EE 735: ASSIGNMENT 4 REPORT

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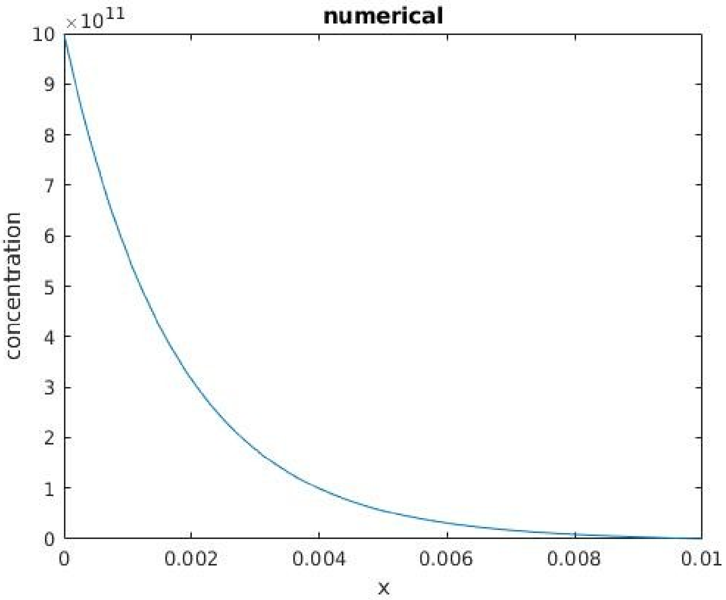
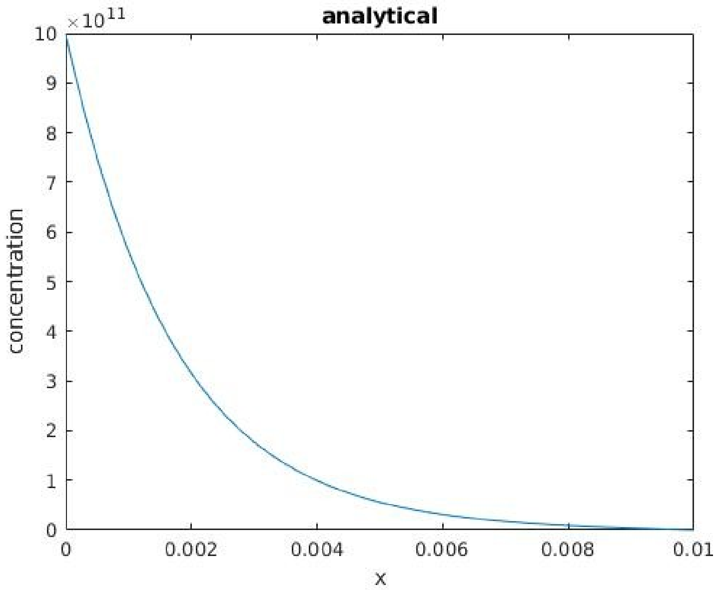
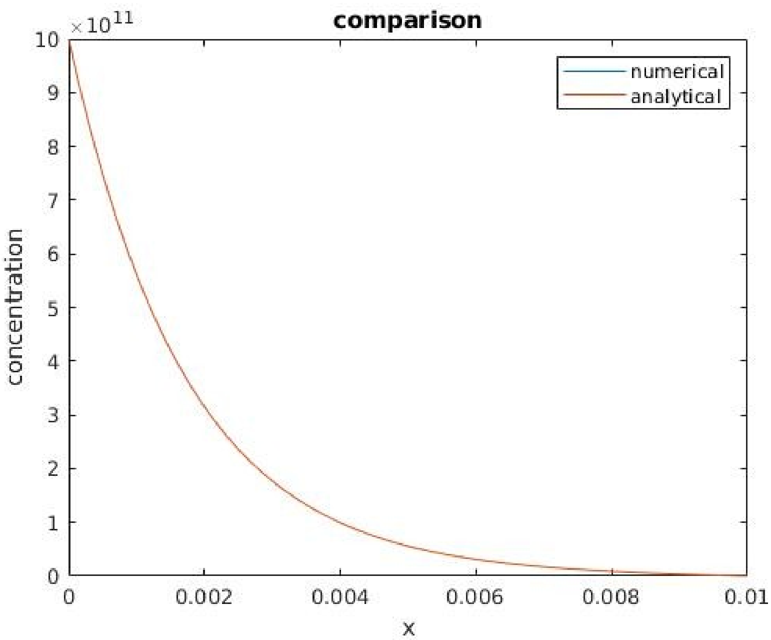
Note: Analytical solutions of all problems are at end. All concentrations (meaning density) are in cm^{-3} and x is in cm in plots.

Q1 a)



