ENCH 445 -- Problem Set #2

Problem 1. The Antoine equation for the vapor pressure of component i as a function of the temperature can be expressed as:

$$\text{Log}_{10}(P_{i,sat}) = A_i - B_i/(T + C_i)$$

With the pressure given in millimeters of mercury (760 mm Hg = 1 atm) and the temperature in °C, the Antoine constants for n-hexane and benzene are as follows:

	n-hexane	benzene
A_i	7.0105	7.201
B_i	1246.33	1415.08
C_i	232.988	248.03

Assume that the liquid phase activity coefficients can be described by regular solution theory and that the vapor phase is an ideal gas. Note that parameters needed to employ regulation solution theory are given in a table elsewhere in this document. You may neglect the effect of temperature on regular solution theory parameters.

Perform the following calculations:

    a. Construct an y-x equilibrium diagram for n-hexane and benzene at 20.2 kPa (0.2 atm) where x denotes the mole fraction of hexane in the liquid and y denotes the mole fraction of hexane in the vapor.

    b. Construct an y-x equilibrium diagram for n-hexane and benzene at 50 °C.

Problem 2. If a 40 mole-% ethanol, 60 mole-% water mixture at 60 °C and 1 atm is heated:

    a. At what temperature does it first begin to boil? What is the composition of the first bubble of vapor?

    b. At what temperature would it stop boiling (assume no material is removed)? What is the composition of the last droplet of liquid?

    c. At 82 °C, what fraction of the original mixture is liquid?

    d. When 80% has been vaporized, what is the temperature, and what are the liquid and vapor compositions?

Use the data in Fig. 2-3 of the Wankat textbook to solve this problem.

Problem 3. A storage tank contains n-butane, n-pentane, and n-hexane at 45°C and 140 kPa. Under these conditions separate liquid and vapor phases exist and are in equilibrium. If the liquid phase contains 0.10 mole fraction of n-butane, find the composition of the liquid and vapor phases. Use the DePriester charts in the Wankat textbook (see Figs. 2-11 and 2-12) to obtain any needed equilibrium data.

Problem 4. We wish to partly separate a mixture that is 45 mole-% benzene and 55 mole-% toluene in a single stage flash unit. The feed rate to the unit is 700 moles/hr. Equilibrium data for the benzene-toluene system can be approximated with a constant relative volatility of 2.5 where benzene is more volatile. The flash unit operates at 1 atm.

      a. Plot a y-x diagram for this system, where y and x indicate the mole fraction of benzene in the vapor and liquid, respectively.

      b. If 60 % of the feed is vaporized, find the liquid and vapor compositions.

      c. If we desire a vapor composition of 60 mole % benzene, what is the corresponding liquid composition, and what are the liquid and vapor flow rates?

Do the following problems from Chapter 2 of the Wankat textbook (4th ed.):

Problem 5. Chapter 2: D8

Problem 6. Chapter 2: D18

Problem 7. Chapter 2: D19

Note that some or all of these final three problems may require a computer solution. If you are using an older edition of the Wankat textbook, make sure you are working on the correct problems (see attached problems taken from the 4th ed. of Wankat).

Values of solubility parameters at 298 K† (data from Hildebrand et al., 1970, and Gardon, 1966)

	V, cm^3/mol	δ, (cal/cm^3)$^{1/2}$		V, cm^3/mol	δ, (cal/cm^3)$^{1/2}$
Water	18	23.2	Ethyl bromide	76	8.9
Ethylene glycol	56	15.7	Carbon tetrachloride	97	8.6
Phenol	88	14.5	Ethyl chloride	73	8.5
Methanol	40	14.5	Cyclohexane	109	8.2
Dimethyl sulfoxide	71	13.4	Cyclopentane	95	8.1
Nitromethane	54	12.6	Perfluorobenzene	115	8.1
Acetic acid	57	12.6	n-Hexadecane	295	8.0
Dimethyl formamide	77	12.1	Ethylene (169 K)	46	7.9
Acetonitrile	53	11.9	Methylcyclohexane	128	7.85
Furfural	83	10.9	CF$_4$ (145 K)	45	7.7
Aniline	91	10.8	n-Nonane	180	7.65
Benzaldehyde	101	10.8	Ethane (184 K)	55	7.6
Pyridine	81	10.7	Propylene (225 K)	69	7.6
Acrylonitrile	67	10.5	n-Octane	164	7.55
n-Butanol	92	10.4	Diethyl ether	105	7.5
Carbon disulfide	61	10.0	n-Heptane	147	7.45
Dioxane	86	10.0	n-Hexane	132	7.3
Acetone	74	9.9	cis-2-Butene	91	7.2
Nitrobenzene	108	9.9	Butadiene	88	7.1
Naphthalene	123	9.9	n-Pentane	116	7.05
1,2-Dichloroethane	79	9.8	$trans$-2-Butene	91	7.0
Chlorobenzene	102	9.5	Isooctane	166	6.85
Ethyl iodide	81	9.4	Methane (112 K)	38	6.8
Chloroform	81	9.3	2-Methylbutane	117	6.75
Styrene	115	9.3	Isobutene	94	6.7
Benzene	89	9.15	1-Butene	95	6.7
Ethyl acetate	99	9.1	Neopentane	122	6.25
o-Xylene	121	9.0	Perfluorocyclohexane	170	6.0
Toluene	107	8.9	Perfluoro-n-heptane	227	5.7

