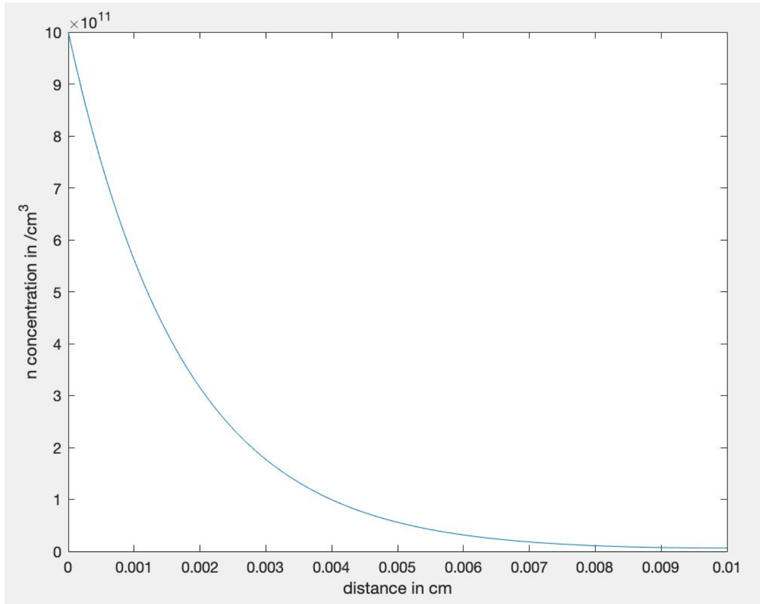


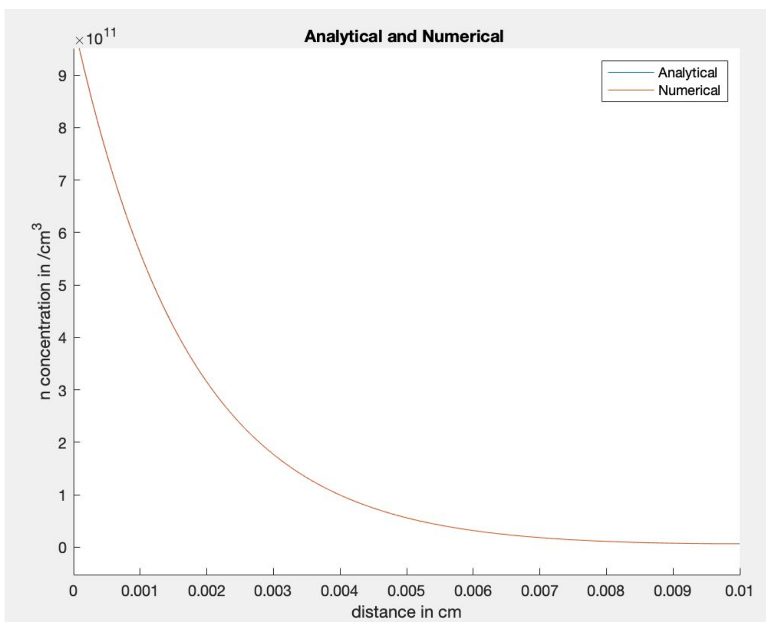


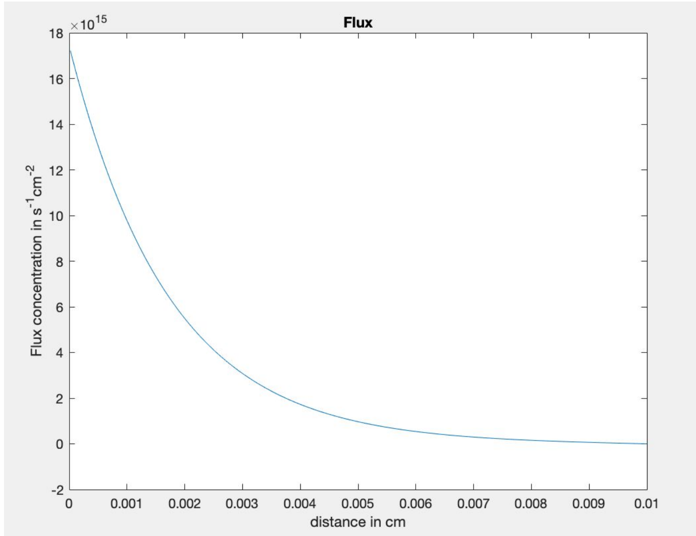
We can see that the analytical and the numerical solution is very close to each other.
Numerical calculation
I divided the x axis in m points with equal spacing h. Each point will have a unique concentration (n) which solve the given differential equation. This can be interpreted as system of linear equation and can be represented as AX=B. We can solve by just taking A inverse.