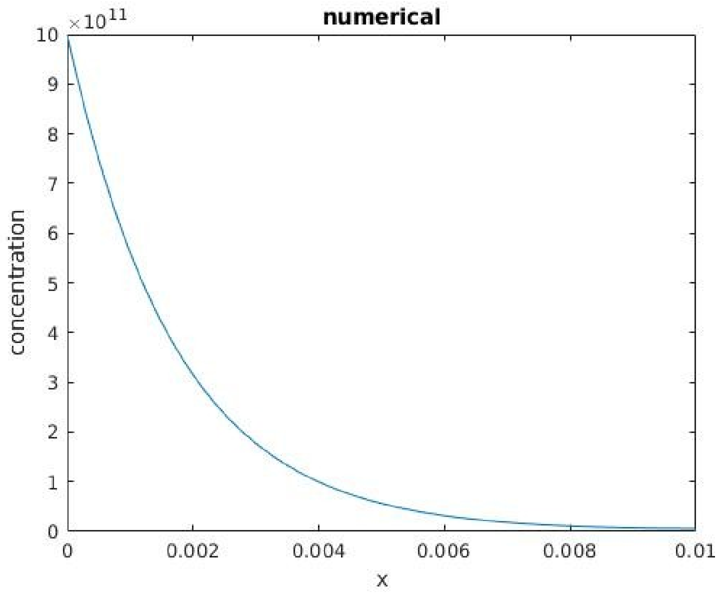


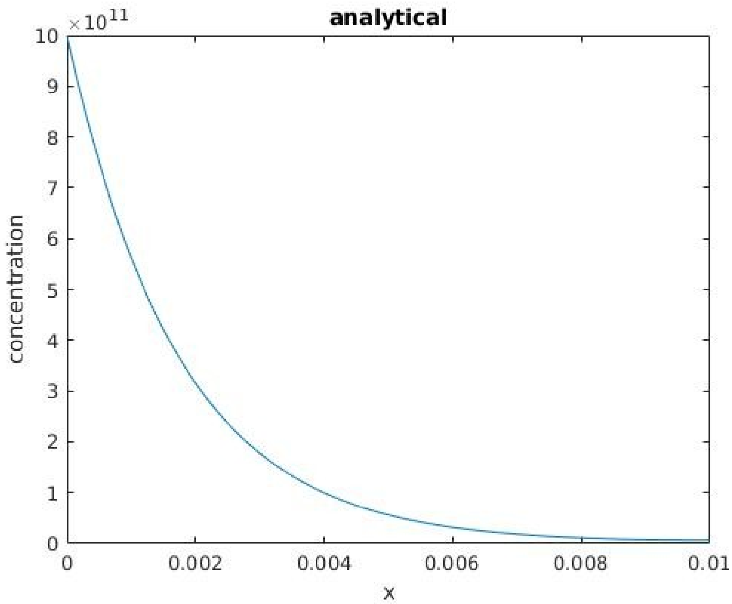
Comparing these two plots by plotting them together, we see that they superimpose each other



flux at A = $-1.72709*10^{16}$
flux at B = $-1.07696*10^{14}$
flux from A to B =
flux at B – flux at A =
$1.71632*10^{16}$

Q1 b)





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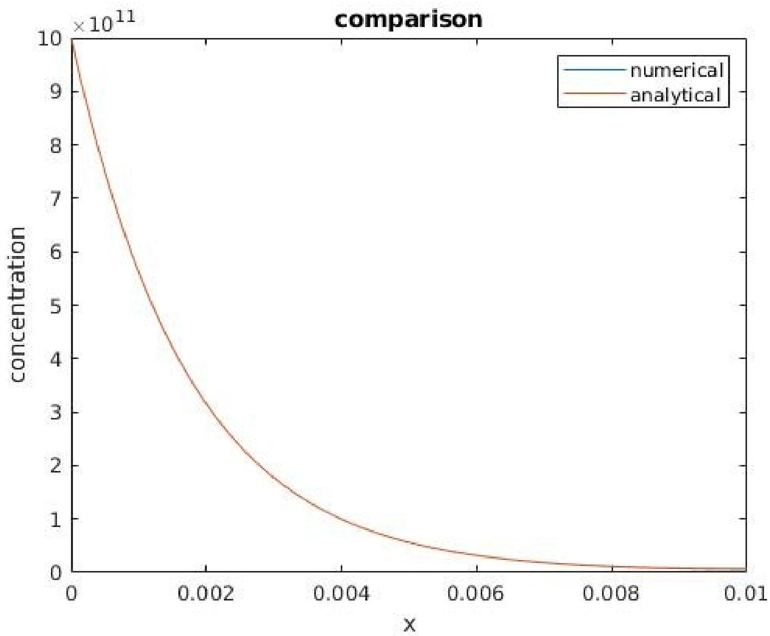
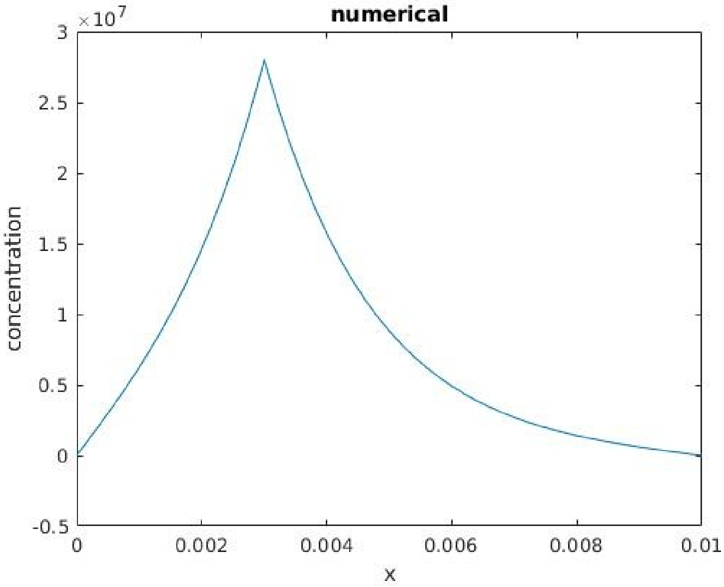
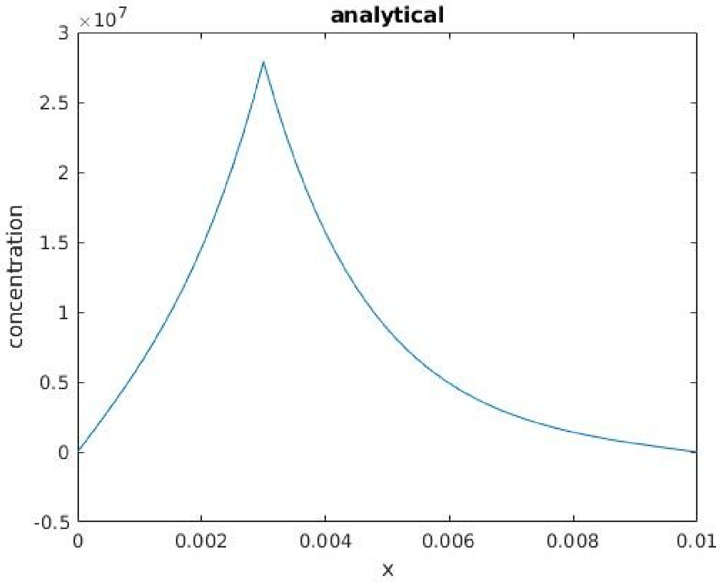


flux at A = $-1.7270*10^{16}$
flux at B = $-5.8944*10^{12}$
flux from A to B =
flux at B – flux at A =
$1.72643*10^{16}$

