

Q1: A solvent contaminated with 0.03 kmol/m^3 of a fatty acid is to be purified by passing it through a fixed bed of activated carbon which will adsorb the acid (but not the solvent). The operation is isothermal and equilibrium is maintained between the liquid and the solid. *Here adsorption is dominant over diffusive transport.* The bed has a diameter of 0.15 m , porosity of 0.4 , and initially free of adsorbate.

Calculate the length of the bed to give 1 hr of operation when the fluid is fed at 0.1 L/s ($10^{-4} \text{ m}^3/\text{s}$). Use an equilibrium fixed bed theory for the calculations of three types of isotherm:

(a) $q = 10C$

(b) $q = 3\sqrt{C}$ – use the mean slope in this case

(c) $q = 10^4 C^2$ – consider breakthrough concentration as 10% of feed inlet.

[10]

Q2: Hard water containing 500 ppm (by weight) MgCO_3 and 50 ppm NaCl is to be softened in a fixed, gel resin bed with a cation capacity of 2.3 eq/L of bed volume. The bed is 2.6 m in diameter and packed to a height of 3.05 m , with a wetted-resin void fraction of 0.38 . During loading, the recommended throughput is 10.18 L/s-m^2 . During displacement, regeneration, and washing, flow rate is reduced to 1.018 L/s-m^2 . The displacement and regeneration solutions are water-saturated with NaCl (26 wt%). Determine: (a) feed flow rate, L/minute; (b) loading time to breakthrough, h; (c) loading wave-front velocity, cm/minute; (d) regeneration solution flow rate, L/minute; and (e) displacement time (in h), and (f) additional time for regeneration (in h)

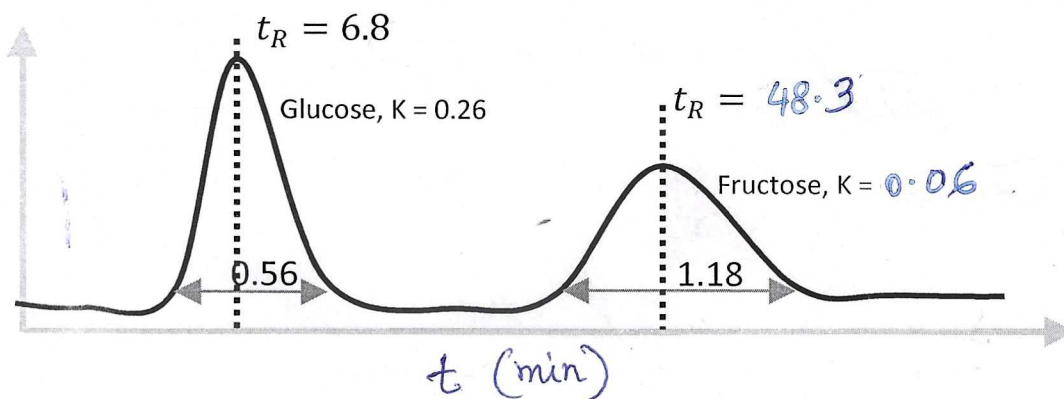
The equilibrium constant $K_{\text{Mg}^{2+}, \text{Na}^+} = 3.3/2$

[10]

Q3: Chromatographic separation of glucose and fructose separation is performed in C18 RP zorbax column of $200 \text{ mm (L)} \times 1 \text{ mm (ID)}$. The column bed porosity is 0.3 , and the particle inclusion porosity is 0.5 . The chromatogram is shown below. What is the flow rate of the solute injection used here? Calculate the number of theoretical plates (N) and the resolution (R) of glucose separation?

The adsorption isotherms are linear and independent, $q_i = K_i c_i$

[10]



Solution to MT2 test QP 1 (11 Nov 2023)

- Q1: For adsorption dominated (over diffusion) transport in fixed bed, the species transport eqn:

$$\epsilon \left(\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial z} \right) = -(1-\epsilon) \frac{\partial q}{\partial t}$$

where ϵ is the fixed bed porosity.

Now since, equilibrium is established in this case,

$$\frac{\partial q}{\partial t} = \underbrace{\frac{\partial q}{\partial c}}_{q'(c)} \cdot \frac{\partial c}{\partial t}$$

(& no mass transfer resistance to transfer of molecules of adsorbate from bulk fluid to adsorption site)

$$\text{So, } \frac{\partial c}{\partial t} + u \frac{\partial c}{\partial z} = -\frac{1}{m} q'(c) \frac{\partial c}{\partial t}$$

$$\text{where } m = \frac{\epsilon}{1-\epsilon}$$

the isotherm $q(c)$ is ^{based on} equilibrium isotherm relation.

