Oving 2

Oppg 1

Den en-dimensjonelle diffusjonsligningen:

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

1a)

Fourier-transformer begge sider:

$$\int_{-\infty}^{\infty} \frac{\partial c(x,t)}{\partial t} \cdot e^{-i2\pi kx} dx = D\int_{-\infty}^{\infty} \frac{\partial^2 c(x,t)}{\partial x^2} \cdot e^{-i2\pi kx} dx$$

Venstre side:

$$\begin{aligned} &\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\partial c(x,t)}{\partial t} \cdot e^{-ikx} dx \\ &= \frac{\partial}{\partial t} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} c(x,t) \cdot e^{-ikx} dx \\ &= \frac{\partial}{\partial t} \tilde{c}(k,t) \end{aligned}$$

der $\tilde{c}(k,t)$ er Den fouriertransformerte $c(x,t)$

Høyre side:

$$D\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\partial^2 c(x,t)}{\partial x^2} \cdot e^{-ikx} dx$$

Delvis integrasjon:

$$\int F\frac{\partial G}{\partial x} dx = (FG)\Big|_{-\infty}^{+\infty} - \int \frac{\partial F}{\partial x} G dx$$

Anta at $c(\plusmn\infty, t) = 0$ som gir mening når vi har en punktkilde. Dvs at (FG)-leddet alltid blir 0. Deriveringen av e^{-ikx} henter bare ut en konstant $(-ik)$

$$= D\frac{1}{\sqrt{2\pi}} \left(0 - \int_{-\infty}^{\infty} \frac{\partial c(x,t)}{\partial x} \cdot e^{-ikx} \cdot (-ik) dx \right)$$

$$= D\frac{1}{\sqrt{2\pi}} (ik) \int_{-\infty}^{\infty} \frac{\partial c(x,t)}{\partial x} \cdot e^{-ikx} dx$$

etter samme logikk:

$$= D(ik)^2 \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} c(x,t) \cdot e^{-ikx} dx$$

$$= -Dk^2\tilde{c}(k,t)$$

Det finnes visst en regneregel for fouriertransformasjoner som viser det jeg viste over
VS = HS

$$\frac{\partial}{\partial t}\tilde{c}(k,t) = -Dk^2\tilde{c}(k,t)$$

Og vi har diff-ligningen vi var ute etter.

1b)

$$\frac{\partial}{\partial t}\tilde{c}(k,t) = -Dk^2\tilde{c}(k,t)$$

matte-lifehack

$$\frac{1}{\tilde{c}(k,t)}\partial\tilde{c}(k,t) = -Dk^2\partial t$$

$$\int \frac{1}{\tilde{c}(k,t)}\partial\tilde{c}(k,t) = \int -Dk^2\partial t$$

$$\ln(\tilde{c}(k,t)) = -Dk^2\int \partial t = -Dk^2 t + C_1$$

$$\tilde{c}(k,t) = e^{-Dk^2t}e^{C_1} = C_2 e^{-Dk^2t}$$

Grensebetingelse for å finne C_2:
Vi vet at $c(x,0) = \delta(0 \cdot c_0)$. Merk at i oppgaveteksten kaller de c_0 for c.

$$\tilde{c}(k,0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{ikx} \cdot c(x,0)dx$$

$$= \frac{1}{\sqrt{2\pi}}\left(e^{ikx} \cdot c_0\right)\Big|^{x=0} = \frac{c_0}{\sqrt{2\pi}}$$

Sett inn i funksjonen fra over:

$$\tilde{c}(k,0) = C_2 \cdot 1 = \frac{c_0}{\sqrt{2\pi}}$$

$$\implies C_2 = \frac{c_0}{\sqrt{2\pi}}$$

$$\implies \tilde{c}(k,t) = \frac{c_0}{\sqrt{2\pi}}e^{-Dk^2t}$$

Fouriertransformere tilbake:

$$c(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \frac{c_0}{\sqrt{2\pi}}e^{-Dk^2t} \cdot e^{ikx}dk$$

$$= \frac{c_0}{\sqrt{4\pi^2}}\int_{-\infty}^{+\infty} e^{-Dk^2t+ikx}dk$$

Regel fra rottmann s 155

$$\int_{-\infty}^{+\infty} e^{-ax^2-bx-c}dx = \sqrt{\frac{\pi}{a}}\exp\left(\frac{b^2-ac}{a}\right)$$