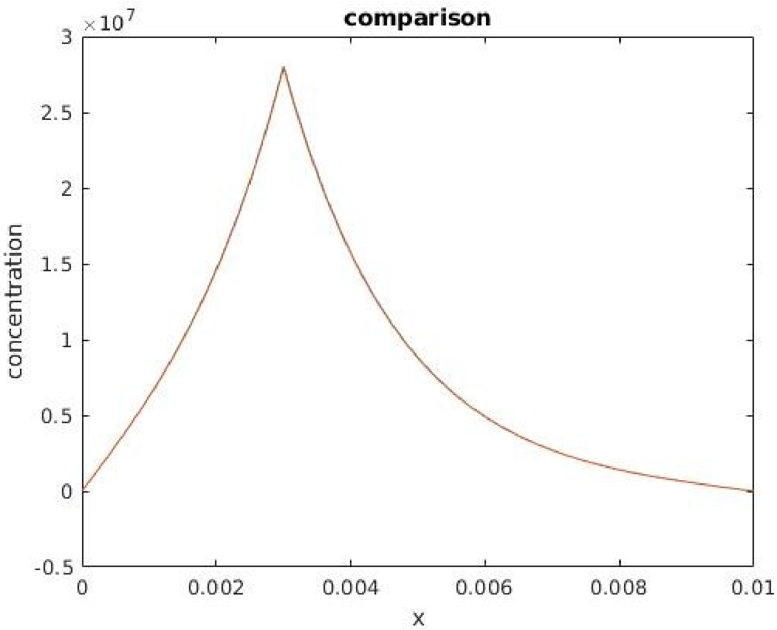
Using this boundary results in nearly same flux at A and same flux from A to B. However, flux at B changes due to this boundary condition as outgoing flux becomes a function of density at B.

Q1 c)





Comparing these two plots by plotting them together, we see that they superimpose each other



flux at A = $1.7736 * 10^{11}$
flux at B =$-1.7067 * 10^{10}$

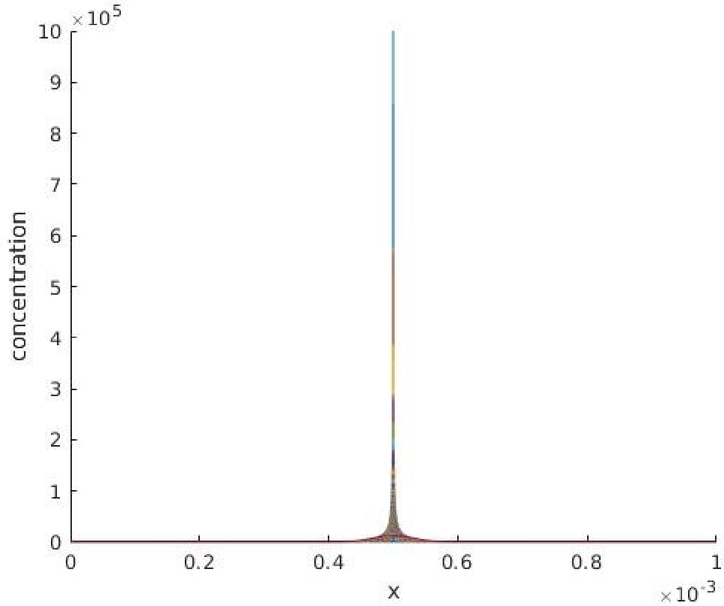
Q2

We take N = 1001 gridpoints from x = 0 to 10^{-3} cm. So, h = 10^{-6} cm

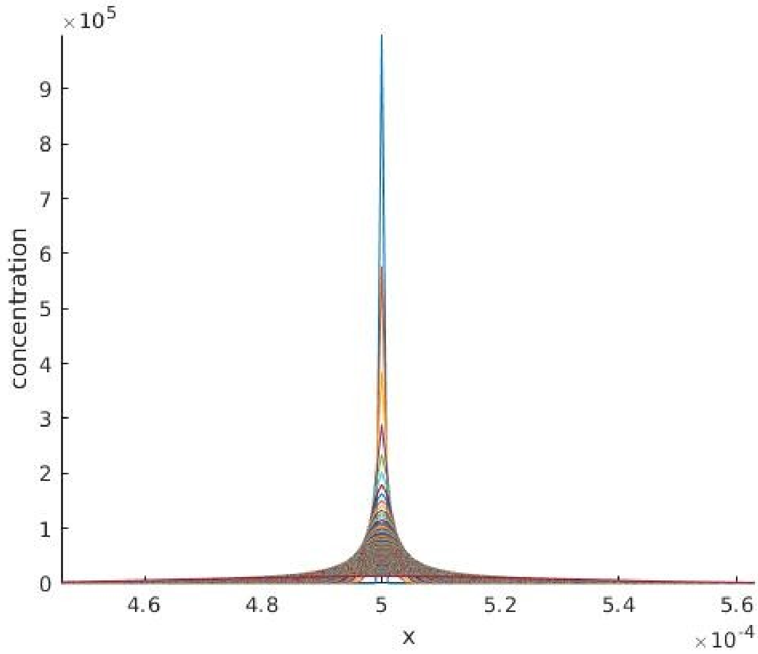
This gives us p = $5*10^{-9}$ sec

Running for 1000 such time steps, means we run till = $5*10^{-6}$ sec

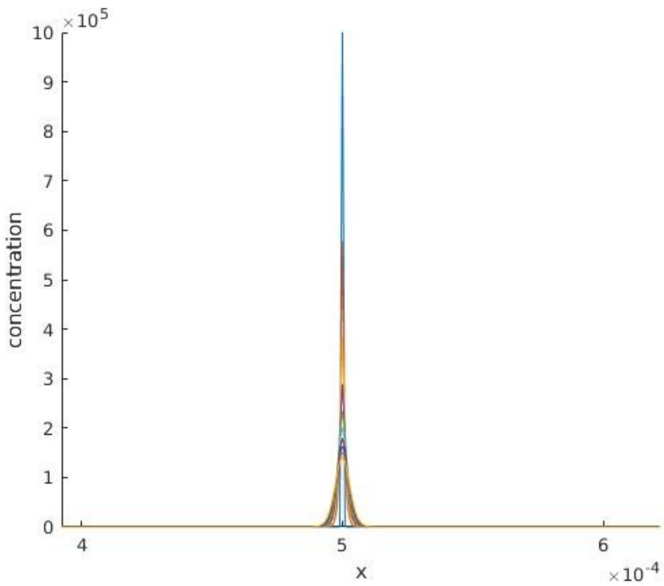
All 1001 graphs:



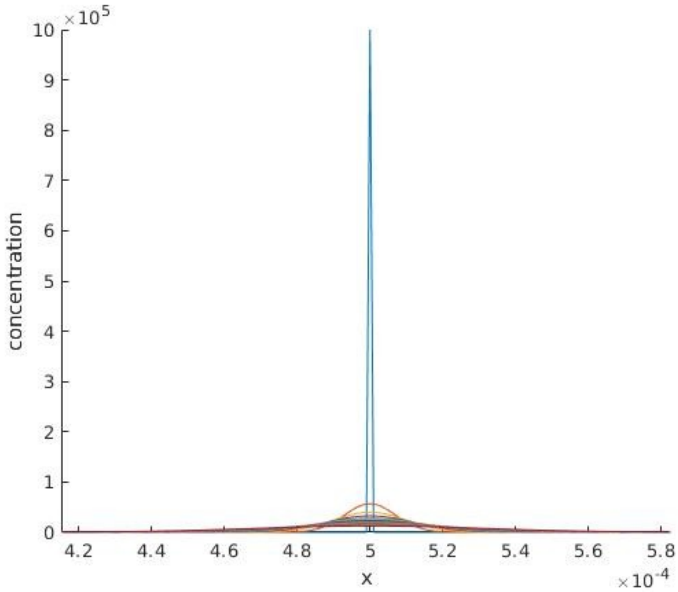
Zoomed plot:



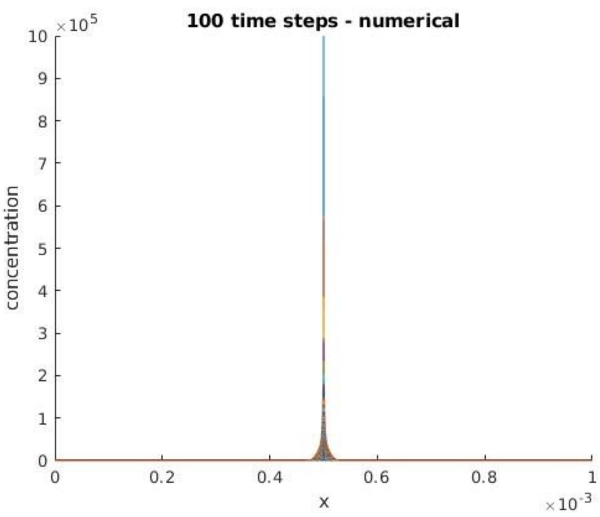
1st 10 plots:

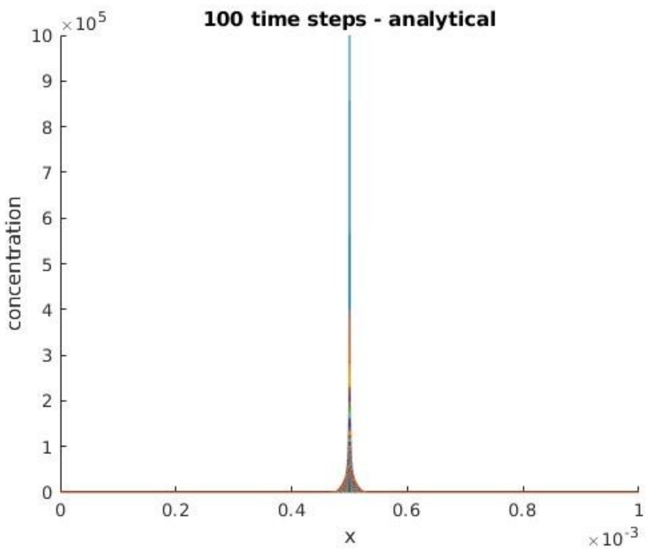


plots after 0.25us intervals (21 plots)



Comparison with analytical:





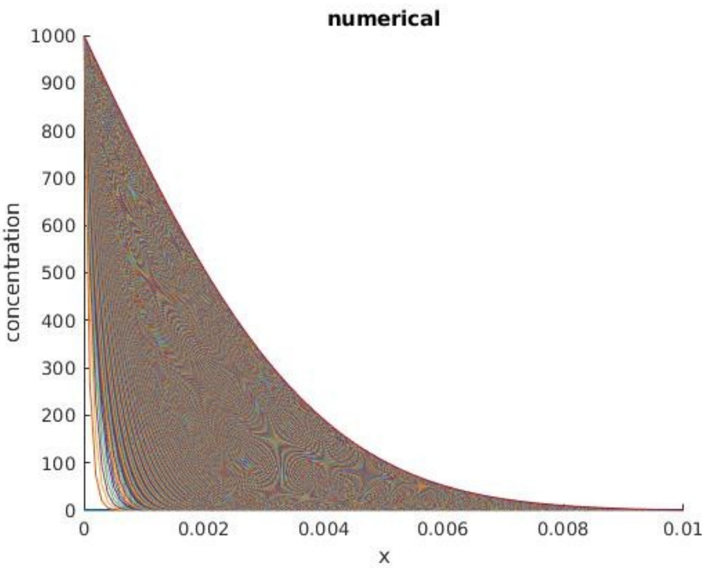
I don't get exactly matched numbers, but their order is same as that of analytical.

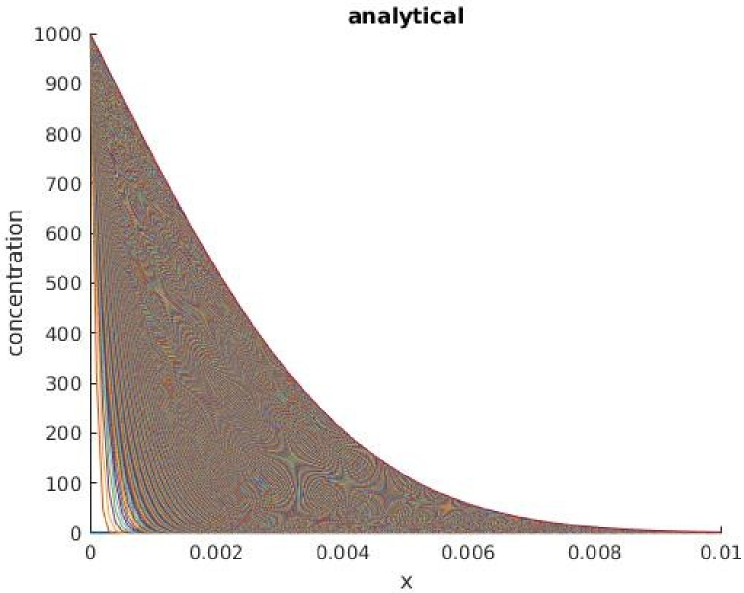
As we see in our analytical solution, we have a gaussian profile with $sigma^2 = 2*D*t$, i.e. profile has a variance which is time dependent. As time passes and variance increases, we see the graph has flattened more which is expected due to diffusion. Increasing D too results in faster flattening as compared to this graph.

