<u>Problem Set #5</u>

Given:

-C_F = 0.0177 lb H_2O/lb dry air, concentration of water in the air feed stream
-P = 1atm
-T = 80ºF
-v = 100 ft/min, superficial velocity
-D = 2.8 mm, diameter of spherical particles made of silica gel inside bed
-ρ_b = 39 lb/ft^3 bed, bed density
-H = 5 ft, bed height
-q = 15.9p, linear absorption isotherm for water vapor where q [=] lb H_2O/lb gel and p [=] atm, is the partial pressure of water vapor
-D_e = 0.05 cm^2/s, effective diffusivity of water vapor in the adsorbent particle
-C_{out} = 0.0009 lb H_2O/lb dry air, concentration of water in the outlet stream at breakthrough
-process is isothermal and isobaric

Objective:

Compare the equilibrium and mass-transfer models for a fixed-bed adsorption of water from air using silica gel.

In order to start this problem, we must first determine the weight and mole fraction of water in the inlet stream, the partial pressure of water, and the molecular weight and density of the air/water mixture.

To determine the weight fraction of water in the inlet stream, we know from C_F that for every lb of dry air there is 0.0177 lb of H_2O. Therefore the weight fraction of water would be the weight of water vapor divided by the weight of the solution (which is made up of water vapor and air).

$$\frac{0.0177lb\_H_2O}{0.0177lb\_H_2O + 1lb\_air} = 0.01739 \text{ or } \mathbf{1.739\ wt\%\ water}$$

To find the mole fraction, we use a similar equation but must convert lbs to moles to that the water and air can be compared on the same basis. First we must convert lbs to moles.

$$0.0177lb\_H_2O \times \frac{453.5924g}{1lb\_H_2O} \times \frac{1mol\_H_2O}{18.02g} = 0.4455mol\_H_2O$$

$$1lb\_air \times \frac{453.5924g}{1lb\_air} \times \frac{1mol\_air}{28.97g} = 15.6573mol\_air$$

Again, we can use the same equation as above to calculate the mole fraction of water.

$$\frac{0.4455mol\_H_2O}{0.4455mol\_H_2O + 15.6573mol\_air} = 0.0277$$

Therefore the **mole fraction of water is 0.0277 and the mole fraction of air is 0.9723**.

To calculate the partial pressure of water, we use Dalton's Law making the assumptions that the solution is ideal and that the liquid phase contains only pure water (x_w = 1). Also, since P, the total pressure of the system is equal to 1atm the equation further reduces to the following

$$y_w = P_w = 0.0277atm$$

The average molecular weight of the solution is determined by the following equation.

$$MW_{solution} = \sum_i MW_i y_i = MW_w y_w + MW_a y_a = 28.67 \frac{g}{mol\_solution}$$

The density of the solution can be determined by using the ideal gas law.

$$\rho = \frac{PMW_{solution}}{RT} = \frac{(1atm)\left(28.67\frac{kg}{kmol}\right)}{\left(\frac{0.082m^3 - atm}{mol - K}\right)(299.82K)} = 1.166\frac{kg}{m^3} \text{ or } 0.07279\frac{lb}{ft^3 bed}$$

Equilibrium Model:
In the equilibrium model, we assume that there is 100% utilization of the bed. In order to determine the time for breakthrough, we first need to determine the amount of water adsorbed by the bed.

From the adsorption isotherm, q = 15.9p we can q which is the amount of H_2O per lb of silica gel. p is the partial pressure of water, which was previously determined to be 0.0277 atm. Plugging into the equation, we obtain q = 0.44043 $\frac{lb\_H_2O}{lb\_silica\_gel}$.

To determine the total amount of water adsorbed by the bed we need to know the amount of silica gel in the bed. This can be found by multiplying the bed density by the volume of the bed. The volume is the cross-sectional area of the bed multiplied by the height of the bed.

$$\rho_b V = 39\frac{lb}{ft^3 bed} \times (1ft^2)(5ft) = 195lb\_silica\_gel$$

By multiplying q by the amount of silica gel in the bed, we find that at equilibrium, **the bed can adsorb 85.8839 lb of H_2O**.