$$C(x) = -9.66 * 10^6 * e^{\frac{x}{\sqrt{D\tau}}} + 10^{12} * e^{\frac{-x}{\sqrt{D\tau}}}\ cm^{-3}$$

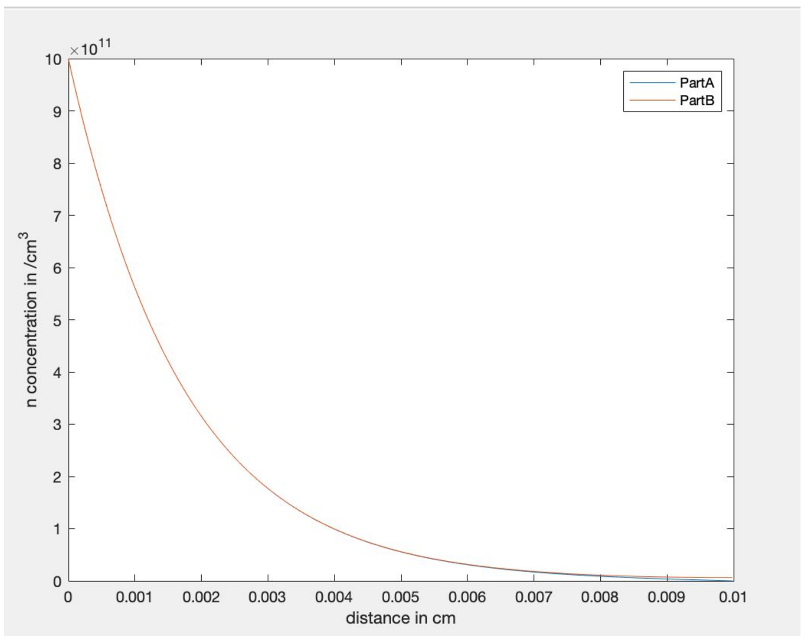
b. For the configuration in part (a), assume that the boundary condition at B is such that $J = kn$, where J is the particle flux (outgoing), k = 10^3 cm/s, and n is the particle density. Assume τ=10-7 s Find the particle profile from A to B and the particle flux at B. Explore the implications of this change in boundary conditions at B.


×10^11
n concentration in /cm^3
distance in cm


Analytical and Numerical
×10^11
Analytical
Numerical
n concentration in /cm^3
distance in cm



Flux at A = 1.7*10^16 cm^-2 s-1
Flux at B = 1.2*10^12 cm^-2 s-1



We can concentration of particle at point B when we add flux at that point.
Particle concentration at point B = 6.3303e+09 cm^-3 (Part B)
Particle concentration at point B =0 (Part A)