Q3.

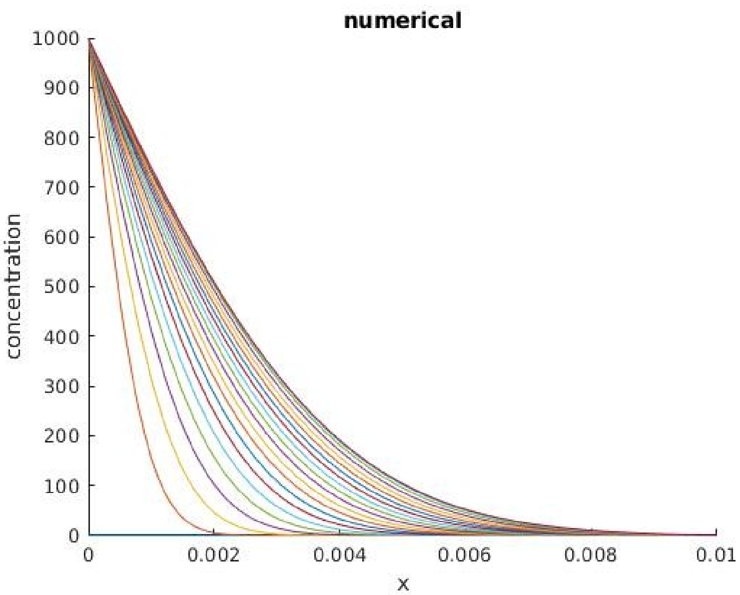
We take N = 101 gridpoints from x = 0 to 10^{-2} cm. So, h = 10^{-4} cm
This gives us p = $1.6667*10^{-10}$ sec
Running for 1000 such time steps, means we run till = $1.6667*10^{-7}$ sec

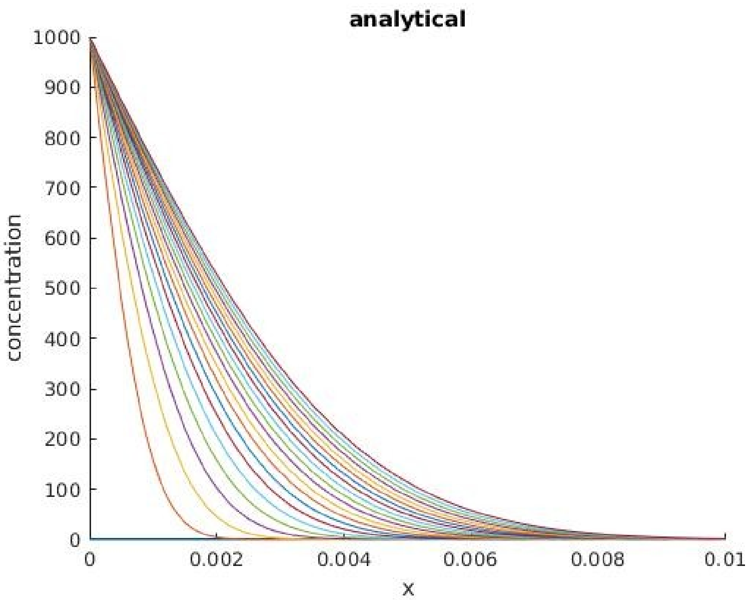
Plotting all 1001 plots and comparing with analytical:(1st plot all 0-inital)



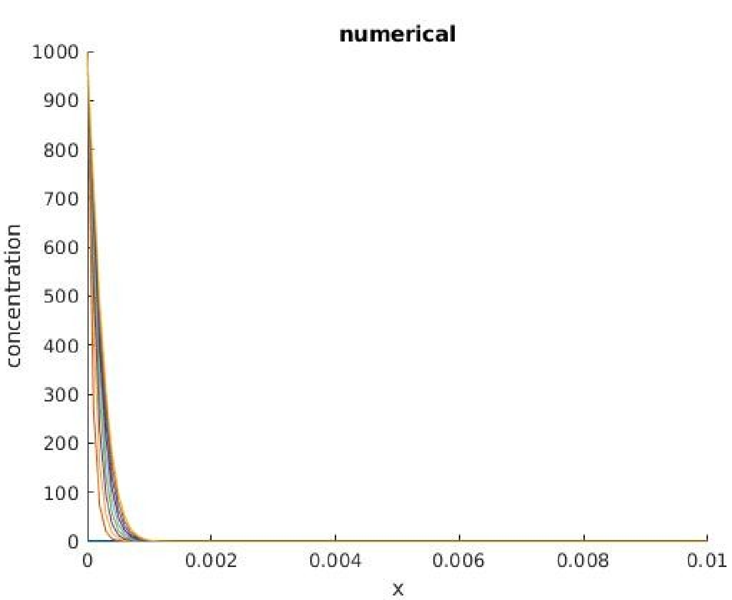


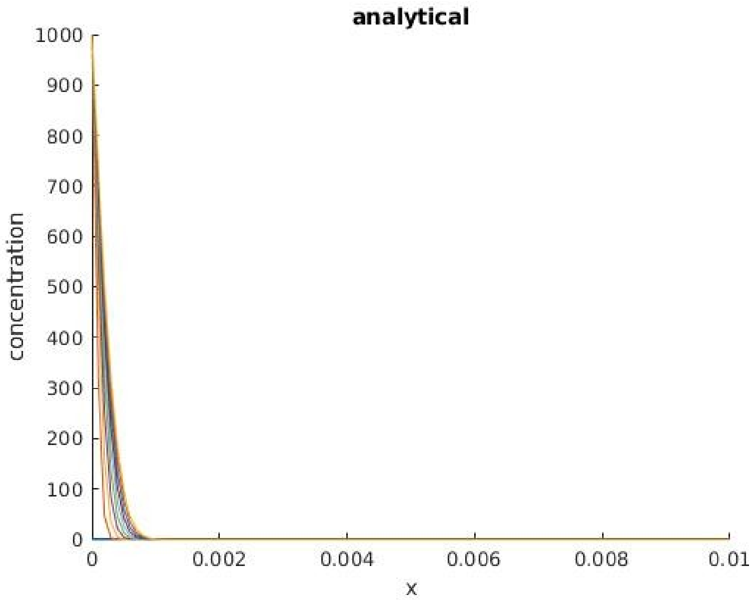
plots after 2.5ms intervals (21 plots) (1st plot all 0-inital)



