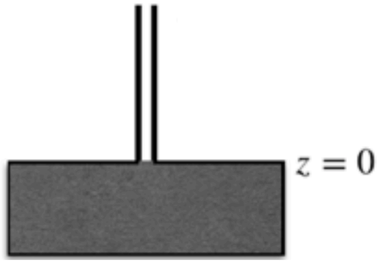
In-class exercise problem

A container filled with liquid aniline (molar mass: 93.13 g/mol) is stored in a large room. The container has a cylindrical tube with length of 10 cm and a diameter of 1 cm. Initially, the cylindrical tube is filled with air (pressure of 1 atm), and aniline is prevented from evaporation. At time t = 0, the evaporation of aniline is allowed.

- Saturation vapor pressure of aniline: 10 kPa
- The diffusion coefficient of the aniline vapor in air: 9×10^{-2} cm^2/s.
- Aniline vapor can be treated as ideal gas.
- Assume a concentration of 0 at z = 10 cm, and saturation conditions at z =0.



1. Neglecting convection, calculate the partial pressure of aniline vapor at z =1.5 cm after 25 seconds.

2. Estimate the error in neglecting convection.

When convection is neglected;

$$\frac{c(z,t) - c_S}{c_\infty - c_S} = erf\ \zeta$$

$c_\infty = 0$

t = 25 s, z = 0.015 m

D = 9×10^{-2} cm^2/s

$$\Rightarrow \zeta = 0.5$$

$$\Rightarrow \frac{c(z,t) - c_S}{0 - c_S} = erf\ \zeta$$

$$\Rightarrow \frac{c(z,t)}{c_S} = (1 - erf\ \zeta) = 0.48$$

Partial pressure = 4.8 kPa

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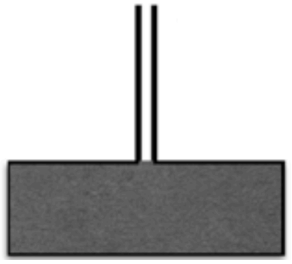
When convection is considered $\bar{V}_1 c_1^{sat} = \left(1 + \frac{1}{\sqrt{\pi}(1+\text{erf }\phi)\phi e^{\phi^2}}\right)^{-1}$

In vapor phase, $\bar{V}_1 c_1^{sat} = y_1^{sat} = 10/100 = 0.1$



$$\Rightarrow \left(1 + \frac{1}{\sqrt{\pi}(1+\text{erf }\phi)\phi e^{\phi^2}}\right) = 10$$

$$\Rightarrow \frac{1}{\sqrt{\pi}(1+\text{erf }\phi)\phi e^{\phi^2}} = 9$$

$$\Rightarrow \sqrt{\pi}(1+\text{erf }\phi)\phi e^{\phi^2} = \frac{1}{9} = 0.11$$

$$\Rightarrow (1+\text{erf }\phi)\phi e^{\phi^2} = 0.06$$

ϕ is positive (dimensionless velocity), $\Rightarrow 1 + \text{erf }\phi > 1$, also $\exp(\phi^2) > 1$

$\Rightarrow \phi$ is small ≈ 0.06

Check LHS; $(1 + erf 0.06)0.06e^{0.06*0.06} = 0.064$

$LHS \approx RHS$

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$$\frac{c_1}{c_1^{sat}} = \frac{1 - \text{erf}\,(\zeta - \phi)}{1 + \text{erf}\,\phi} \qquad \zeta = 0.5 \qquad \phi = 0.06$$

$$\frac{c_1}{c_1^{sat}} = \frac{1 - \text{erf}\,0.44}{1 + \text{erf}\,0.06} = 0.5$$

Partial pressure comes out to be 5.0 kPa

Neglecting convection, we got partial pressure of 4.8 kPa

Very small error because y_1^{sat} is only 0.1

Exercise problem 1: calculate mean-free path, mean velocity and D of helium at 1 atm and 25 °C.

