Question:

Jasmone ($C_{11}H_{16}O$) is a valuable material in the perfume industry, used in many soap and cosmetics. Suppose we are recovering this material from a **water** suspension (concentration of jasmone in water is 5mM) by an extraction with **benzene**. The local mass transfer coefficient in water is $3.0 \cdot 10^{-4}\,\frac{cm}{s}$ and the local mass transfer coefficient in benzene is $2.4 \cdot 10^{-3}\,\frac{cm}{s}$. The interfacial concentrations are in equilibrium according to the following equation $C_{j,benzene} = 170\ C_{j,water}$.

a) Calculate the interfacial concentration of jasmone in water and in benzene

b) Calculate the molar flux

c) Determine if one side is limiting the mass transport using the partition coefficients

d) Draw the qualitative liquid/liquid **concentration diagram**, which means identify the concentration values, in bulk and at the interface, along with the direction of the molar flux (in the exam sheets, not here).

e) Qualitatively identify bulk, equilibrium and interface concentrations in the **equilibrium diagram** (in the exam sheets, not here).

f) Can you briefly explain in which cases we introduce the overall mass transfer coefficient? Do the equilibrium concentration have any physical meaning?

Solution:

a) If we equate the local fluxes of jasmone:

$$n_j = k_W^{loc}\left(C_{j,W,b} - C_{j,W,o}\right) = k_B^{loc}\left(C_{j,B,o} - C_{j,B,b}\right)(\boldsymbol{Eq.1})$$

Also, it is given that the interface concentration are in equilibrium as per the following relation:

$$C_{j,B,o} = 170 * C_{j,W,o}\ (\boldsymbol{Eq.2})$$

In order to solve for $C_{j,W,o}$:

$$k_W^{loc}\left(C_{j,W,b} - C_{j,W,o}\right) = k_B^{loc}(170 * C_{j,W,o} - C_{j,B,b})$$

Thus, we get

$$C_{j,W,o} = \frac{\left(k_W^{loc} C_{j,w,b} + k_B^{loc} C_{j,B,b}\right)}{\left(170 k_B^{loc} + k_W^{loc}\right)}(\boldsymbol{Eq.3})$$

If we put the values from the question,

$$C_{j,W,o} = \frac{(3 \times 10^{-6} \times 0.005 + 2.4 \times 10^{-5} \times 0)}{(170 \times 2.4 \times 10^{-5} + 3 \times 10^{-6})}$$

$$C_{j,W,o} = 3.6 \times 10^{-6} M$$

Since $C_{j,W,o}$ is in equilibrium with $C_{j,B,o}$ as per $\boldsymbol{Eq.2}$,

$$C_{j,B,o} = 170 * C_{j,W,o} = 0.612 \times 10^{-3} M$$

b) In order to solve for the molar flux, we can use the $(\boldsymbol{Eq.1})$

$$n_j = k_W^{loc}\left(C_{j,W,b} - C_{j,W,o}\right)$$

$$n_j = 3 \times 10^{-6} m/s \ \times (0.005 - 0.0000036) \times 10^3 mol/m^3$$

$$n_j = 0.015 \times 10^{-3} mol/m^2 s$$

c) To determine if mass transfer is limited on one side, we have to calculate m_{B}, m_{W} and m_{avg}

$$m_{\mathrm{B}} = \frac{\mathrm{c_{j,B,0}} - \mathrm{c}_{\mathrm{j,B,b}}^{eq}}{\mathrm{c_{j,W,0}} - \mathrm{c_{j,W,b}}} = \frac{0.612 \times 10^{-3} - 170 \times 0.005}{3.6 \times 10^{-6} - 0.005} = 170$$