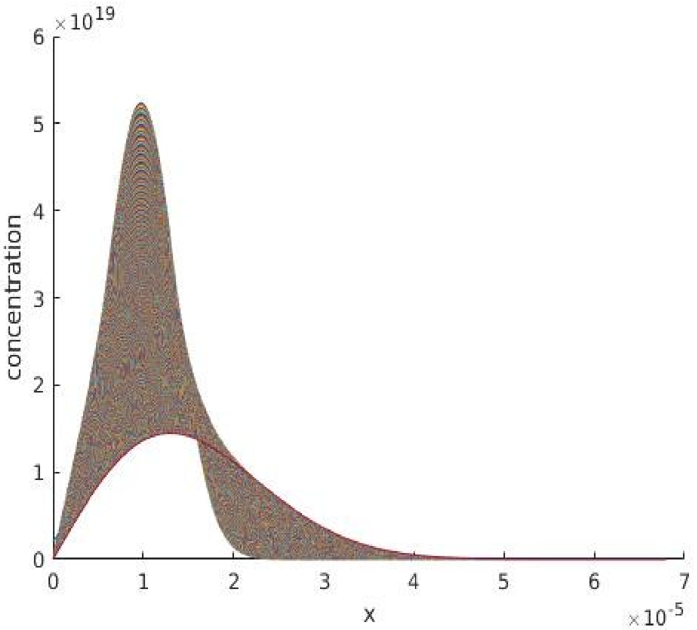


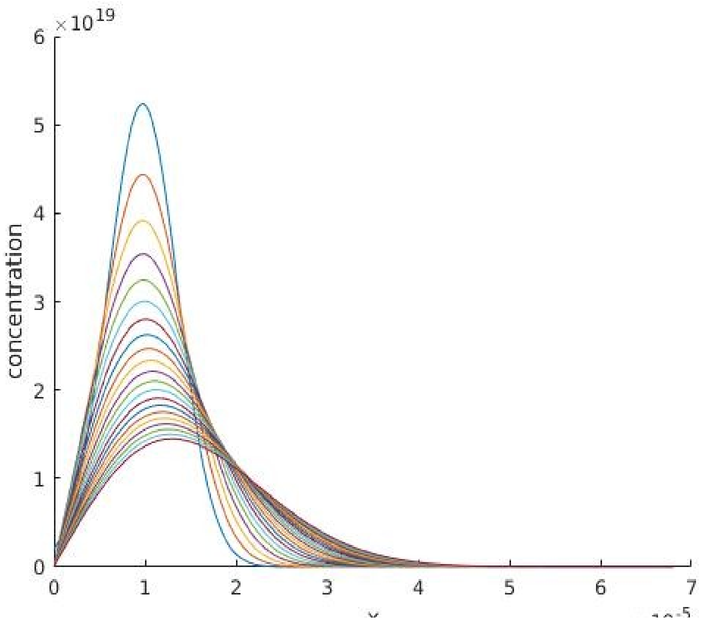
1st 10 plots:





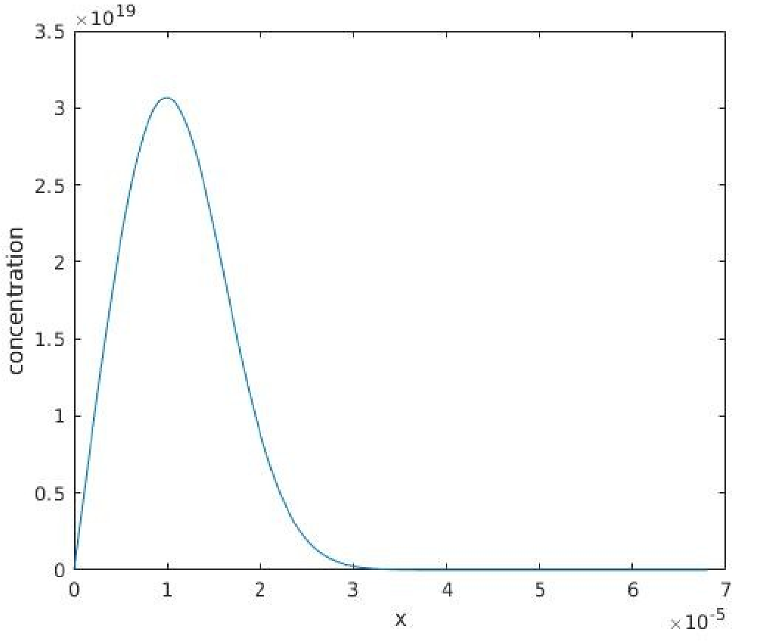
Q4.
Ea = 3.69 eV, D_0 = 10.5 cm^2/sec
Keeping neumann boundary conditions at right boundary and keeping left boundary at n=0 (using neumann boundary at left boundary also doesn't change thermal budget