0.04×10 9×10

Q1a $C(x) = Ae^{\frac{x}{\sqrt{DT}}} + B^{\frac{-x}{\sqrt{DT}}}$

BC1 $C(0) = 10^{12}\ cm^{-3}$

$A + B = 10^{12}\ cm^{-3}$ — ①

BC2

$C(100\times10^{-4}) = 0$

$A = -B\ e^{\frac{-2\times100\times10^{-4}}{\sqrt{DT}}}$ — ②

from 1 & 2 $\cancel{A=}$

$A = -9.6648\times10^{6}\ cm^{-3}$
$B = 1.0\times10^{12}\ cm^{-3}$

Q2b = $C(x) = Ae^{x/\sqrt{DT}} + Be^{-x/\sqrt{DT}}$

BC1 $C(0) = 10^{12}$

$A + B = 10^{12}\ cm^{-3}$

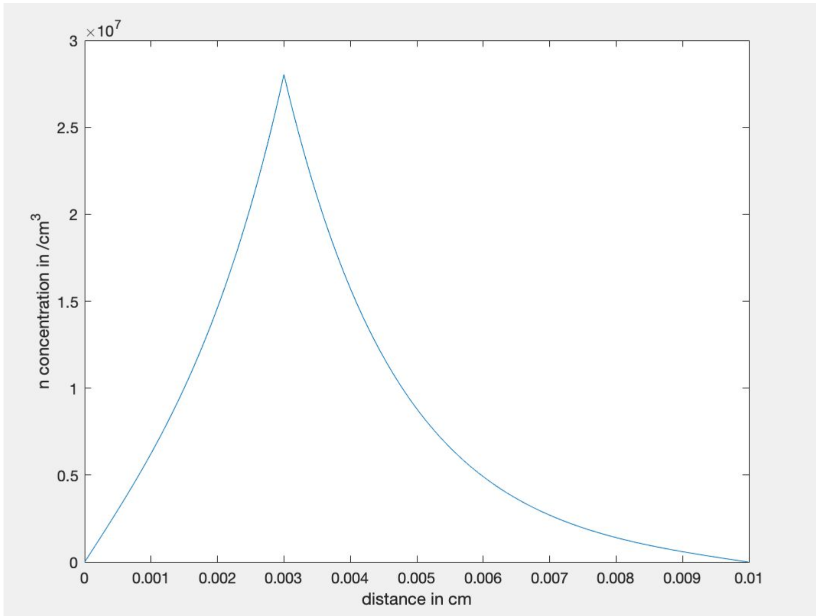
BC2

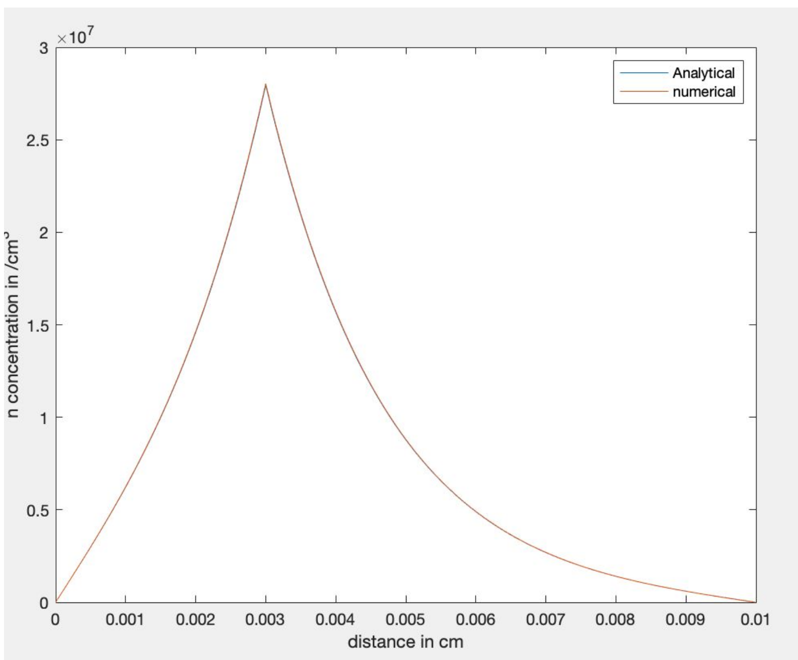
$J = kn_D = \frac{D}{\sqrt{D\tau}}\left(Ae^{\frac{x}{\sqrt{DT}}} - Be^{\frac{-x}{\sqrt{DT}}}\right)\Big|_{x=10}$