$$\text{Also, } \left. \frac{\partial c}{\partial t} \right|_z = - \left(\frac{\partial c}{\partial z} \right)_t \underbrace{\left(\frac{\partial z}{\partial t} \right)_c}_{\text{this represents wave front of MTZ}}$$

$$\therefore \left\{ u - \left[1 + \frac{1}{m} q'(c) \right] \frac{\partial z}{\partial t} \right\} \frac{\partial c}{\partial z} = 0$$

$$\text{Hence, } \left(\frac{\partial z}{\partial t} \right)_c = \frac{u}{1 + \frac{1}{m} q'(c)}$$

- For a constant pattern wave front propagation, only the leading zone has to be considered. Thus, above eqn can be integrated at constant c , to give

$$\frac{ut}{1 + \frac{1}{m} q'(c)} = z - z_0$$

where z_0 is the position of c initially. For a bed initially free of adsorbate, $z_0 = 0$ for all values of c .

$$\text{For (a), } q = 10c, \text{ so } q'(c) = 10$$

$$u = 10^{-4} / [(\pi/4)(0.15^2 \epsilon)] \text{ m/s}$$

$$\text{for } \epsilon = 0.4, \quad m = \frac{\epsilon}{1-\epsilon} = \frac{0.4}{0.6}$$

$$\text{Here } t = 3600 \text{ s, } z = \left(\frac{4 \times 10^{-4}}{\pi \cdot 0.15^2 \cdot 0.4} \right) \frac{3600}{1 + 10(0.6/0.4)} = 3.18 \text{ m}$$

For case (b), $q = 3\sqrt{C}$, $q' = 1.5/\sqrt{C}$

As C increases, $q'(C)$ decreases and points of higher conc. are predicted to move a greater distance in a given time than lower concentrations. It is not possible for points of high conc. to overtake low conc., and since $z_0 = 0 \forall C$, the adsorption wave propagate as a step change (similar to previous case)

$$\text{Mean slope of } q' \sim \frac{q(C_0)}{C_0}$$

$$\therefore z = \frac{u t}{1 + \frac{1}{m} \frac{q(C_0)}{C_0}} = \left(\frac{4 \times 10^{-4}}{\pi \cdot 0.15^2 \cdot 0.4} \right) \left(\frac{3600}{1 + (0.6/0.4)(3/\sqrt{6})} \right)$$
$$= 1.88 \text{ m}$$

For case (c): $q = 10^4 C^2$, $q'(C) = 2 \times 10^4 C$

As C increases, $q'(C)$ increases such that, in a given time, z for lower concentrations is greater than for high conc. For the breakthrough conc.,

$$C = 0.1 C_0 = 0.003 \text{ kmol/m}^3,$$

$$q'(C=0.003) = 60$$

$$\text{Hence, } z = \left(\frac{4 \times 10^{-4}}{\pi \cdot 0.15^2 \cdot 0.4} \right) \left(\frac{3600}{1 + (0.6/0.4) q'(C)} \right)$$
$$= 0.55 \text{ m}$$

Q9. MW of $\text{MgCO}_3 = 83.43$ (you can consider 83)

$$\text{Conc. of } \text{MgCO}_3 \text{ in feed} = \frac{500}{83.43 \times 10^3} = 0.006 \text{ mol/L} \\ \text{or } 0.012 \text{ eq/L}$$

MW of $\text{NaCl} = 58.45$ (you can consider 58)

$$\text{Conc. of } \text{NaCl} \text{ in feed} = \frac{50}{58.45 \times 10^3} = 0.000855 \text{ mol/L} \\ \text{or eq/L}$$

(a) Bed cross-section area $= \pi D^2/4 = 5.31 \text{ m}^2$

$$\text{Feed solution flow rate} = 10.18(5.31) \approx 54 \text{ L/s or } 3240 \text{ L/min}$$

(b) Behind the loading wave front:

$$x_{\text{Mg}^{2+}} = \frac{0.012}{0.012 + 0.000855} = 0.9335$$

Since no NaCl in the feed is exchanged:

$$C = 0.012 \text{ eq/L and } Q = 2.3 \text{ eq/L}$$

$$\text{Here } K_{\text{Mg}^{2+}, \text{Na}^+} = 3.3/2 = 1.65$$

The equilibrium relation between Mg^{2+} (and Na^+) is,

$$K \left(\frac{Q}{C} \right) = \frac{y_{\text{Mg}^{2+}} (1 - x_{\text{Mg}^{2+}})^2}{x_{\text{Mg}^{2+}} (1 - y_{\text{Mg}^{2+}})^2}$$

$$\Rightarrow 1.65 \left(\frac{2.3}{0.012} \right) = \frac{y_{\text{Mg}^{2+}} (1 - 0.9335)^2}{0.9335 (1 - y_{\text{Mg}^{2+}})^2}$$