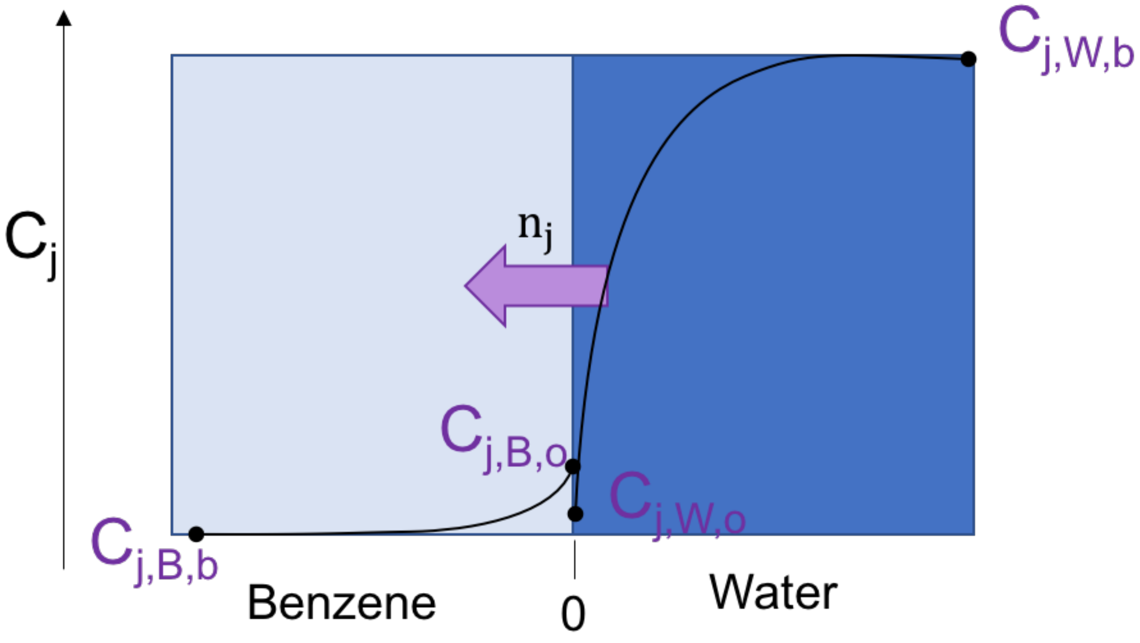
$$m_{\mathrm{W}} = \frac{\mathrm{c_{j,B,b}} - \mathrm{c_{j,B,0}}}{\mathrm{c}_{\mathrm{j,W}}^{eq} - \mathrm{c_{j,W,0}}} = \frac{0 - 0.612 \times 10^{-3}}{0 - 3.6 \times 10^{-6}} = 170$$

$$m_{avg} = \tfrac{1}{2}(m_{\mathrm{B}} + m_{\mathrm{W}}) = \tfrac{1}{2}(170 + 170) = 170$$

$$\boldsymbol{\frac{k_W^{loc}}{m_{avg} k_{\mathrm{B}}^{loc}} = \frac{3 \times 10^{-6} \frac{m}{s}}{170 \times 2.4 \times 10^{-5} \frac{m}{s}} = 0.0007}$$

Since $\boldsymbol{\frac{k_W^{loc}}{m_{avg} k_{\mathrm{B}}^{loc}}} \ll \mathbf{1,}$ the mass transfer is controlled by the water phase.

d)



