PROBLEMS

Problem 3.1

Use the Redlich-Kwong equation to estimate the molar volumes of saturated vapor and saturated liquid of methyl chloride at 60°C and 13.76 bar

$$P = \frac{RT}{V-b} - \frac{a}{T^{0.5}V(V+b)}$$

Data: $a = 1.5641\times 10^8$ cm^6 bar mol^{-2}K$^{1/2}$, $b = 44.891$ cm^3 mol^{-1} and $R = 83.14$.

Problem 3.2

Consider a binary system of components 1 and 2, with component 1 being the more volatile one. For a pressure P and a liquid composition x of component 1 the bubble point calculations consist in determining the temperature T and the vapor composition y.

Assuming ideal solutions in both liquid and vapor phases show that the pressure and vapor composition y are given by

$$P(T) = xP^s{}_1(T) + (1-x)P^s{}_2(T)$$

$$y = xP_1{}^s/P$$

where P_i^s are the vapor pressure given by the simple Antoine relation

$$\ln(P_i^s) = A_i + B_i/(T+Ci) \qquad i = 1,2$$

For a pressure P and liquid composition x the objective is then to find the temperature that satisfies

$$f(T) = P - (xP^s{}_1(T) + (1-x)P^s{}_2(T)) = 0$$

Perform the calculations for a mixture of acetonitrile and nitromethane at a pressure of 70 kPa. The mole fraction of acetonitrile is 0.6.

Data:

Acetonitrile: A =14.2724   B= 2945.47   C=224.0

Nitromethane :A =14.2403   B=2972.64   C=209.0=2 ‘

Problem 3.3

A heavy hydrocarbon oil which has Cp = 2.3 kJ/kg K is being cooled in a heat exchanger from T_1 = 372 K to T_2 = 350 K at a rate of 3630 kg/h. Cooling water enters at T_3 = 288^{o}K and leaves at unknown temperature T_4. Using the log mean temperature difference, the heat transfer between the two streams is given by:

$$mCp(T_1 - T_2) = UA \frac{(T_1 - T_4) - (T_2 - T_3)}{\ln \frac{(T_1 - T_4)}{(T_2 - T_3)}}$$

Calculate the water outlet temperature T_4 if the heat transfer area is 2.66 m^2 and the overall heat transfer coefficient U is 340 W/m^{2}K.

Problem 3.4

The oxidation of carbon monoxide is carried out in excess oxygen in a CSTR containing platinum catalyst particles as follows

$$CO + 1/2\ O_2 \rightarrow CO_2$$

The rate of CO disappearance is

$$-r_A = \frac{kC_A}{1 + KC_A^2}$$

where C_A is the concentration of CO. Given that steady state mole balance equation for CO has the form:

$$C_A/\tau - C_{A0}/\tau + \frac{kC_A}{1+KC_A^2} = 0$$

where τ is the residence time (V/F)

(a)Find the steady state solution for the case:

$$K = 10,\ C_{A0} = 1,\ \tau = 100,\ k = 0.2$$

(b) Show if the value of k is increased to 0.3, three real steady states can be found.

Problem 3.5

The reactions

$$C(s) + 2\,H_2 \rightarrow CH_4$$
$$C(s) + CO_2 \rightarrow 2CO$$

occur during the reduction of carbon. On the basis of the following data calculate the equilibrium composition at 700 ^oC and 10 atm. The feed consists of 30% CO_2 and 70% hydrogen, and the equilibrium constants for the respective reactions at this temperature are $K_1 = 0.13237$ atm^{-1} and $K_2 = 1.07266$ atm

Let reactions be represented as follows:

$$C + 2A \rightarrow B$$
$$C + D \rightarrow 2E$$

Let n_1 and n_2 be equal the moles of C that react in the first and second reactions respectively. The equilibrium equations for the two reactions can be shown to have the forms:

$$K_1 = \frac{p_B}{p_A^2} = \frac{n_1(n_T^o - n_1 + n_2)}{(n_A^o - 2n_1)^2 P}$$

$$K_2 = \frac{p_E^2}{p_D} = \frac{4n_2^2 P}{(n_T^o - n_1 + n_2)(n_D^o - n_2)}$$

where p_i is the partial pressure of component i, n_T^0 is the total moles of the reactants in the feed and n_i^0 is the number of moles of component i in the feed. Solve these two equations for the two unknowns n_1 and n_2.