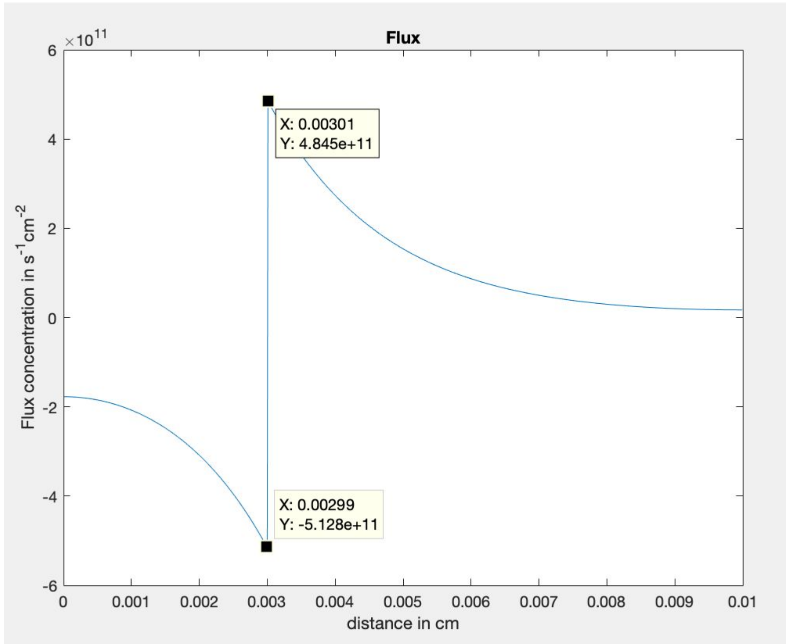
$A = 8.61\times10^{6}\ cm^{-3}$
$B = 9.99\times10^{11}\ cm^{-3}$

$$C(x) = 8.61 * 10^7 * e^{\frac{x}{\sqrt{D\tau}}} + 9.99 * 10^{11} * e^{\frac{-x}{\sqrt{D\tau}}} cm^{-3}$$

c. For the configuration in part (a), assume that a particle flux is introduced at x=30um at the rate of 10^12 cm-2 /s. Assume that the particle density at A and B are held constant at n=0 and τ = 10-7 s. Find the particle profile from A to B, and the flux at A and B.







Flux at A = -1.77*10^11 cm^-2 s-1
Flux at B = 1.71*10^10 cm^-2 s-1

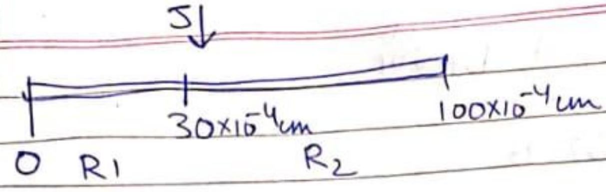
When $0 < x < 30 * 10^{-4}\ cm^{-3}$ **:**

$$C(x) = 5.105 * 10^{6} * e^{\frac{x}{\sqrt{D\tau}}} - 5.105 * 10^{6} * e^{\frac{-x}{\sqrt{D\tau}}} cm^{-3}$$

When $30 * 10^{-4}\ cm^{-3} < x < 100 * 10^{-4}\ cm^{-3}$ **:**

$$C(x) = -1.52 * 10^{3} * e^{\frac{x}{\sqrt{D\tau}}} + 1.58 * 10^{8} * e^{\frac{-x}{\sqrt{D\tau}}} cm^{-3}$$