† Unless otherwise noted.

rate to the first drum is 1000 kmol/h. We desire a liquid product from the first drum that is 30.0 mol% methanol ($x_1 = 0.30$). The second drum operates at a fraction vaporized of $(V/F)_2 = 0.25$. The equilibrium data are in Table 2-7.

a. Sketch the process labeling the different streams.

b. Find the following for the first drum: vapor mole fraction y_1, fraction vaporized $(V/F)_1$, and vapor flow rate V_1.

c. Find the following for the second drum: vapor mole fraction y_2, liquid mole fraction x_2, and vapor flow rate V_2.

D6. One form of the Antoine equation is $\log_{10}(VP) = A - B/(T + C)$ where VP is in mm Hg and T is in °C. For 1-octanol, $A = 6.8379$, $B = 1310.62$, $C = 136.05$.

a. At 1.5 atm and 100°C, what is vapor pressure of 1-octanol in mm Hg?

b. Assuming Raoult's law is valid, what is the K value of 1-octanol at 1.5 atm and 100°C?

D7. Your plant feeds 100 kmol/h of a mixture that is 46.0 mol% ethanol and 54.0 mol % water to a flash drum. Your boss thinks that results will be better with two flash drums (same configuration as in Problem 2.D2.) with $V_1 = 30.0$ kmol/h and $V_2 = 30.0$ kmol/h.

a. Find L_1, L_2, and x_2.

b. Compare x_2 to the liquid mole fraction from a single flash drum with V/F = 0.60.

D8.* You want to flash a mixture with a drum pressure of 2.0 atm and a drum temperature of 25°C. The feed is 2000.0 kmol/h. The feed is 5.0 mol% methane, 10.0 mol% propane, and the rest n-hexane. Find the fraction vaporized, vapor mole fractions, liquid mole fractions, and vapor and liquid flow rates. Use DePriester charts.

D9.* We wish to flash distil an ethanol-water mixture that is 30.0 wt% ethanol and has a feed flow of 1000.0 kg/h. Feed is at 200°C. The flash drum operates at a pressure of 1.0 kg/cm². Find T_{drum}, weight fraction of liquid and vapor products, and liquid and vapor flow rates.

Data:

$C_{PL,EtOH} = 37.96$ at 100°C, kcal/(kmol°C)
$C_{PL,W} = 18.0$, kcal/(kmol°C)
$C_{PV,EtOH} = 14.66 + 3.758 \times 10^{-2}T - 2.091 \times 10^{-5}T^2 + 4.74 \times 10^{-9}T^3$
$C_{PV,W} = 7.88 + 0.32 \times 10^{-2}T - 0.04833 \times 10^{-5}T^2$
Both C_{PV} values are in kcal/(kmol°C), with T in °C.
$\rho_{EtOH} = 0.789$ g/mL, $\rho_W = 1.0$ g/mL, $MW_{EtOH} = 46.07$, $MW_W = 18.016$, $\lambda_{EtOH} = 9.22$ kcal/mol at 351.7 K, and $\lambda_W = 9.7171$ kcal/mol at 373.16 K.
Enthalpy composition diagram at $p = 1$ kg/cm² is in Figure 2-4. Note: Be careful with units.

D10. We have a mixture that is 35.0 mol% n-butane with unknown amounts of propane and n-hexane. We are able to operate a flash drum at 400 kPa and 70°C with $x_{C6} = 0.7$. Find the mole fraction of n-hexane in the feed, z_{C6}, and the value of V/F.

D11. An equilibrium mixture of ethylene and propylene is at 2500.0 kPa and 25°C. Find the vapor and liquid mole fractions of ethylene. Note: This is not a guess-and-check problem.

D12. Find h_{total} and D for a horizontal flash drum for Problem 2.D1c. Use $h_{total}/D = 4$.

D13. We flash distil a mixture that is 36% ethane (C2) and 64% n-butane (C4). The flash drum operates as an equilibrium stage. We measure the outlet concentrations of

60

ethane as $x_{C2} = 0.088$ and y_{C2}
not trial and error.

D14. A flash drum is separating a
n-butane (C4), and 40.0 mol%
partially liquid and partially v
The flash drum is at 3.0 bar an
mole fractions.