Problem 3.6

Ethane (A) is dehydrogenated to ethylene(B) and acetylene(C) in the following pair of catalytic reactions :

$$A \leftarrow\rightarrow B + D$$

$$A \leftarrow\rightarrow C + D$$

D is hydrogen. The reaction take place at 977°C and 1 atm and proceed to a point such the product gas composition satisfies the following equations:

$$\frac{y_B y_D}{y_A} = 3.75 \qquad \frac{y_C y_D^2}{y_A} = 0.135$$

where y_i denotes mole fraction.

Taking 100 mole ethane fed to the reactor as a basis and using extent of reactions ζ_1, ζ_2, it can be shown that the equilibrium relations take the form:

$$\frac{\zeta_1(\zeta_1 + 2\zeta_2)}{(100 - \zeta_1 - \zeta_2)(100 + \zeta_1 + 2\zeta_2)} = 3.75$$

$$\frac{\zeta_2(\zeta_1 + 2\zeta_2)^2}{(100 - \zeta_1 - \zeta_2)(100 + \zeta_1 + 2\zeta_2)} = 0.135$$

Solve for the extent of reactions and determine the composition of the reactor product.

Problem 3.7

A furnace gas at a temperature T_G radiates heat Q to the outer surface of a pipe whose temperature is T_S. The heat is conducted through a the pipe wall to the inner surface T_W and then through a film to a process stream having temperature T_P. Analyzing this system, the following equations are established:

Radiant heat flux

$$Q = a\,(T_G^4 - T_S^4)$$

Conduction through pipe wall

$$Q = b(T_S - T_W)$$

Conduction through film

$$Q = c\,(T_W - T_P)$$

where $a = 1.2\times 10^{-9}$, $b = 70 + 0.07\,(T_S + T_W)$, $c = 6$

Calculate Q, T_S and T_W for $T_P = 900\ ^{\circ}\mathrm{K}$ and $T_G = 1500$

Problem 3.8

An empirical relation between the coefficient of the fluid friction with the pipe c_f and the Reynold's number is

$$\frac{1}{c_f^{0.5}} = 4.04 + 3.94\ln(\mathrm{Re}\,c_f^{0.5})$$

For values of Re = 10^3 to 10^5 in steps of 5000, solve the given equation for c_f .

Problem 3.9

The entropy change for a complete conversion of the reaction

$$1/3\ (N_2 + H_2 \rightarrow (2/3)\ NH_3$$

at any T has the form

$$\Delta S^{o} = -66.2 - 21.6\ \ln(T/298) + 23.9\times 10^{-3}(T-298) - 3.41\times 10^{-6}(T^2-298^2)$$

Find the temperature that corresponds to an entropy change of −76.1 kJ/K.

Problem 3.10

Solve the equation of state

$$(P + \frac{a}{v^2})(v - b) - RT = 0$$

for *v*. Given

$T = 535^oR$, $R = 0.6689$ (psia)(ft^3)/(lb)(^{o}R), P = 720 psia

$a = 33.012$ (psia)(ft^3)/lb^2

$b = 0.0427$ ft^3/lb

Initial guess $v = 0.249$

Problem 3.11

A gaseous mixture has the following composition (in mole percent): methane 20%, C_2H_4, 30%, N_2 50%. at 90 atm pressure and 100^{o}C. Calculate the molar volume of this gas using the Van der Waals' equation using averaged constants:

$$V^3 - (b + \frac{RT}{P})V^2 + \frac{a}{P}V - \frac{ab}{P} = 0$$

Additional data needed are :

a (atm)(cm^3/mol)^2 for CH_4 is 2.25×10^6, for C_2H_4 is 4.48×10^6, *for* N_2 is 1.35×10^6.

b (cm^3 /mol) : for CH_4 is 42.8, for C_2H_4 is 57.2, for N_2 is 38.6.