where

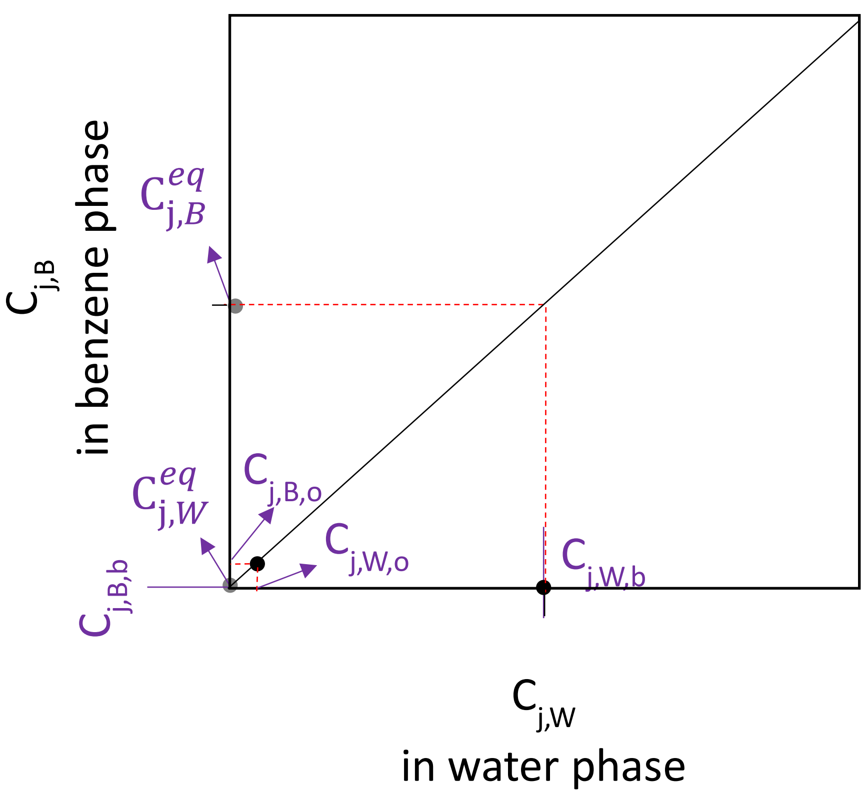
$$C_{j,W,b} = 0.005M$$

$$C_{j,W,o} = 0.0000036M$$

$$C_{j,B,b} = 0$$

$$C_{j,B,o} = 0.0006M$$

e) The graph below is quantitative, a qualitative version is also accepted considering the challenge in positioning $C_{j,B,b}$ and $C_{j,w,eq}$ at the origin.



$$C_{j,W}^{eq} = \frac{C_{j,B,b}}{170} = 0$$

$$C_{j,B}^{eq} = 170 \times C_{j,W,b} = 0.85M$$

f)

The interface concentrations are not normally known and only the bulk concentrations and local mass transfer co-efficients are known in real life problems. Hence, it is easier to have overall mass transfer coefficients relating the bulk concentrations. In order to convert the local mass transfer to overall mass transfer coeffiecients, we use theoretical values as equilibrium concentration. These equilibrium concentrations do not physically appear anywhere in the system and is just a simplification to solve the problems.

Indeed, for the sake of knowledge, if we rigorously solve the equations of local mass transfer coefficient to relate the flux to known bulk concentrations, interface equilibrium relation (solubility curve) and local mass transfer co-efficients, we can derive the theoretical equilibrium concentrations as shown below:

$$n_j = k_B^{loc}\left(C_{j,B,o} - C_{J,B,b}\right) = K_B\left(C_{j,B}^{eq} - C_{j,B,b}\right)\boldsymbol{Eq.5}$$

If we express $\boldsymbol{C_{j,B,o}}$ in terms of known quantities like k_B^{loc}, $k_W^{loc}$and $C_{J,W,b}$, from $\boldsymbol{Eq.2}$ and $\boldsymbol{Eq.3}$, for the first term of the equation with the local mass transfer coefficient we get

$$n_j = k_B^{loc}\left(\frac{\left(170k_W^{loc}C_{j,W,b} + 170k_B^{loc}C_{j,B,b}\right)}{170k_B^{loc} + k_w^{loc}} - C_{J,B,b}\right)$$

$$n_j = k_B^{loc}\left(\frac{\left(170k_W^{loc}C_{j,W,b} + 170k_B^{loc}C_{j,B,b}\right) - \left(170k_B^{loc}C_{j,B,b} + k_W^{loc}C_{j,B,b}\right)}{170k_B^{loc} + k_w^{loc}}\right)$$

$$n_j = k_B^{loc}\left(\frac{170k_W^{loc}C_{j,W,b} - k_W^{loc}C_{j,B,b}}{170k_B^{loc} + k_w^{loc}}\right)$$

$$n_j = \left(\frac{k_B^{loc}k_W^{loc}}{170k_B^{loc} + k_w^{loc}}\right)\left(170C_{j,W,b} - C_{j,B,b}\right)$$

$$n_j = \left(\frac{1}{\frac{170}{k_W^{loc}} + \frac{1}{k_B^{loc}}}\right)\left(170C_{j,W,b} - C_{j,B,b}\right)$$

This equation when equated to the overall mass transfer coefficient from $\boldsymbol{Eq.5,}$

$$\left(\frac{1}{\frac{170}{k_W^{loc}} + \frac{1}{k_B^{loc}}}\right)\left(170C_{j,W,b} - C_{j,B,b}\right) = K_B\left(C_{j,B}^{eq} - C_{j,B,b}\right)$$

Thus, we get

$$\frac{1}{K_B} = \frac{170}{k_W^{loc}} + \frac{1}{k_B^{loc}}$$

and

$$C_{j,B}^{eq} = 170C_{j,W,b}$$

Basically, in order to use the overall mass transfer coefficient and equation 5 to be valid, we MUST impose that $C_{j,B}^{eq}$,which is the theoretical concentration of jasmone in benzene, is in equilibrium with the concentration of jasmone in water bulk