$$\text{Solving for } y_{\text{Mg}^{2+}} = 0.9961$$

$$\text{Bed volume} = (5.31)(3.05) = 16.195 \text{ m}^3 \text{ or } 16,195 \text{ L}$$

$$\text{Total bed capacity} = 2.3(16195) = 37248 \text{ eq}$$

$$\text{Mg}^{2+} \text{ adsorbed by resin} = 0.9961(37248) = 37103 \text{ eq}$$

$$\text{Mg}^{2+} \text{ entering bed in feed solution}$$

$$= 0.012(3240) = 38.88 \text{ eq/min}$$

$$\therefore t_L = \frac{37103}{38.88} = 954.3 \text{ min (or } 15.9 \text{ h)}$$

$$(c) u_L = L/t_L = 3.05/954.3 = 0.0032 \text{ m/min (or } 0.32 \text{ cm/min)}$$

(d) Flow rate of regeneration solution .

$$= \left(\frac{1.018}{10.18} \right) (3240) = 324 \text{ L/min}$$

(e) Displacement time = time for 324 L/min to displace liquid in the voids. Void volume = $(0.38) 16195$
 $= 6154 \text{ L}$

$$\text{and } t_D = 6154/324 = 19 \text{ min}$$

(f) For 26% NaCl, density can be considered as 1.2 g/cc

Flow of Na^+ in regenerated solution

$$= \frac{324 (1000) (1.2) 0.26}{58.45} = 1729 \text{ eq/min}$$

$$\text{NaCl conc. in regenerating solution} = \frac{1729}{324} = 5.34 \text{ eq/L}$$

$$\therefore \frac{Q}{C_R} K_{Mg^{2+}, Na^+} = 1.65 \left(\frac{2.3}{5.34} \right) = 0.71$$

Since it is less than 1, but not much less than 1. Therefore, regeneration wave front may not sharpen rapidly, considering a shock-wave like front. Thus, no additional time is needed for regeneration.

Q3. For pulse chromatography input, the output profile is gaussian in nature, with solute mean residence time, $t_R = \frac{L}{\omega v_i}$

where ω is the fraction of solute in the moving phase @ equilibrium and v_i is the interstitial solution velocity.

$$\omega = \frac{1}{1 + \frac{1-\epsilon_b}{\epsilon_b} \cdot \frac{1}{\alpha}} \quad \left[\text{where } \alpha = \frac{1}{\epsilon_p} \quad (\epsilon_p: \text{inclusion porosity}) \right]$$

Alternatively, $t_R = \frac{L}{u_i}$

where u_i is the wave front velocity (assuming const. ideal wave front in equilibrium)

$$u_i = \frac{v_i}{1 + \frac{1-\epsilon_b}{\epsilon_b} K} = \frac{v_i}{1 + \frac{1-\epsilon_b}{\epsilon_b} K} \quad (\text{for linear isotherm})$$

Thus, the superficial solution velocity $u_s \equiv \epsilon_b u_i$

(a) Here (using glucose peak information)

$$t_R = 6.8 \text{ min}, \quad L = 200 \text{ mm}, \quad \epsilon_b = 0.3, \quad K = 0.26$$

$$u_i = L/t_R = \frac{200}{6.8} = 29.4 \text{ mm/min or } 2.94 \text{ cm/min}$$

$$\therefore v_i = 2.94 \left(1 + \frac{1-0.3}{0.3} (0.26) \right) = 4.72 \text{ cm/min}$$

$$\text{and hence, } u_s = 0.3 (4.72) = 1.417 \text{ cm/min}$$

$$\therefore \text{flow rate} \equiv u_s \left(\frac{\pi D^2}{4} \right) = 1.417 \left(\frac{\pi 0.1^2}{4} \right) = 0.011 \text{ ml/min}$$

(b) The standard deviation, $\sigma^2 = \frac{t_R H}{u_i}$

where H is the height of each (theoretical) chromatographic plate.

From the gaussian curve, it is known that $4\sigma = \text{peak base width}$

$$\therefore \frac{t_B^2}{16} = t_R H / u_i = \frac{t_R^2}{N} \quad \left[\because L = N H \right]$$

or, $N = 16 \left(\frac{t_R^2}{t_B^2} \right)$ # plates

From the information present in the chromatogram,

$$N = 16 \left(\frac{6.8^2}{0.56^2} \right) \approx 2359$$

(c) Resolution R of two solutes is defined by the ratio of peak separation relative to the average peak width.

$$R = \frac{|t_{R1} - t_{R2}|}{(t_{B1} + t_{B2})/2} = \frac{|6.8 - 48.3|}{(0.56 + 1.18)/2} = 47.7$$

Alternatively, $R \equiv \frac{\delta \sqrt{N}}{4}$

where δ is the fractional difference in wave front velocities in the fluid phase ~~tt~~

$$\delta = 2 \frac{|u_i - u_j|}{u_i + u_j}$$