Problem 3.12

Given that the vapor pressure of methyl chloride at 60^{o}C is 13.76 bar, use the Redlich/kwong equation to estimate the molar volumes of saturated vapor and saturated liquid at these condition. The Redlich/kwong equation is: :

$$P = \frac{RT}{V - b} - \frac{a}{T^{0.5}V(V + b)}$$

Data:

R = 83.14, P = 13.76bar, T = 333.15°K, $a = 1.5641\times 10^8$ cm^6 bar mol^{-2}K$^{1/2}$, b = 44.891 cm^3 mol^{-1} .

Problem 3.13

The rate of thermal decomposition of ethane to ethylene and hydrogen was found to be first order with respect to ethane and the following expression for the rate constant was given:

$$\log(k) = 15.21 - 15970/T$$

where T is in °K and k has the units of s^{-1}. You are required to find the conversion of ethane which can be achieved in a plug-flow reactor which is operated isothermally at 750°C and 1 atm pressure with V/v^o_T = 4 s, where V is the total volume of the reactor and v^o_T is the volumetric flow rate of the feed at the reactor conditions . The feed consists of pure ethane. The design equation for this problem has the following form:

$$dx/dV = k(1-x)/v_T^0(1+x)$$

Separation of variables followed by integration over the volume V gives the nonlinear algebraic equation in term of the conversion x :

$$-2\ln(1-x) - x = k\, V/v^o_T$$

At the reactor condition, the design equation becomes

$$-2\ln(1-x) - x = 1.292$$

Problem 3.14

An equimolar mixture of benzene and toluene is stored at 1000 mm Hg . Below what temperature will the mixture exist as a single liquid phase (Bubble point)? Above what temperature will it exist as a single gas phase (Dew point)? Assuming Raoult's law is sufficiently accurate for this system, the K values for benzene is given as

$$\ln(K_1) = 9.2675 - \frac{2948.78}{T - 44.5633}$$

and for toluene

$$\ln(K_2) = 9.3587 - \frac{3242.38}{T - 47.1806}$$

For bubble point calculations, you need to solve the equation

$$f(T) = \sum_{i=1}^{2} K_i x_i - 1 = 0$$

where x_i is the mole fraction of component *i*. For the dew point calculations solve

$$f(T) = \sum_{i=1}^{2} \frac{K_i}{x_i} - 1 = 0$$

Problem 3.15

In the isothermal flash, the following specifications are made: T_F, P, X_i and F. It is required to find V, L,y_i and x_i. The independent equations required to describe this flash process are as follows:

Equilibrium relationships:

$$y_i = K_i x_i, \qquad \sum x_i = 1, \qquad \sum y_1 = 1$$

Component Material Balance:

$$F\,X_i = V\,y_i + L\,x_i$$

(a) Show that this system of nonlinear equations can be reduced to the following single equation in trem V:

$$f(V) = \sum \frac{X_i}{1 - \frac{V}{F}(1 - K_i)} - 1 = 0$$

(b) It is proposed to flash the following feed at a specific temperature T_F = 100^{o}F and a pressure P = 1 atm

If the feed rate to the flash drum is 100 mol/h, compute the vapor and liquid rates V and L leaving the flash as well as the respective mole fractions y_i and x_i of these streams.

Component	K_i	x_i
1	K_1 = 0.01T/3P	1/3
2	K_2 = 0.02T/1P	1/3
3	K_3 = 0.03T/2P	1/3

Problem 3.16

Liquid methanol is to be burned with an excess air . The engineer designing the furnace must calculate the highest temperature that the furnace walls will have to withstand so that an appropriate material of construction can be chosen. The methanol is assumed to be fed at 25°C and the air enters at 100°C. The energy balance calculations show that the adiabatic flame temperature of the furnace is given by:

$$7.535\times 10^{-12}T^4 - 1.393\times 10^{-8}T^3 - 4.913\times 10^{-5}T^2 - 0.4738T + 681.7 = 0$$

Solve the resulted equation for the adiabatic flame temperature.