I vårt tilfelle er $a = Dt$, $b = \frac{-ix}{2}$, $c = 0$

$$c(x,t) = \frac{c_0}{\sqrt{4\pi^2}}\sqrt{\frac{\pi}{Dt}}\exp\left(\frac{-x^2}{4Dt}\right) = \frac{c_0}{\sqrt{4\pi Dt}}e^{-x^2/Dt}$$

1c)

Her er det ikke så godt å vite hva man skal frem til dessverre

Vi begynner med at

$$c(x,t) = \mathcal{F}^{-1}[\tilde{c}(k,t)] = \mathcal{F}^{-1}[e^{-Dk^2t}\cdot\tilde{c}(k,0)]$$

konvolusjonsteoremet sier at

$$\mathcal{F}^{-1}[G\cdot H] = \mathcal{F}^{-1}[G] * \mathcal{F}^{-1}[H]$$

Dermed har vi

$$c(x,t) = \mathcal{F}^{-1}[e^{-Dk^2t}] * \mathcal{F}^{-1}[\tilde{c}(k,0)]$$

Første ledd i konvolusjonen

$$\mathcal{F}^{-1}[e^{-Dk^2t}] = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{-Dk^2t}e^{ikt}dk$$

som etter samme rottmann-formel som i oppgave 1b blir

$$\mathcal{F}^{-1}[e^{-Dk^2t}] = \frac{1}{\sqrt{2\pi}}\sqrt{\frac{\pi}{Dt}}\exp\left(\frac{-x^2}{4Dt}\right) = \frac{1}{\sqrt{2Dt}}e^{-x^2/4Dt}$$

For en eller annen grunn mangler angivelig jeg et ledd $1/\sqrt{2\pi}$ TODO
Andre ledd i konvolusjonen:

$$\mathcal{F}^{-1}[\tilde{c}(k,0)] = c(x,0)$$

per definisjon. Dermed får vi at (herfra og ned er korrigert for en feil over) TODO

$$c(x,t) = \mathcal{F}^{-1}[e^{-Dk^2t}] * \mathcal{F}^{-1}[\tilde{c}(k,0)] = c(x,0) * \frac{1}{\sqrt{4\pi Dt}}e^{-x^2/4Dt}$$

$$= \int_{-\infty}^{+\infty} c(z-x,0)\cdot\frac{1}{\sqrt{4\pi Dt}}e^{-z^2/4Dt}dz$$

1d)

Jeg nekter å kalle denne oppgaven 1B)

$$c(x,0) = \begin{cases} c_0 & \text{når x} < 0 \\ 0 & \text{ellers}\end{cases}$$

$$c(x-z,0) = \begin{cases} c_0 & \text{når } x-z<0 \\ 0 & \text{ellers} \end{cases}$$

dermed:

$$c(x,t) = \int_{-\infty}^{+\infty} c(z-x,0) \cdot \frac{1}{\sqrt{4\pi Dt}} e^{-z^2/4Dt} dz$$

$$= \int_{x}^{+\infty} c(z-x,0) \cdot \frac{1}{\sqrt{4\pi Dt}} e^{-z^2/4Dt} dz$$

Her kunne vi trengt mellomregning TODO

$$= \left[\frac{c_0\sqrt{\pi}}{\sqrt{4\pi Dt}} \frac{\sqrt{4Dt}}{2} erf\left(\frac{1}{\sqrt{4Dt}} z\right)\right]_x^\infty$$

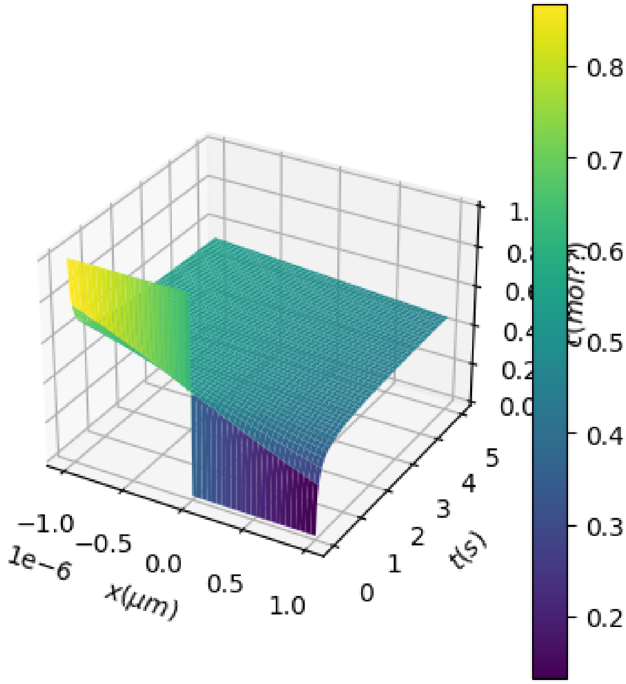
$$= \left[\frac{c_0}{2} erf\left(\frac{1}{\sqrt{4Dt}} z\right)\right]_x^\infty$$