Q1.C



$R_1 = x : 0 < x < 30\times10^{-4}$ cm

$$C(x) = A e^{+\frac{x}{\sqrt{D\tau}}} + B e^{-\frac{x}{\sqrt{D\tau}}}$$

R_2 $30\times10^{-4} < x < 100\times10^{-4}$

$$C(x) = C\, e^{+\frac{x}{\sqrt{DT}}} + D e^{-\frac{x}{\sqrt{DT}}}$$

BC (1)

$$C(0) = 0 \Rightarrow A = -B$$

BC (2)

$$C(100\times10^{-4}) = 0 \Rightarrow D = \frac{C\, e^{\frac{100\times10^{-4}}{\sqrt{DT}}}}{e^{-\frac{100\times10^{-4}}{\sqrt{DT}}}}$$

$$D = -1.0347\times10^{5}\times C$$

BC (3)

$$C^{-}(30\times10^{-4}) = C^{+}(30\times10^{-4})$$

$$A\left[e^{\frac{x}{\sqrt{DT}}} - e^{-\frac{x}{\sqrt{DT}}}\right]_{\text{At } x = 30\times10^{-4}} = C\left[e^{\frac{x}{\sqrt{DT}}} - 1.03\times10^{5}\, e^{-\frac{x}{\sqrt{DT}}}\right]$$