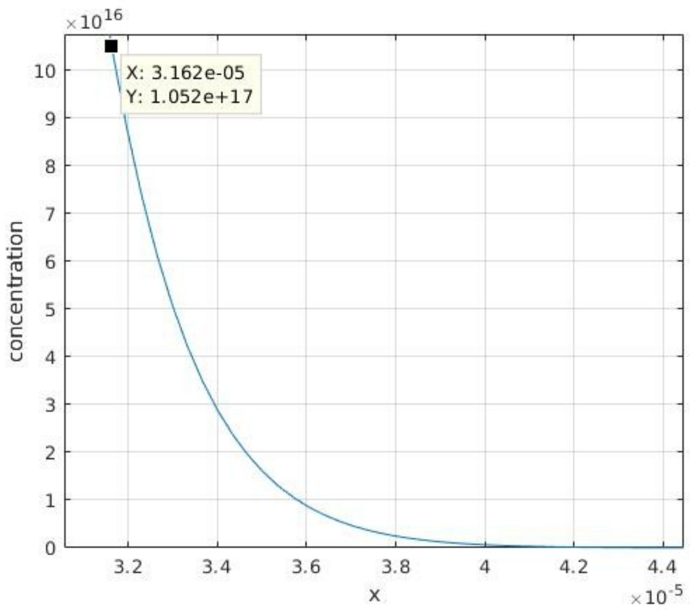


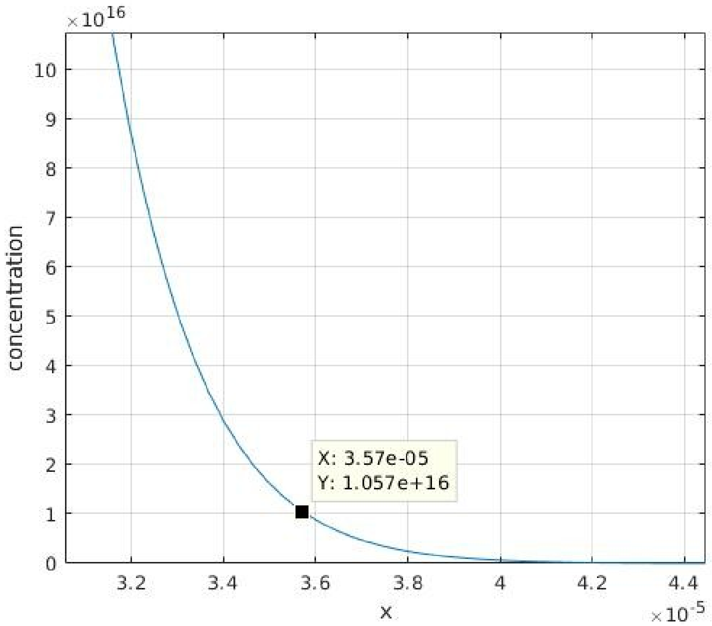


Thermal Budget = 1.36408*10^{-11} cm^2

At 1000 degrees celsius, when slope roll off is 40nm/decade at junction depth:







(slight error in answer due to numerical inaccuracies)

time (sec)	D (cm^2/sec)	Temperacture (celsius)
512.0253	$2.6641*10^{-14}$	1000
$1.4132*10^{12}$	$9.6526*10^{-24}$	500
0.0392	$3.4804*10^{-10}$	1500

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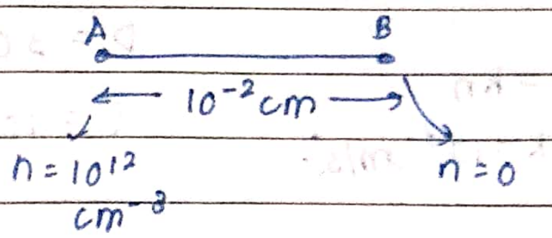
Page No.
Date

Analytical Solutions.

Q1·a)



$D = 30\,cm^2/s$

$\tau = 10^{-7}\ s$

$$\frac{D\,d^2n}{dx^2} = \frac{n}{\tau}$$

Let $n(x) = Ae^{\alpha x} + Be^{-\alpha x}$

$$D\alpha^2(Ae^{\alpha x} + Be^{-\alpha x}) = \frac{1}{\tau}(Ae^{\alpha x} + Be^{-\alpha x})$$

$$\therefore \alpha^2 = \frac{1}{D\tau} \Rightarrow \alpha = \frac{1}{\sqrt{D\tau}} = \frac{1}{\sqrt{30\times10^{-7}}} = 577.35$$

Boundary conditions:

$n(0) = A + B = 10^{12}$

$n(10^{-2}) = Ae^{5.7735} + Be^{-5.7735} = 0.$

$\Rightarrow 321.568\,A + (3.1088\times10^{-3})B = 0.$

~~321.6569~~

$\cancel{321.6569}B = 321.569\times10^{12}$

$\therefore B = 1.0000096\times10^{12}$

$\therefore A = -9.665\times10^{6}.$

$$n(x) = 10^6\left[-9.665\,e^{577.35x} + 1.0000096\times10^6\times e^{-577.35x}\right]$$

$$\therefore n(x) = 10^6\left[-9.665\,e^{577.35x} + 1.0000096\times10^6\,e^{-577.35x}\right]$$

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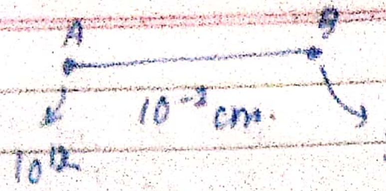
Q 1 (b)



$J = kn$

$k = 10^{3}$ cm/s.

$D = 30\ cm^2/s$

$\tau = 10^{-7}$.

$$\frac{D\, d^2 n}{dx^2} = \frac{n}{\tau}.$$

Let $n(x) = Ae^{\alpha x} + Be^{-\alpha x}$.

Substituting

$$D\left(A\alpha^2 e^{\alpha x} + B\alpha^2 e^{-\alpha x}\right) = \frac{Ae^{\alpha x} + Be^{-\alpha x}}{\tau}.$$

$$\therefore D\alpha^2 = \frac{1}{\tau} \Rightarrow \alpha = \frac{1}{\sqrt{D\tau}} = \frac{1}{\sqrt{30 \times 10^{-7}}} = 577.35$$

$n(0) = A + B = 10^{12}$.

$J = D\frac{dn}{dx} = kn \rightarrow$ at point B

$$\therefore D\alpha\left(Ae^{\alpha x} - Be^{-\alpha x}\right)\Big|_{x=10^{-2}} = k\left(Ae^{\alpha x} + Be^{-\alpha x}\right)\Big|_{x=10^{-2}}$$

$$1.732 \times 10^{4}\left(321.66A - (3.1088 \times 10^{-3})B\right)$$

$$= 10^{3}\left(321.66A + (3.1088 \times 10^{-3})B\right).$$

$\Rightarrow 5249.5A - 0.05695B = 0$.