$$\frac{c_0}{2} - \frac{c_0}{2} erf\left(\frac{1}{\sqrt{4Dt}} x\right)$$

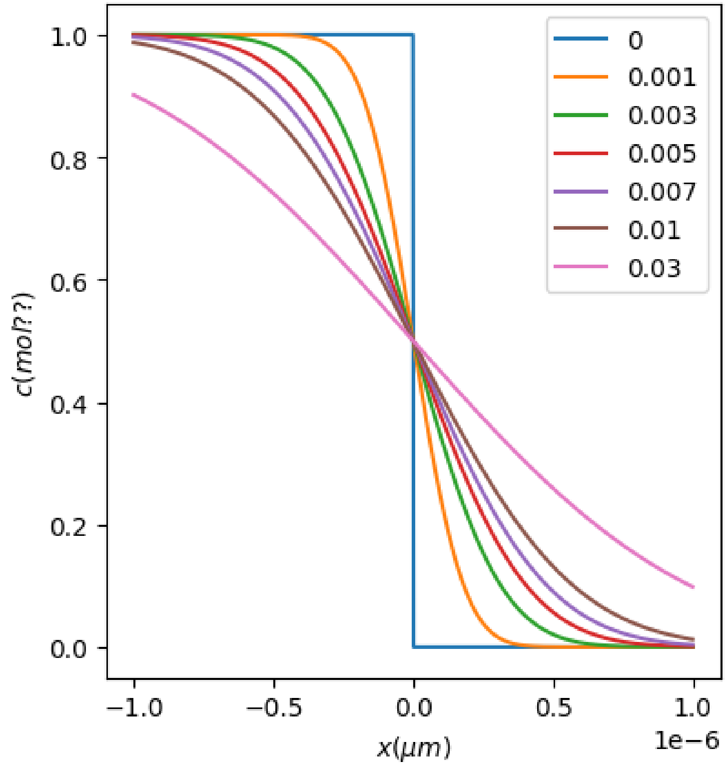
In [18]:

```
from scipy.special import erf
import numpy as np
import matplotlib.pyplot as plt
from matplotlib import cm



D = 1e-11  # m^2/s
c_0 = 1
c = lambda x, t: c_0 / 2 - c_0 / 2 * erf(x / np.sqrt(4 * D * t))
x1d = np.linspace(-1, 1, 1000) * 1e-6
t1d = np.linspace(0, 5, 1000)
x, t = np.meshgrid(x1d, t1d)
cs = c(x, t)
fig = plt.figure(figsize=plt.figaspect(0.5))
ax = fig.add_subplot(1, 2, 1, projection="3d")
ax.set_xlabel("$x(\mu m)$")
ax.set_ylabel("$t(s)$")
ax.set_zlabel("$c(mol??)$")
surf = ax.plot_surface(x, t, cs, cmap=cm.viridis)
ax2 = fig.add_subplot(1, 2, 2)
ax2.set_xlabel("$x(\mu m)$")
ax2.set_ylabel("$c(mol??)$")
# for ts in range(0, len(t1d)):
#    ax2.plot(x1d, c(x1d, ts))
ts = [0, 0.001, 0.003, 0.005, 0.007, 0.010, 0.030]
for tee in ts:
    ax2.plot(x1d, c(x1d, tee))
ax2.legend(ts)

fig.colorbar(surf, ax=ax)
plt.show()
```

```
C:\Users\ivism\AppData\Local\Temp\ipykernel_17240\1741507609.py:9: RuntimeWarning: divide by zer
o encountered in divide
  c = lambda x, t: c_0 / 2 - c_0 / 2 * erf(x / np.sqrt(4 * D * t))
```



0.8
0.7
0.6
0.5
0.4
0.3
0.2
−1.0
−0.5
0.0
0.5
1.0
1e−6
x(μm)
0
1
2
3
4
5
t(s)



1.0
0.8
0.6
0.4
0.2
0.0
c(mol??)
−1.0
−0.5
0.0
0.5
1.0
1e−6
x(μm)
0
0.001
0.003
0.005
0.007
0.01
0.03