$$A = -2.992\times10^{-4}\times C$$

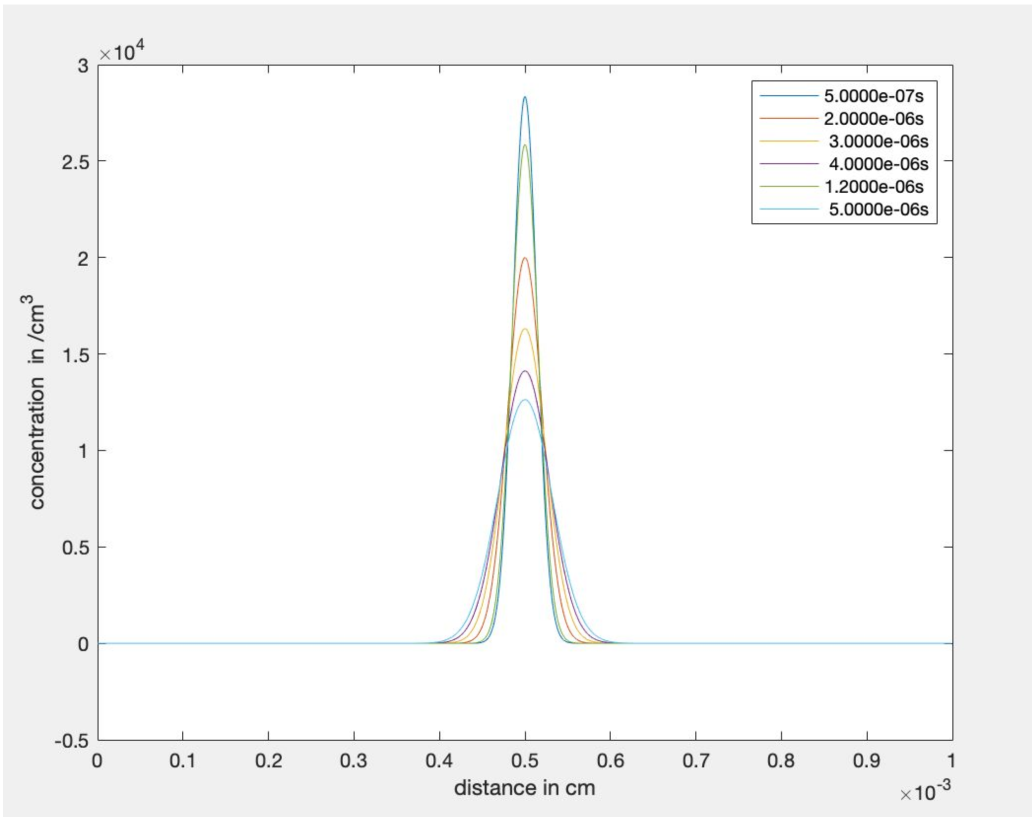
BC 4

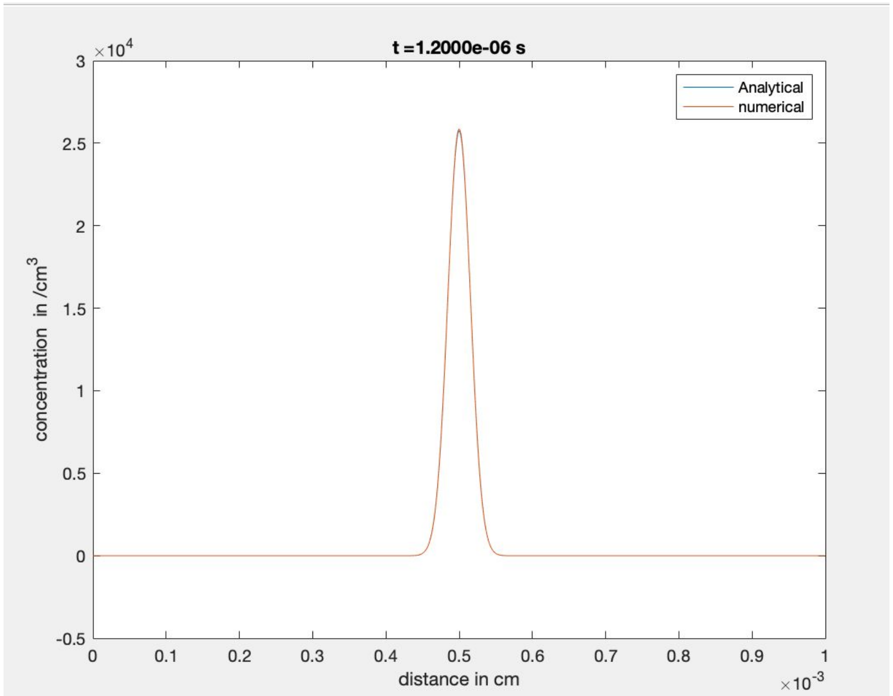
$$-D\left[\left.\frac{dC}{dx}\right|^{R_2}_{x=30\times10^{-4}} - \left.\frac{dC}{dx}\right|^{R_1}_{x=30\times10^{-4}}\right] = 10^{12}$$

$$\frac{A}{\sqrt{D\tau}}\left[e^{\frac{30\times10^{-4}}{\sqrt{DT}}} + e^{\frac{-30\times10^{-4}}{\sqrt{DT}}} - (-2.992\times10^{-4})\left(e^{\frac{30\times10^{-4}}{\sqrt{DT}}} + 1.034 e^{-30}\right.\right.$$

$$\boxed{A = 5.105\times10^{6}\ cm^{-3}} \quad = 10^{12}$$

2 Consider a region of length 10 μm. Assume perfectly absorbing boundary conditions at x=0 and x=10, at time t = 0, assume that particles are injected at x=5μm such that the density is 10^6 cm^{-3} (i.e., the injection is a delta function in both space and time). Using the formalism described, plot the evolution of particle density over the specified domain (use D = 10^{-4} cm^2 /s). Compare with analytical results. Explore the significance of the parameter $\sqrt{Dt}$.





Numerical solution : Now the concentration will change with time as well as in x direction. We need to satisfy Courant–Friedrichs–Lewy (CFL) condition. Thus