$A = 1.085 \times 10^{7}$

$B = 9.99989 \times 10^{11}$

$$\therefore n(x) = 10^{7}\left[1.085e^{577.35x} + 9.99989 \times 10^{4} e^{-577.35x}\right]$$

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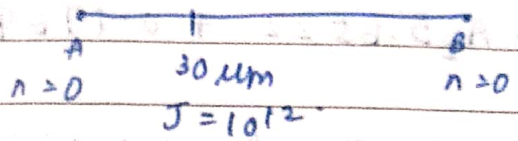
Q1(c).



$n_1(x) = A_1 e^{\alpha x} + B_1 e^{-\alpha x}$ $\quad 0 \le x \le 30\,\mu m$

$n_2(x) = A_2 e^{\alpha x} + B_2 e^{-\alpha x}$ $\quad 30 \le x \le 100\,\mu m.$

Boundary conditions.

① $n_1(0) \Rightarrow A_1 + B_1 = 0.$

② $n_2(100\,\mu m) \Rightarrow A_2 e^{\alpha 10^{-2}} + B_2 e^{-\alpha 10^{-2}} = 0.$

At 30 um boundary.

③ $$D\frac{\partial n_1}{\partial x}\Big|_{x=30^-\mu m} - D\frac{\partial n_2}{\partial x}\Big|_{x=30^+\mu m} = 10^{12}.$$

(sum of fluxes at 30^- um and 30^+ um)

④ $n_1(30\,\mu m) = n_2(30\,\mu m).$

note: $$D\frac{\partial^2 n}{\partial x^2} = \frac{n}{\tau}.$$

$$\alpha^2 D(Ae^{\alpha x} + Be^{-\alpha x}) = \frac{1}{\tau}(Ae^{\alpha x} + Be^{-\alpha x})$$

Hence, $$\alpha = \frac{1}{\sqrt{D\tau}} = \frac{1}{\sqrt{30 \times 10^{-7}}} = 577.35$$

Now, using boundary conditions.

⑤ $A_1 + B_1 = 0$

⑥ $321.66\,A_2 + (3.1088 \times 10^{-3})\,B_2 = 0$

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(7) $\alpha 3D \left[A_1 5.6522 - 0.1769 B_1 - A_2 5.6522 + 0.1769 B_2 \right] = 10^{12}$

(8) $5.6522 A_1 + 0.1769 B_1 = 5.6522 A_2 + 0.1769 B_2$

Solving:

$A_1 = -B_1$

$A_2 = -9.6648 \times 10^{-6} B_2$.

$577.35 \times 30 \left[-5.8291 B_1 + 0.176954 B_2 \right] = 10^{12}$

$-5.4753 B_1 = 0.17684 B_2$.

$\Rightarrow B_2 = -30.9619 B_1$

$B_1 = -5.105 \times 10^6$.

$\Rightarrow A_1 = 5.105 \times 10^6$.

$\Rightarrow B_2 = 1.58 \times 10^8$.

$\Rightarrow A_2 = -1527.836$

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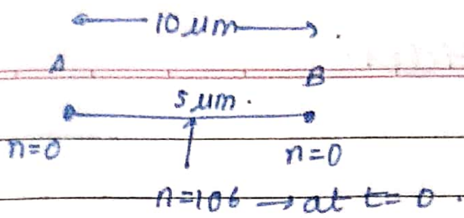
Page No.
Date

Q2.



$$\left(\frac{d^2}{dx^2} - \frac{1}{D}\frac{d}{dt}\right) n = \delta(x - x')$$

↳ source term delta function in space at time t=0.

↓ Fourier transform.

$$-k^2 c(k,t) - \frac{1}{D}\frac{dc(k,t)}{dt} = 0.$$

$$c(k,t) = c(k,t=0)\exp(-k^2 D t)$$

initial condition:

$c(k,0) = c(k,t=0)$

$$c(k,t=0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \delta(x-x')\exp(-ikx)\,dx$$

$$= \frac{\exp(-ikx')}{2\pi}$$ ($x' = 5\,\mu m$ here)

Taking inverse fourier transform

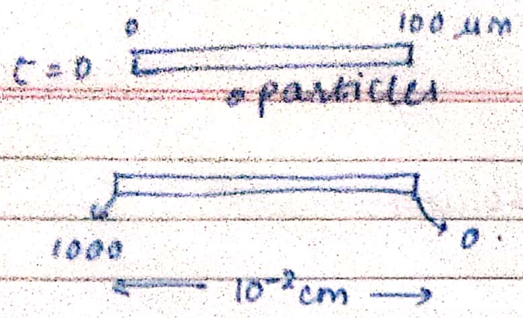
$$c(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp(ik(x-x'))\exp(-k^2 D t)\,dk.$$

$$\Rightarrow c(x,t) = \frac{1}{(4\pi D t)^{0.5}} \exp\left(-(x-x')^2/4Dt\right).$$

$D = 10^{-4}\ cm^2/s.$ ↳ (note at $t\to\infty$ $c(x,t)\to 0$).

$$\therefore c(x,t) = \frac{1}{(4\pi\, 10^{-4} t)^{0.5}} \exp\left(-(x - 5\times10^{-4})^2/(4\times10^{-4}\times t)\right)$$

3.



infinite ~~time~~ source : $g(0^{+}, t) = M \quad \forall \; t > 0.$

$$c(x,t) = \frac{2}{(4\pi D t)^{0.5}} \int_0^{\infty} M \exp\left(-\frac{(x+x')^2}{4tD}\right) dx'$$

$$x + x' = p$$
$$dx' = dp$$

$$\therefore C(x,t) = \frac{2}{(4\pi D t)^{0.5}} \int_x^{\infty} M \exp\left(\frac{-p^2}{4Dt}\right) dp.$$

$$\frac{p}{\sqrt{4Dt}} = q$$
$$\frac{dp}{\sqrt{4Dt}} = dq.$$

$$c(x,t) = \frac{2}{\sqrt{\pi}} \int_{x/\sqrt{4Dt}}^{\infty} M \exp(-q^2)\, dq.$$

$$\because \operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-t^2} dt.$$

$$\therefore C(x,t) = M \left(\operatorname{erfc}\left(\frac{x}{\sqrt{4Dt}}\right)\right).$$

$$\therefore C(x,t) = M \left[\operatorname{erfc}\left(\frac{x}{\sqrt{4Dt}}\right)\right].$$

$M = 10^3$, $D = 30\,cm^2/s$.

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