Øving 9

1

Experimental equilibrium data for adsorption of methane on Calgon PCB activated carbon are listed in a table below:

T = 296 K		T = 373 K			T = 480 K	
p (kPa)	*q (mol/kg)*	*p (kPa)*	*q (mol/kg)*	*p/q*	*p (kPa)*	*q (mol/kg)*
275.8	2.030	482.7	1.115	432.7	637.8	0.357
1137.6	4.082	1123.8	1.851	607.0	1296.2	0.758
2413.1	5.041	1620.3	2.231	726.3	2378.7	1.205
3757.6	5.398	1999.5	2.543	786.3	3709.3	1.606
5240.0	5.577	3447.4	3.168	1088.3	5329.6	1.918
6274.2	5.621	4929.7	3.480	1416.6	6246.6	2.075
6687.9	5.621	6157.0	3.681	1672.8	6687.9	2.142
		6584.4	3.770	1746.6		

1. Find out what type of adsorption isotherm gives a good fit to the data at T=373K.
2. Find the value of the adsorption equilibrium constant for T=373K. **Answer:** (5.395 x 10^{-4} kPa)$^{-1}$
3. Check if the equilibrium constant follows the Arrhenius type of T-dependency if
   $K_A(296) = 2.045\,.10^{-3}\ (kPa)^{-1}$
   $K_A(480) = 1.888\,.10^{-4}\ (kPa)^{-1}$

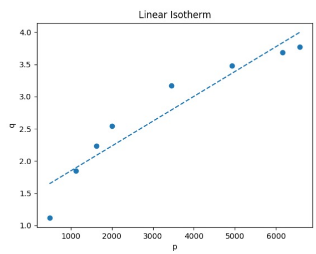
Hint: Plot $\ln K_A = 1/T$

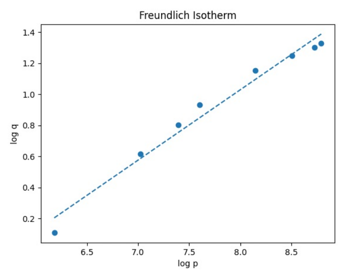
1)

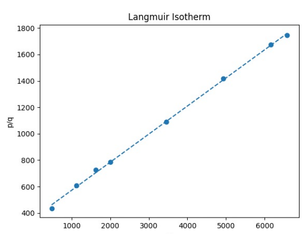
If linear: $q = kp$

If freundlich $\log q = \log k + \frac{1}{n} \log p$

If Langmuir $\frac{p}{q} = \frac{1}{q_m K} + \frac{p}{q_m}$







Langmuir isotherm fits best

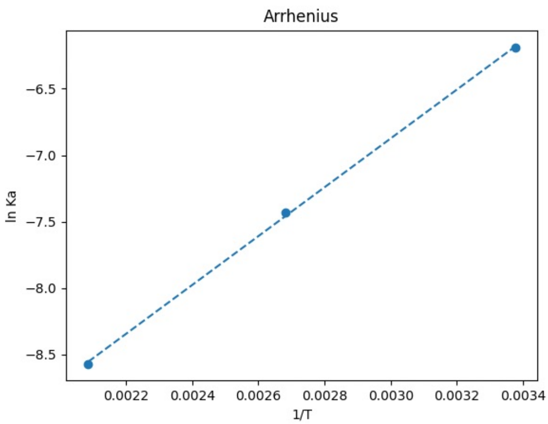
2) Extracting the constants from the regression of the langmuir isotherm gives:

$$\frac{1}{q_m K} = 359 \quad \text{and} \quad \frac{1}{q_m} = 0{,}213$$

$$\Rightarrow q_m = 4{,}70 \text{ mol/kg}$$

$$\underline{\underline{K = 5{,}93 \cdot 10^{-4} \text{ kPa}^{-1}}}$$

3) We check if plotting $\ln K_a$ vs. $1/T$ gives a straight line



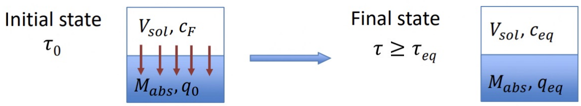
$\Rightarrow$ <u>It does appear to follow Arrhenius-type dependency</u>

