Exercise 4.1.

Calculate depth of penetration for typical gas ($D = 1 \left[\frac{cm^2}{s}\right]$), liquid ($D = 10^{-5} \left[\frac{cm^2}{s}\right]$) and solid in high temperature ($D = 10^{-10} \left[\frac{cm^2}{s}\right]$) for:

- 1 second
- 1 hour
- 1 day
- 1 month

Solution:

$$\boldsymbol{x = \sqrt{2Dt}}$$

[cm]	D[cm^2/s]	1 sekunda	1 godzina	1 dzień	1 miesiąc
gaz	1	1,414	84,85	415,69	2276,84
ciecz	$1 \cdot 10^{-5}$	0,00447	0,268	1,315	7,20
ciało stałe	$1 \cdot 10^{-10}$	1,414E-05	0,00085	0,004157	0,0228

Exercise 4.2.

Prove that the function $c_i(x,t) = \frac{M}{2\sqrt{D\pi t}} e^{-(x-\mu)^2/4Dt}$ fulfills a diffusion equation:

$$\frac{\partial c_i}{\partial t} = D_i \frac{d^2 c_i}{dx^2}$$

Solution:

$$\frac{\partial c_i}{\partial t} = \frac{\partial}{\partial t}\left(\frac{M}{2\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}}\right) = \frac{M(x-\mu)^2}{8Dt^2\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}} - \frac{M}{4t\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}}$$

$$\frac{\partial c_i}{\partial x} = \frac{\partial}{\partial x}\left(\frac{M}{2\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}}\right) = -\frac{M(x-\mu)}{4Dt\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}}$$

$$\frac{\partial^2 c_i}{\partial x^2} = \frac{\partial}{\partial x}\left(-\frac{M(x-\mu)}{4Dt\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}}\right) = \frac{M(x-\mu)^2}{8D^2t^2\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}} - \frac{M}{4Dt\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}}$$

$$\frac{M(x-\mu)^2}{8Dt^2\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}} - \frac{M}{4t\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}} = (?) = D\left[\frac{M(x-\mu)^2}{8D^2t^2\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}} - \frac{M}{4Dt\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}}\right]$$

$$\frac{M(x-\mu)^2}{8Dt^2\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}} - \frac{M}{4t\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}} = \frac{M(x-\mu)^2}{8Dt^2\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}} - \frac{M}{4t\sqrt{D\pi t}} e^{-\frac{(x-\mu)^2}{4Dt}}$$

Exercise 4.3.

Find concentration c(x) for a closed system of length *d* in a steady state, if c(x, t=0) was given by equation:

$$c(x, t = 0) = 10 + \frac{20x}{d}$$

For:

- Neumann boundary conditions J(0,t)=J(d,t)=0
- Dirichlet boundary conditions

Neumann

Steady state:

$$\frac{\partial ..}{\partial t} = 0$$

Diffusion equation:

$$\frac{\partial c}{\partial t} = 0 = -\frac{\partial J}{\partial x} \quad \Rightarrow \quad J(x) = const$$

from boundary conditions:

$$J = 0 \quad \Rightarrow \quad -D\frac{\partial c}{\partial x} = 0 \quad \Rightarrow \quad c = const$$

$$c(t \to \infty) = \frac{1}{d}\int_0^d 10 + \frac{20x}{d}dx = \frac{1}{d}\left[10x + \frac{10x^2}{d}\right]_0^d = \frac{1}{d}[10d + 10d] = 20$$

Dirichlet

$$c(0, t) = 10$$

$$c(d, t) = 30$$

Steady state:

$$\frac{\partial ..}{\partial t} = 0$$

Diffusion equation:

$$\frac{\partial c}{\partial t} = 0 = -\frac{\partial J}{\partial x} \quad \Rightarrow \quad J(x) = const$$

$$J = const \quad \Rightarrow \quad -D\frac{\partial c}{\partial x} = const \quad \Rightarrow \quad c = Ax + B$$

from boundary conditions:

$$B = 10$$

$$A = \frac{20}{d}$$

As a result:

$$c(x, t \to \infty) = \frac{20}{d}x + 10$$

Exercise 4.4.

Temperature distribution in an isolated rod of length l=10cm, is in t=0 given by:

$$T(x,0) = 5\left(x - \frac{l}{3}\right)^2$$

Calculate temperature distribution in a steady state, assuming Dirichlet boundary conditions.