$$p = \frac{h*h}{2*D}$$

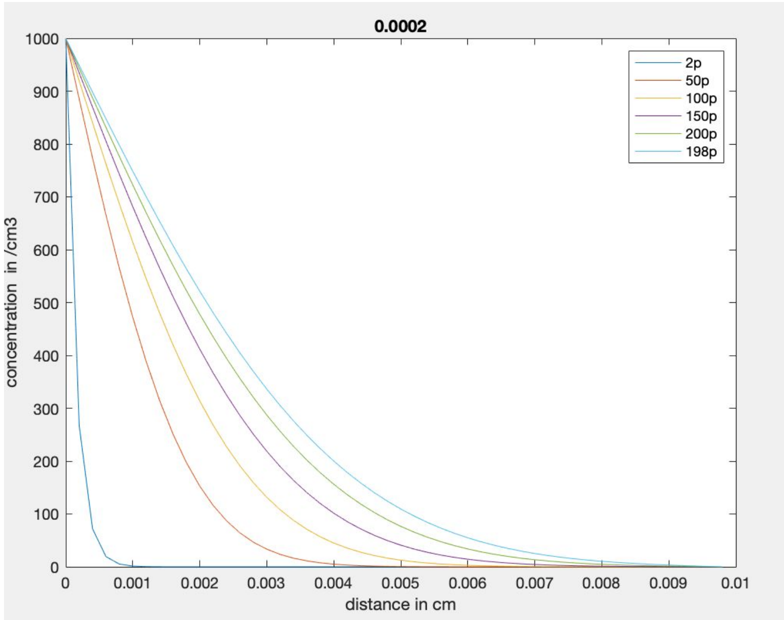
We are applying S *δ(x,t) at t = 0. We know that the integral of δ(x,t) direc function is 1. But in numerical analysis we are applying the source for one step i.e for h. Thus we have to apply S/h for the first iteration so that its integral is S which would have been same in case we applied S *δ(x,t)

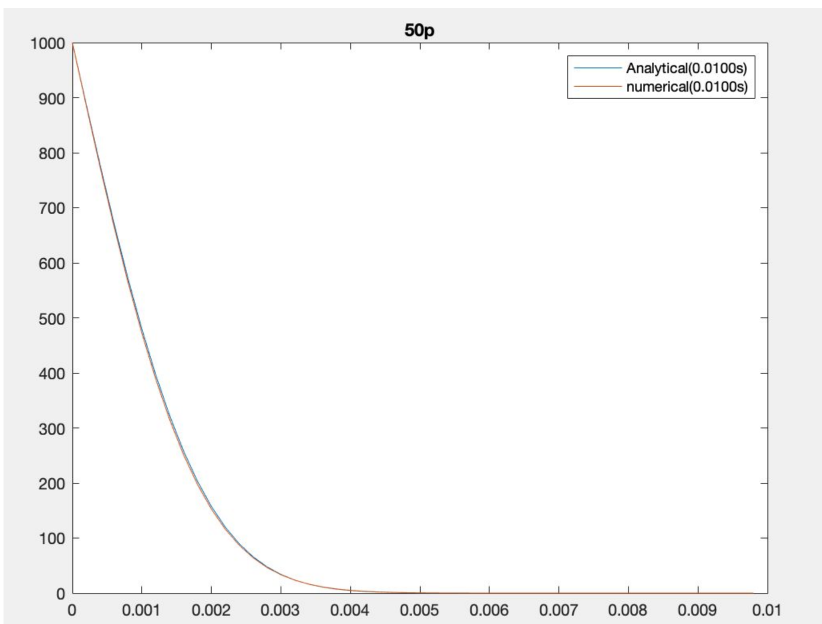
At any time τ0 the doping concentration across the x axis can be found by solving a system of linear equation AX=B where A is 1000* 1000 matrix Xis the concentration and B depends on concentration at time= τ0 - p.

The sqrt(D*t) term signifies the variance of the particle distribution.

$$C(x,t) = \frac{M}{(4\pi Dt)^{0.5}} * exp(-(X-X')^2/4Dt)$$

3 Consider a region of length 100um. Assume that the region is devoid of any particles at time t=0. Also assume perfectly absorbing boundary condition at x=100um. Solve for the diffusion of particles from the side x=0 as a function of time under the assumption that n(x=0,t)=1000. Plot the space and temporal evolution of the particle density profile. (Note that this scenario is very similar to doping of a semiconductor to form a PN junction diode). Compare the numerical solution with the analytical solution