2

A wastewater solution having a volume of 1.0 m³ contains 0.21 kg phenol/m³ of solution (0.21 g/L). A total of 1.40 kg of fresh granular activated carbon is added to the solution, which is then mixed thoroughly to reach equilibrium. The adsorption isotherm is given by: $q = 0.199c^{0.229}$

a) Plot the equilibrium and the operation lines. **Hint:** Arrange the equilibrium line so that they become a straight line.
b) Based on the plot. What are the final equilibrium values? **Answer:** $c_{eq} = 0.06\ kg\ phenol/m^3$, $q_{eq} = 0.1054\ kg\ phenol/kg\ adsorbent$
c) Calculate the final equilibrium values with a numerical method. **Hint:** Combine the equilibrium and operating line.
d) What percent of phenol is extracted? **Answer:** 70 %.

From power point:



a) + b) Balance over the system (before and after adsorption)

$$V_{sol} \cdot c_F + M_{abs} \cdot q_0 = V_{sol} \cdot c_{eq} + M_{abs} \cdot q_{eq}$$

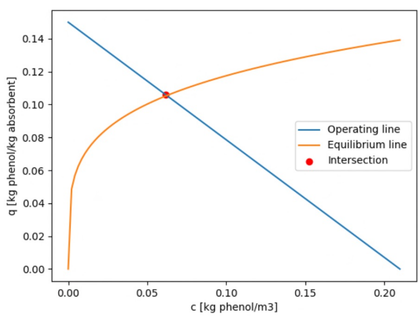
Solve for q_{eq} => operating line.

$$q_{eq} = q_0 + c_F \frac{V_{sol}}{M_{abs}} - c_{eq} \cdot \frac{V_{sol}}{M_{abs}} \quad \Big/ \quad c_F = 0{,}21,\ q_0 = 0,\ V_{sol} = 1,\ M_{abs} = 1{,}40$$

$$\Rightarrow q_{eq} = 0{,}15 - \frac{5}{7} c_{eq}$$

From the assignment => eq. line

$$q_{eq} = 0{,}199\, c_{eq}^{0{,}229}$$



$$\Rightarrow \underline{\underline{c_{eq} = 0{,}06\ kg\ phenol/m^3,\ q_{eq} = 0{,}1054\ kg\ phenol/kg\ absorbent}}$$

c) This was done in python using scipy.optimize.brentq,

Optimizing:

$$0{,}15 - \frac{5}{7} C_{eq} - 0{,}199\, c_{eq}^{0{,}229} = 0$$

$\Rightarrow$ $\underline{\underline{C_{eq} = 0{,}0624 \text{ kg phenol/m}^3,\ q_{eq} = 0{,}10544 \text{ kg phenol/kg absorbent}}}$

d)

$$\underline{\underline{\% \text{ exracted} = \frac{C_F - C_{eq}}{C_F} \cdot 100\% = 70{,}3\%}}$$

$\boxed{3}$

A 1 m high column is packed with activated alumina. The column initially contains pure liquid cyclohexane solvent. At time $\tau = 0$ a feed puls that contains 0.0001mol/L anthracene and 0.0002mol/L naphthalene in cyclohexane is injected for a 10 minutes time interval. The superficial velocity is 20 cm/min for both the feed and the purge step. Use the solute movement theory assuming linear adsorption isotherm and construct the outlet concentration profiles. Predict the exit times for the two components anthracene and naphthalene.

Data: Bulk density with air as fluid is 642.6kg/m^3, The adsorbent particle porosity is 0.51 and the bed void fraction is 0.39. Density of cyclohexane is 0.78 kg/L. The adsorption equilibrium constants are 22.0 L/kg adsorbent for anthracene and 16.0 L/kg adsorbent for naphthalene. Consider no sterically hindering effects.

We know the height of the column is 1m $\Rightarrow$ need to find the velocity

$$u_A = \frac{dz}{d\tau} \Rightarrow \tau_A = \frac{L}{u_A}$$

From solute movement theory:

$$u_A = \frac{V}{1 + K_d \frac{\varepsilon_p(1-\varepsilon_e)}{\varepsilon_e} + \frac{(1-\varepsilon_e)(1-\varepsilon_p)\rho_s}{\varepsilon_e} \cdot \frac{dq}{dc_A}} \qquad (1)$$

Given: $K_d = 1$ (no sterically hindering effects), $\varepsilon_p = 0{,}51$, $\varepsilon_e = 0{,}39$

Assuming linear isotherm: $\frac{dq}{dc_A} = K_A$ (given)