By determining the flow rate of water, which is the mass flow rate multiplied by the weight fraction of water, we can determine what time breakthrough will occur. Given the superficial velocity, we can multiple by the cross-sectional area to get the volumetric flow rate, Q. **Q = 100 ft^3/min.** The mass flow rate, F, is equal to the volumetric flow rate multiplied by the density of the solution. **F = 7.279 lb/min**. By multiplying the mass flow rate by the weight fraction of water determined earlier, we find that **the flow rate of water is 0.1264 lb H_2O/min**.

Knowing the amount of water the bed can adsorb and the water flow rate, we determine **the breakthrough time to be $t_{breakthrough}$ = 679.46 min.**

Mass-Transfer Model:
In the mass-transfer model, we must use the Klinkenberg equation to determine the time that breakthrough occurs. We must first determine the overall mass transfer coefficient using the following equation.

$$\frac{1}{kK} = \frac{R_p}{3k_c} + \frac{R_p{}^2}{15D_e}$$ where R_p = 0.0014 m and D_e = 5.0E-6 m^2/s

k_c can be determined using the following correlation

$$k_c = \frac{D_{water}}{D_p}\left[2 + 1.1\left(\frac{D_p G}{\mu}\right)^{0.6}\left(\frac{\mu}{\rho D_{water}}\right)^{0.33}\right]$$ where D_{water} = 0.26E-4 m^2/s and μ = 1.75E-5 kg/m-s.

From unit analysis, we can see the G, the velocity of the fluid must have the units kg/m^2-s in order for the Reynolds number to be dimensionless.

$$G = 7.279\frac{lb}{\min} \times \frac{1}{1ft^2} \times \frac{0.4536kg}{1lb} \times \frac{10.7639ft^2}{1m^2} \times \frac{1\min}{60\sec} = 0.5923\frac{kg}{m^2 - s}$$

All other values in the equation are known, by plugging in we can get k_c, the mass transfer coefficient.

$$k_c = \frac{0.26\times10^{-4}\ \frac{m^2}{s}}{2.8\times10^{-3}\,m}\left[2+1.1\left(\frac{\left(2.8\times10^{-3}\,m\right)\left(0.5923\,\frac{kg}{m^2-s}\right)}{1.75\times10^{-5}\ \frac{kg}{m-s}}\right)^{0.6}\left(\frac{1.75\times10^{-5}\ \frac{kg}{m-s}}{\left(1.1667\,\frac{kg}{m^3}\right)\left(0.26\times10^{-4}\ \frac{m^2}{s}\right)}\right)^{0.33}\right] = 0.149\,\frac{m}{s}$$

Finally, before solving for k, the overall transfer coefficient, we need to convert the units of K.

K must be in the units $\dfrac{\frac{lb\_H_2O}{ft^3 gel}}{\frac{lb\_H_2O}{ft^3 gas}}$. The K in the given problem statement has the units $\dfrac{lb\_H_2O}{lb\_gel-atm}$.

Prior to converting units, we must first solve for the particle density using equation 15.4.

$$\rho_p = \frac{\rho_b}{1-\varepsilon_b} = \frac{39\,\frac{lb\_gel}{ft^3 bed}}{(1-0.47)\frac{ft^3 gel}{ft^3 bed}} = 73.5849\,\frac{lb\_gel}{ft^3 gel}$$

$$K = \frac{\left(15.9\,\frac{lb\_H_2O}{lb\_gel-atm}\right)\left(73.6\,\frac{lb\_gel}{ft^3 gel}\right)(0.0277\,atm)}{0.001264\,\frac{lb\_H_2O}{ft^3 gas}} = 25645.29\,\frac{\frac{lb\_H_2O}{ft^3 gel}}{\frac{lb\_H_2O}{ft^3 gas}}$$

Finally, we can solve for k by rearranging the above equation.