$$l = \frac{k_B T/P}{\left(\frac{\pi}{4}\sigma^2\right)} = \frac{\text{volume occupied by single molecule}}{\text{cross-sectional area}}$$

$$\bar{v} = \sqrt{\frac{8k_B T}{\pi m}}$$

$$D = \frac{1}{3}\bar{v}\,l = \frac{8}{3}\sqrt{\frac{2}{m}}\left(\frac{k_B T}{\pi}\right)^{3/2}\frac{1}{P\sigma^2}$$

Table 5.1-2 *Lennard–Jones potential parameters found from viscosities*

Substance		σ(Å)	ε_{12}/k_B(K)
He	Helium	2.551	10.2

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$$l = \frac{1.38 * 10^{-23} * 298/101325}{\left(\frac{3.14}{4}(2.55 * 10^{-10})^2\right)} = 7.95 * 10^{-7}\ m = 795\ nm$$

$$\bar{v} = \sqrt{\frac{8 * 1.38 * 10^{-23} * 298}{3.14 * (0.004/(6.023 * 10^{23}))}} = 1256.05\ \ m/s$$

$$D = \frac{1}{3}\bar{v}\,l = \frac{1}{3}1256.05 * 7.95 * 10^{-7} = 3.33 * 10^{-4}\ m^2\ s^{-1} = 3.33\ cm^2\ s^{-1}$$

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Exercise problem 2: In previous problem, calculate how fast a gas molecule is colliding. Also, calculate average distance between molecules and compare to mean free path.

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Time scale for collision is $\approx \frac{l}{\bar{v}} = 0.63 \text{ ns}$

Volume occupied by 1 mole = 22.4 liter

Volume occupied by 1 molecule = 37.2 nm^3

Average distance between molecules = 3.3 nm

Mean free path was calculated as 795 nm

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Exercise problem 3: Calculate D for helium in argon at 1 atm and 25 °C with the Chapman-Enskog theory

$$D_{12} = \frac{1.86 * 10^{-3} * T^{1.5} * (1/M_1 + 1/M_2)^{0.5}}{P\sigma_{12}^2\Omega}$$

D in cm²/s
T in Kelvin
P in atm
M in g/mole
σ_{12} in Angstrom

Table 5.1-2 *Lennard–Jones potential parameters found from viscosities*

Substance		σ(Å)	ε_{12}/k_B(K)
Ar	Argon	3.542	93.3
He	Helium	2.551	10.2

Table 5.1-3 *The collision integral* Ω

k_BT/ε_{12}	Ω	k_BT/ε_{12}	Ω	k_BT/ε_{12}	Ω
0.30	2.662	1.65	1.153	4.0	0.8836
0.40	2.318	1.75	1.128	4.2	0.8740
0.50	2.066	1.85	1.105	4.4	0.8652
0.60	1.877	1.95	1.084	4.6	0.8568
0.70	1.729	2.1	1.057	4.8	0.8492
0.80	1.612	2.3	1.026	5.0	0.8422
0.90	1.517	2.5	0.9996	7	0.7896
1.00	1.439	2.7	0.9770	9	0.7556
1.10	1.375	2.9	0.9576	20	0.6640
1.30	1.273	3.3	0.9256	60	0.5596
1.50	1.198	3.7	0.8998	100	0.5130
1.60	1.167	3.9	0.8888	300	0.4360

Source: Data from Hirschfelder *et al.* (1954).

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D in cm²/s
T in Kelvin
P in atm
M in g/mole
σ_{12} in Angstrom

$$\epsilon_{12}/k_B = \sqrt{\epsilon_1/k_B * \epsilon_2/k_B} = \sqrt{93.3 * 10.2} = 30.8$$

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Substance		σ(Å)	ε_{12}/k_B(K)
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$$\frac{K_B T}{\epsilon_{12}} = 298/30.8 = 9.67$$

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$$\Omega \approx 0.75$$

$$\sigma_{12} = \frac{3.542 + 2.551}{2} = 3.047 \overset{o}{A}$$

$$D_{12} = \frac{1.86 * 10^{-3} * 298^{1.5} * (1/4 + 1/40)^{0.5}}{1 * 3.047^2 * 0.75}$$

$$= 0.72\ cm^2 s^{-1}$$

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