Problem 3.17

One of the most common methods of measuring the diffusion coefficient is to fill a small capillary tube with one liquid, immerse the tube in a second liquid and measure the concentration of molecules of one fluid as it diffuses into the other as a function of time. This may be done by labeling the intruder fluid with radioactive isotopes or by simply observing the color change of, for example, ink diffusing into water .

The relationship between the concentration at a later time, $C(t)$ and the initial concentration at time $t = 0, C_0$ is given by the equation

$$\frac{C(t)}{C_o} = \frac{8}{\pi^2}\sum_{k=1}^{\infty}\frac{1}{(2k+1)^2}\exp\left(\frac{-(2k+1)^2\pi^2 Dt}{4L^2}\right)$$

where L is the length of the capillary tube (m) and t is the time (sec). Once the concentrations $C(t)$, C_0 are measured, this equation is then solved for the diffusion coefficient D. Use Newton method to find the constant D for the case:

Data:

$C(t)/C_0 = 0.5$, $t = 43200$ sec, $L = 0.1$ m, assuming the maximum number of terms in the summation is 50 .

Problem 3.18

Use the modified Raoult's law

$$y_iP = x_i \gamma_i P_i^{sat}$$

to calculate the bubble and dew points for the system propanol(1)/water(2).

The Antoine vapor -pressure equation are:

for propanol

$$P_1^{sat} = \exp(16.678 - \frac{3640.2}{T - 53.54})$$

for water

$$P_2^{sat} = \exp(16.2887 - \frac{3816.44}{T - 46.13})$$

where T is in kelvin and the vapor pressure are in kPa. The activity coefficients γ can be estimated using the Wilson equation:

$$\ln(\gamma_1) = -\ln(x_1 + x_2\Gamma_{12}) + x_2(\frac{\Gamma_{12}}{x_1 + x_2\Gamma_{12}} - \frac{\Gamma_{21}}{x_2 + x_1\Gamma_{21}})$$

$$\ln(\gamma_2) = -\ln(x_2 + x_1\Gamma_{21}) + x_1(\frac{\Gamma_{12}}{x_1 + x_2\Gamma_{12}} - \frac{\Gamma_{21}}{x_2 + x_1\Gamma_{21}})$$

where

$$\Gamma_{12} = \frac{V_2}{V_1}\exp\frac{-a_{12}}{RT}$$

$$\Gamma_{21} = \frac{V_1}{V_2}\exp\frac{-a_{21}}{RT}$$

and the following parameter values are given

$$a_{12} = 437.98,\ a_{21} = 123800 \text{ cal mol}^{-1}$$

$$V_1 = 76.92,\ V_2 = 18.07 \text{ cm}^3 \text{ mol}^{-1}$$

Calculate:

(a) P, y_1, y_2, for $T = 353.15$ K and $x_1 = 0.25$.

(b) P, x_1, x_2, for $T = 353.15$ K and $y_1 = 0.6$.

(c) T, y_1, y_2, for $P = 101.33$ kPa and $x_1 = 0.85$.

(d) T, x_1, x_2, for $P = 101.33$ kPa and $y_1 = 0.4$.

Problem 3.19

Determine the steady-state operating temperature for the following two sets of parametric values and the design equation:

$$v\rho Cp(T_o - T) - UA(T - T_M) = \frac{-V(-\Delta H)k_o e^{-E/RT} C_{Ao}}{v + Vk_o e^{-E/RT}}$$

Case 1:

ρCp = 50 Btu/ft$^{3\,o}$F, $T_0 = T_M = 530^o$R, UA = 500 Btu/h^{o}F, V = 100 ft^3, $-\Delta H = 10^4$ Btu/lbmole, $k_0 = 10^8$ h^{-1} , $E/R = 10^{4\,o}$R, v = 200 ft^3/h, C_{A0} = 0.270 lbmol/ft^3 .

Case 2:

$-\Delta H/\rho C_p = 200^o$K/mol liter, $T_0 = T_M = 350^o$K, $UA/v\rho C_p$ = 1 min^{-1}, v/V = 1 min^{-1}, $k_0 = e^{25}$ min^{-1}, $E/R = 10^4$ K , C_{A0} = 1.0 mol/liter.