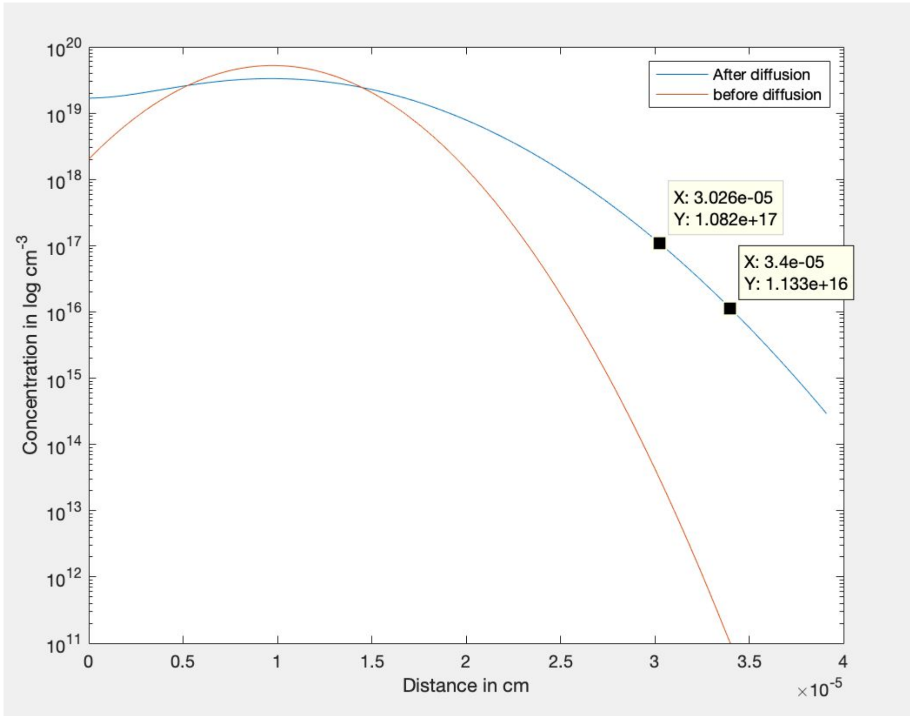


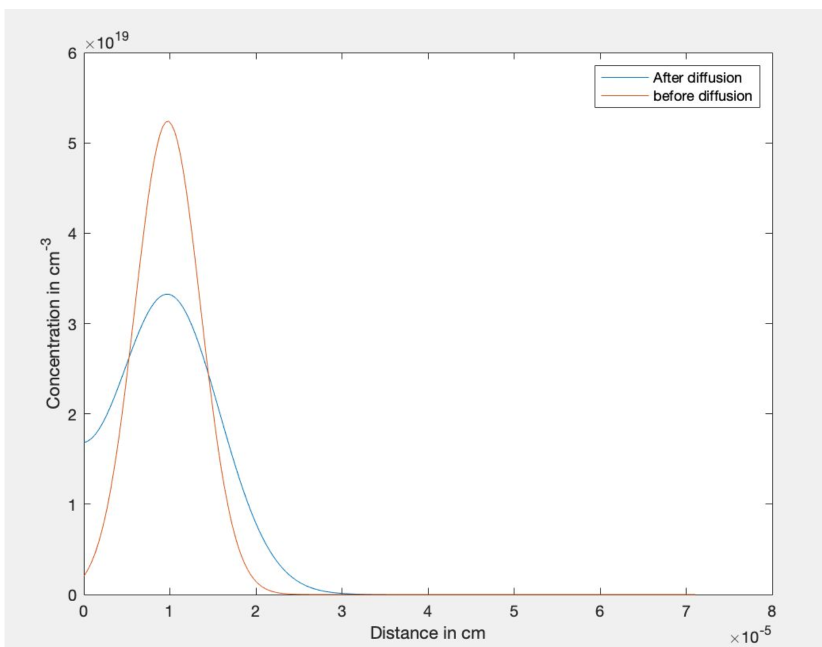


P = 0.0002s

$$C(x,t) \quad = M * (erf(\frac{x}{(4Dt)^{0.5}}) \ + 1)$$

Q4.





Time taken = 205.1128s
D = 5.3541e-14 cm^2
T = 1027 C
Roll off = 4.0800e-06 cm/dec
Thermal Budget : 1.0982e-11 s cm^2