$K_a = 22 \text{ L/kg} = 22 \text{ dm}^3\text{/kg} = 0{,}022 \text{ m}^3\text{/kg}$, $K_n = 0{,}016 \text{ m}^3\text{/kg}$

$$\text{Need } V = \frac{V_s}{\varepsilon_e} = \frac{20 \text{ cm/min}}{0{,}39} = 51{,}28 \text{ cm/min} = 0{,}5128 \text{ m/min}$$

ρ_s: We know ρ_B.

$$\left.\begin{array}{l} \varepsilon_e = 1 - \dfrac{\rho_b}{\rho_p} \Rightarrow \rho_p = \dfrac{\rho_b}{1-\varepsilon_e} \\ \varepsilon_p = 1 - \dfrac{\rho_p}{\rho_s} \Rightarrow \rho_p = \rho_s(1-\varepsilon_p) \end{array}\right\} \rho_s = \frac{\rho_b}{(1-\varepsilon_e)(1-\varepsilon_p)}$$

$$\Rightarrow \rho_s = \frac{642{,}6 \text{ kg/m}^3}{(1-0{,}39)(1-0{,}51)} = 2150 \text{ kg/m}^3$$

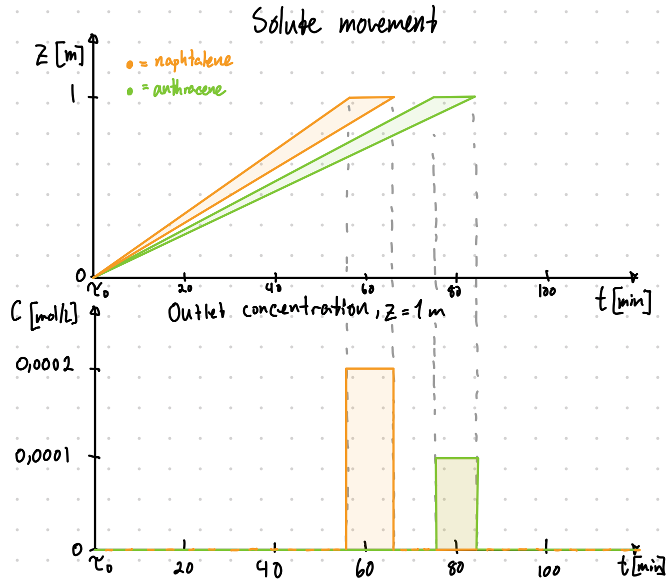
Inserting into 1:

$$u_a = \frac{0{,}5128 \text{ m/min}}{1 + 1 \cdot \frac{0{,}51(1-0{,}39)}{0{,}39} + \frac{(1-0{,}39)(1-0{,}51)}{0{,}39} \cdot 2150 \text{ kg/m}^3 \cdot 0{,}022 \text{ m}^3\text{/kg}} = 0{,}0135 \text{ m/min}$$

$$u_n = \frac{0{,}5128 \text{ m/min}}{1 + 1 \cdot \frac{0{,}51(1-0{,}39)}{0{,}39} + \frac{(1-0{,}39)(1-0{,}51)}{0{,}39} \cdot 2150 \text{ kg/m}^3 \cdot 0{,}016 \text{ m}^3\text{/kg}} = 0{,}0182 \text{ m/min}$$

$$\Rightarrow \tau_A = \frac{1 \text{ m}}{0{,}0135 \text{ m/min}} = \underline{\underline{74 \text{ min}}}$$

$$\tau_n = \frac{1 \text{ m}}{0{,}0182 \text{ m/min}} = \underline{\underline{55 \text{ min}}}$$



4

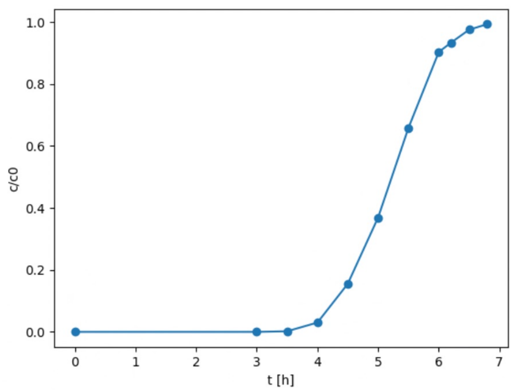
A water stream of alcohol vapor in air from a process was adsorbed by activated carbon particles in a packed bed having a diameter of 4 cm and length of 14 cm containing 79.2 g of carbon. The inlet gas stream having a concentration c_0 of 600 ppm and a density of 0.00115 g/cm³ entered the bed at a flow rate of 754 cm³/s. Table 1 provides data on the concentration measured at the outlet of the column. The break-point concentration is set at $c/c_0 = 0.01$. Do as follows:

a) Determine the break-point time, the total capacity used up to the break point, and the length of the unused bed. **Hint 1:** Start plotting the breakthrough concentration data. **Hint 2:** Use the trapezoidal rule to integrate the relevant equations. **Answer:** $t_u = 3.649\ h$.
b) If the break-point time required for a new column is 6.0 h, what is the new total length of the column required? **Answer:** $t_u = 20.344\ cm$.
c) Determine the saturation loading capacity of the carbon. **Answer:** $saturation\ capacity = 0.123\ g\ alcohol/g\ carbon$.

Table 1. Concentration at the outlet of the column

Time (h)	c/c0
0	0.000
3	0.000
3.5	0.002
4	0.030
4.5	0.155
5	0.396
5.5	0.658
6	0.903
6.2	0.933
6.5	0.975
6.8	0.993

a) Plotting the data:



We find t_b when $C_{out} = 1\%\ C_{in}$

$$\Rightarrow \frac{C}{C_0} = 0{,}01$$

By linear regression, $\underline{\underline{t_b = 3{,}6415\ h}}$

not the same as the provided solution, should I have used some other interpolation rule?

t_d is found when $\frac{C}{C_0} = 1$

By linear regression, $t_d = 6{,}9160\ h$

The column capacity is found from

$$\tau_T = \int_0^{t_d \to \infty} \left(1 - \frac{c}{c_0}\right) dt$$

numerically $\rightarrow$ $$= \underbrace{\int_0^{t_b} \left(1 - \frac{c}{c_0}\right) dt}_{\tau_b} + \underbrace{\int_{t_b}^{t_d} \left(1 - \frac{c}{c_0}\right) dt}_{\tau_d}$$

python, np.trapz $$= 3{,}6415 \text{ h} + 1{,}5490 \text{ h}$$

$$= 5{,}1892 \text{ h}$$

The used bed height is given by:

$$H_b = \frac{\tau_b}{\tau_t} H_T$$

The unused bed height is given by

$$H_{unb} = H_T - H_b = \left(1 - \frac{\tau_b}{\tau_t}\right) H_t = \left(1 - \frac{3{,}6415}{5{,}1892}\right) 14 \text{ cm}$$

$$\underline{\underline{H_{unb} = 4{,}176 \text{ cm}}}$$

b) Assuming that H_{unb} remains constant (which is most likely the case), then only H_b will change:

$$H_b = H_{b,old} \cdot \frac{\tau_{b\,new}}{\tau_{b\,old}} = \frac{\cancel{\tau_{b.old}}}{\tau_{T\,old}} \cdot H_{T_{old}} \cdot \frac{\tau_{b\,new}}{\cancel{\tau_{b.old}}}$$

$$H_b = \frac{6 \text{ h}}{5{,}1892 \text{ h}} \cdot 14 \text{ cm}$$

$$H_b = 16{,}187 \text{ cm}$$

$$H_T = H_b + H_{unb} = (16{,}187 + 4{,}176)\ cm$$

$$\underline{\underline{H_T = 20{,}363\ cm}}$$

c) The column is "full" at t_d, need to find how much alcohol has passed through the column by then.

$$\dot{m}_{air} = 754\ \frac{\cancel{cm^3}}{\cancel{s}} \cdot 0{,}00115\ \frac{g}{\cancel{cm^3}} \cdot 3600\ \frac{\cancel{s}}{h} = \underline{3121{,}56\ g/h}$$

$$\dot{m}_{OH} = \dot{m}_{air} \cdot \frac{660\ g\ OH}{10^6\ g\ air} = \qquad g/h$$

$$m_{OH,\,absorbed} = 1{,}873\ g/\cancel{h} \cdot 5{,}1892\ \cancel{h} = \underline{9{,}719\ g}$$

$$\Rightarrow \text{Saturation capacity} = \frac{9{,}719\ g\ OH}{79{,}2\ g\ C} = \underline{\underline{0{,}123\ \frac{g\ OH}{g\ C}}}$$