$$k = \frac{1}{K\left[\frac{R_p}{3k_c}+\frac{R_p{}^2}{15D_e}\right]} = \frac{1}{25645.29\left[\frac{0.0014m}{3\left(0.149\,\frac{m}{s}\right)}+\frac{(0.0014m)^2}{15\left(5\times10^{-6}\ \frac{m^2}{s}\right)}\right]} = 0.00133\,\frac{1}{s}$$

With all variables known, we can now solve for the breakthrough time for the mass-transfer model. We first use the length to determine the value of ξ at breakthrough. At breakthrough the length traveled in the bed is the height of the bed, therefore z = 5 ft or 1.524 m.

$$\xi = \frac{kKz}{u}\left(\frac{1-\varepsilon_b}{\varepsilon_b}\right) = \frac{\left(0.00133\,\frac{1}{s}\right)(25645.29)(1.524m)}{1.08\,\frac{m}{s}}\left(\frac{1-0.47}{0.47}\right) = 35.6134$$

where u is the interstitial velocity $u = \dfrac{v}{\varepsilon_b} = \dfrac{100\,\frac{ft}{\min}}{0.47} = 213\,\dfrac{ft}{\min}\times\dfrac{1m}{3.2808\,ft}\times\dfrac{1\min}{60\sec} = 1.08\,\dfrac{m}{s}$

Since, we know that at breakthrough the value of $\dfrac{C}{C_F} = 0.05$, we are left with one unknown in the Klinkenberg equation, t. Using excel solver, we can solve the following equation for t

$$\frac{C}{C_F} = \frac{1}{2}\left[1 + erf\left(\sqrt{\tau} - \sqrt{\xi} + \frac{1}{8\sqrt{\tau}} + \frac{1}{8\sqrt{\xi}}\right)\right]$$

$$0.05 = \frac{1}{2}\left[1 + erf\left(\sqrt{\tau} - \sqrt{35.6134} + \frac{1}{8\sqrt{\tau}} + \frac{1}{8\sqrt{35.6134}}\right)\right] \text{ where } \tau = k\left(t - \frac{z}{u}\right)$$

Solving, we find that $\mathbf{t_{breakthrough}}$ **= 476.91 minutes.**

Mass-Transfer Zone:
To find the mass transfer zone, we need to find the length the front has traveled within the bed when $t = t_{breakthrough}$ and $\frac{C}{C_F} = 0.95$. Again we use the Klinkenberg equation, but solve for z instead of t.

$$0.95 = \frac{1}{2}\left[1 + erf\left(\sqrt{\tau} - \sqrt{\xi} + \frac{1}{8\sqrt{\tau}} + \frac{1}{8\sqrt{\xi}}\right)\right]$$

Using Excel solver, we find that z = 0.7159. Therefore the mass transfer zone is the difference between the length at $\frac{C}{C_F} = 0.05$ and the length at $\frac{C}{C_F} = 0.95$.