Solution:

$$\frac{\partial T}{\partial t} = 0 = -\frac{\partial Q}{\partial x} \quad \Rightarrow \quad Q = const \quad \Rightarrow \quad \frac{\partial T}{\partial x} = const \quad \Rightarrow \quad T = Ax + b$$

From boundary conditions:

$$T(0,t) = 5\left(-\frac{10}{3}\right)^2 = 55{,}56\ [K]$$

$$T(l,0) = 5\left(10 - \frac{10}{3}\right)^2 = 222{,}22[K]$$

$$b = 55{,}56[K]$$

$$A = \frac{222{,}22 - 55{,}56}{10} = 16{,}66\left[\frac{K}{cm}\right]$$

Ostatecznie:

$$T(x, t \to \infty) = 16{,}66x + 55{,}56$$

Exercise 4.5.

Sample of thickness l=20[cm] has following boundary conditions:

- On left side: NBC J(0,t)=0,0005$\left[\frac{mol}{cm^2 s}\right]$
- On right side: DBC c(l,t)=0,005$\left[\frac{mol}{cm^3}\right]$

Find a steady state concentration profile for diffusion coefficient $D = 10^{-5}\left[\frac{cm^2}{s}\right]$.

Solution:

$$\frac{\partial c}{\partial t} = 0 = -\frac{\partial J}{\partial x} \quad \Rightarrow \quad J = const$$

From NBC:

$$J(x,t) = 0{,}0005 \left[\frac{mol}{cm^2 s}\right]$$

$$J = -D\frac{\partial c}{\partial x} \quad \Rightarrow \quad c = \int -\frac{J}{D}dx = -\frac{J}{D}x + A$$

From DBC:

$$c(l,t) = -\frac{J}{D}l + A \quad \Rightarrow \quad A = c(l,t) + \frac{J}{D}l$$

Finally:

$$c(x,t) = \frac{J}{D}(l - x) + c(l,t)$$

$$c(x,t) = 2(20 - x) + 0{,}005$$

Exercise 4.6.

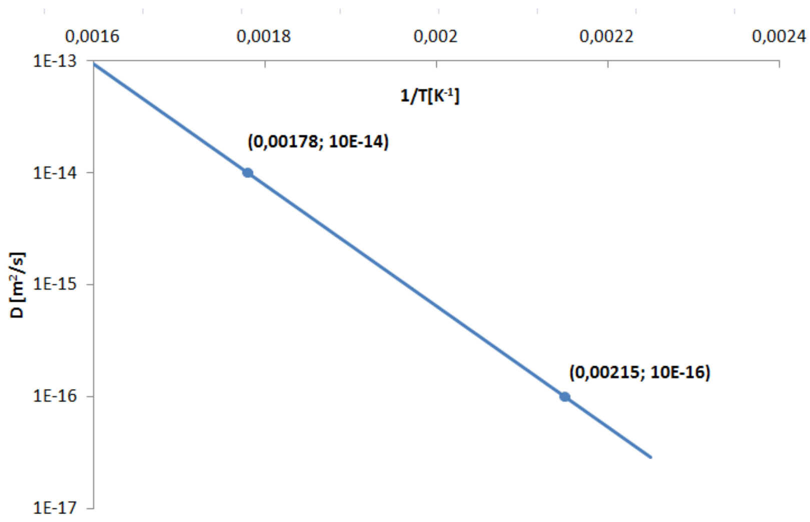
On the plot below it can be seen how the self-diffusion coefficient of Pb depends on the temperature (or to be more precise 1/T). Knowing, that the diffusion coefficient can be described by the Arrhenius relation:

$$D = D^0 \exp\left(-\frac{\Delta H}{k_B T}\right)$$

find:

- value of the enthalpy of activation
- depth of penetration in 450K after two days
- depth of penetration in 550K after two days

Value of D^0 equals $4{,}1868\cdot10^{-5}$ [m^2/s]



Solution:

$$lnD = lnD^0 - \frac{\Delta H}{k}\frac{1}{T}$$

Enthalpy of activation

$$\Delta H = -k * \frac{ln(10^{-14}) - ln(10^{-16})}{0{,}00215 - 0{,}00178} = -8{,}61733 \cdot 10^{-5\cdot} \frac{-36{,}8414 + 32{,}2362}{0{,}00037} = 1{,}073\ eV$$

D in 450K:

$$D = (4{,}1868 \cdot 10^{-5}) \cdot \exp\left(-\frac{1{,}07255}{8{,}61733 \cdot 10^{-5\cdot} \cdot 450}\right) = 4{,}07 \cdot 10^{-17}$$

Depth of penetration 450K:

$$x = \sqrt{4{,}07 \cdot 10^{-17} \cdot 20000} = 3{,}752[\mu m]$$

D in 550K:

$$D = (4{,}1868 \cdot 10^{-5}) \cdot \exp\left(-\frac{1{,}07255}{8{,}61733 \cdot 10^{-5\cdot} \cdot 550}\right) = 6{,}22 \cdot 10^{-15}$$

Depth of penetration 550K:

$$x = \sqrt{4{,}07 \cdot 10^{-17} \cdot 20000} = 46{,}367[\mu m]$$