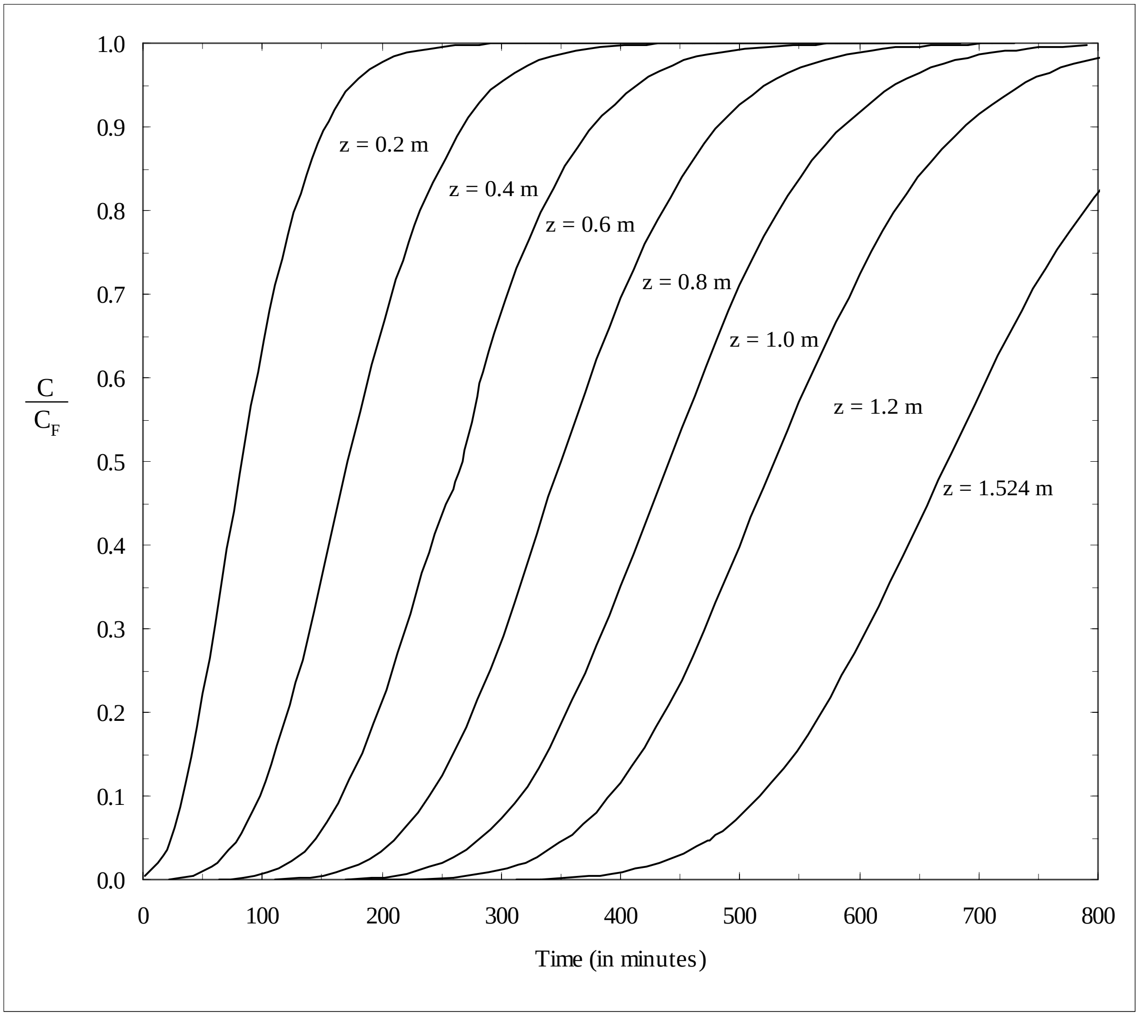
$$MTZ = 1.524m - 0.7159m = 0.8081m$$

Average Loading of bed:
In order to find the average loading of the bed we must solve the following integral.

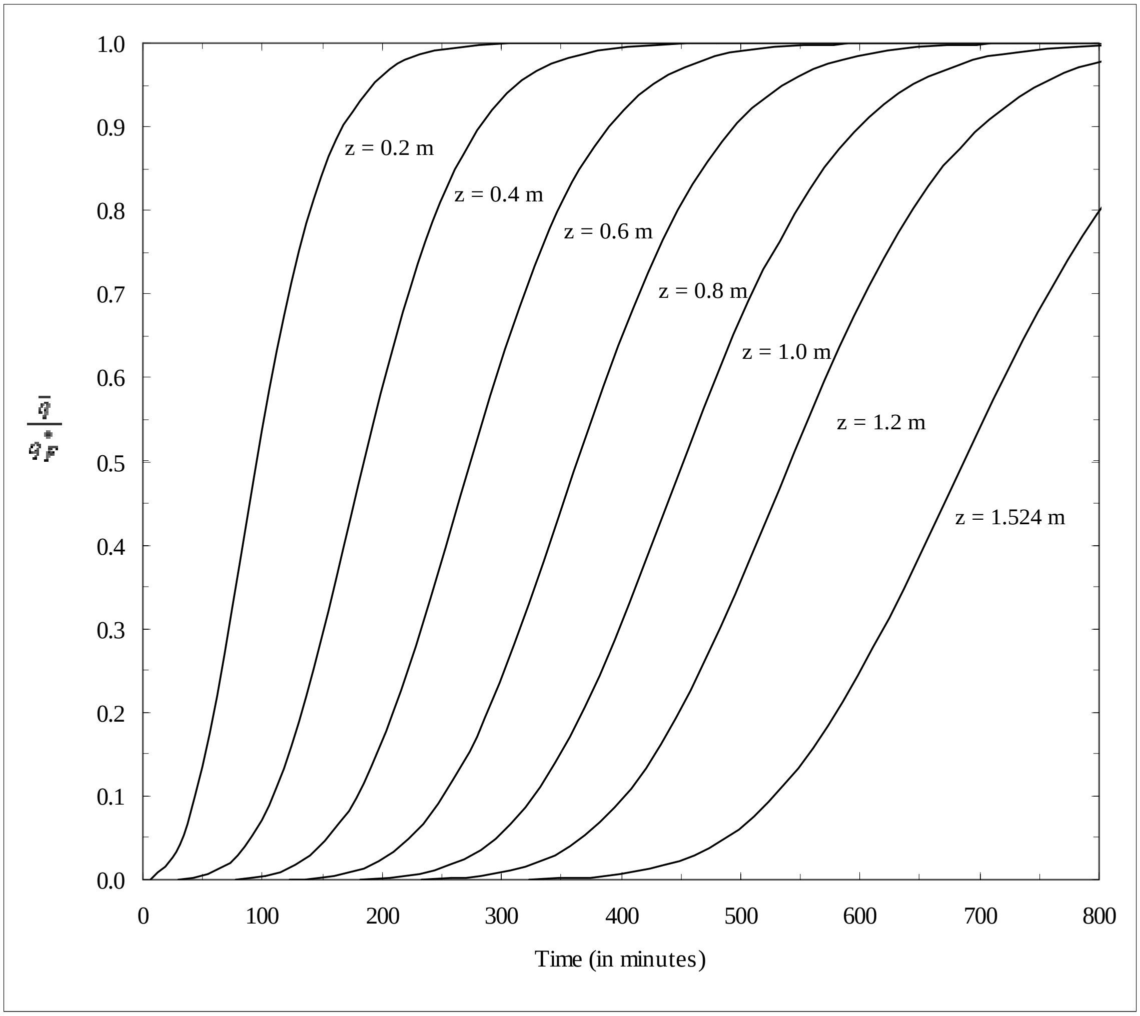
$$\bar{q}_{avg} = \frac{\int_0^z \bar{q}dz}{z} \text{ where } \bar{q} = q_F^* \frac{1}{2}\left[1 + erf\left(\sqrt{\tau} - \sqrt{\xi} - \frac{1}{8\sqrt{\tau}} - + \frac{1}{8\sqrt{\xi}}\right)\right] \text{ and } q_F^* = Kc_F = 0.44\frac{lb\_H_2O}{lb\_silica\_gel}$$

Using $t = t_{breakthrough}$, we have $\bar{q}$ as a function of z. To obtain the average, we can use the trapezoidal rule and sum up the values of $\bar{q}$ at various z and divide by the total height of the bed. From this method, we get $\bar{q}_{avg} = 0.2863$ and that **65 % of the bed is utilized at breakthrough**.

Below are the graphs of the profile in the bed at various times and lengths.



1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
C / C_F
0
100
200
300
400
500
600
700
800
Time (in minutes)
z = 0.2 m
z = 0.4 m
z = 0.6 m
z = 0.8 m
z = 1.0 m
z = 1.2 m
z = 1.524 m



Point Breakdown:
2 points: calculation of mass transfer coefficients and equilibrium constant with correct units
2 points: calculation of breakthrough time for Klinkenberg model
2 points: calculation of breakthrough time for equilibrium model
1 point: determining the mass transfer zone (MTZ)
1 point: calculation of the average loading of the bed
1 point: graph of breakthrough curves, i.e. C/C_F vs. time or tau at various values of z
1 point: graph of either adsorbent loading profile or adsorbent breakthrough curves