D15.* We have a flash drum separat
n-butane. The ratio of isobu
$z_{nC4} = 0.8$). The mole fraction
flash drum operates at a press
is operating at V/F = 0.4, wha
feed be?

D16. A feed that is 50.0 mol% me
25.0 mol% n-hexane is flash
drum temperature = 10°C. Us

D17. We are separating a mixture
$p = 1$ atm. Equilibrium data a

a. 1000.0 kmol/day of a fee
the feed is vaporized, find
products.

b. Repeat part a for a feed ra

c. If feed is 30.0 mol% aceto
the highest possible vapor

d. If we want to obtain a liqu
of the feed, what must the

D18.* 10.0 kmol/h of a feed that is 1
n-hexane is flash distilled at a
85.0 mol% n-hexane. Use De
answer is within 0.5°C of the
a simultaneous mass and ener

D19.* A flash drum operating at 30
tane, 25.0 mol% n-pentane,
n-hexane in the liquid. F = 10

D20. 200.0 kmol/h of a feed that is
a pair of flash drums. The vap
$2 (F_2 = V_1)$. If $y_2 = 0.45$ and V
are at 1.0 atm.

D21. We wish to flash distil a feed t
drum operates $p_{drum} = 700.0$ k

a. Find V/F, V, L, liquid mol
b. Find the dimensions in me
vapor is an ideal gas to ca
Be careful of units. Arbi
72.15. Liquid densities are

ethane as $x_{C2} = 0.088$ and $y_{C2} = 0.546$. Find x_{C4}, y_{C4}, T_{drum}, p_{drum}, and V/F. Note: This is not trial and error.

D14. A flash drum is separating a mixture that is 12.0 mol% methane (C1), 48.0 mol% n-butane (C4), and 40.0 mol% n-pentane (C5). Feed rate is 122.0 kmol/h. The feed is partially liquid and partially vapor at a pressure of 5.0 bar and temperature of 50.4°C. The flash drum is at 3.0 bar and T = 36°C. Find V/F, the K values, and vapor and liquid mole fractions.

D15.* We have a flash drum separating 50.0 kmol/h of a mixture of ethane, isobutane, and n-butane. The ratio of isobutane to n-butane is held constant at 0.8 (that is, $z_{iC4}/z_{nC4} = 0.8$). The mole fractions of all three components in the feed can change. The flash drum operates at a pressure of 100 kPa and a temperature of 20°C. If the drum is operating at V/F = 0.4, what must the mole fractions of all three components in the feed be?

D16. A feed that is 50.0 mol% methane, 10.0 mol% n-butane, 15.0 mol% n-pentane, and 25.0 mol% n-hexane is flash distilled. F = 150.0 kmol/h. Drum pressure = 250.0 kPa, drum temperature = 10°C. Use the DePriester charts. Find V/F, x_i, y_i, V, and L.

D17. We are separating a mixture of acetone (MVC) from ethanol by flash distillation at p = 1 atm. Equilibrium data are listed in Problem 4.D7. Solve graphically.
   a. 1000.0 kmol/day of a feed that is 70.0 mol% acetone is flash distilled. If 40% of the feed is vaporized, find the flow rates and mole fractions of the vapor and liquid products.
   b. Repeat part a for a feed rate of 5000.0 kmol/day.
   c. If feed is 30.0 mol% acetone, what are the lowest possible liquid mole fraction and the highest possible vapor mole fraction?
   d. If we want to obtain a liquid product that is 40.0 mol% acetone while flashing 60% of the feed, what must the mole fraction of the feed be?

D18.* 10.0 kmol/h of a feed that is 10.0 mol% propane, 30.0 mol% n-butane, and 60.0 mol% n-hexane is flash distilled at a drum pressure of 200.0 kPa. We desire a liquid that is 85.0 mol% n-hexane. Use DePriester charts. Find T_{drum} and V/F. Continue until your answer is within 0.5°C of the correct answer. Note: This is a single trial and error, *not* a simultaneous mass and energy balance convergence problem.

D19.* A flash drum operating at 300.0 kPa is separating a mixture that is 40.0 mol% isobutane, 25.0 mol% n-pentane, and 35.0 mol% n-hexane. We wish a 90% recovery of n-hexane in the liquid. F = 1000.0 kmol/h. Find T_{drum}, x_j, y_j, V/F.

D20. 200.0 kmol/h of a feed that is 10.0 mol% ethanol and 90.0 mol% water is separated in a pair of flash drums. The vapor from drum 1 is partially condensed and fed to drum 2 ($F_2 = V_1$). If $y_2 = 0.45$ and $V_2/F_2 = 0.6$, find V_1, L_1, V_2, L_2, x_1, y_1, and x_2. Both drums are at 1.0 atm.

D21. We wish to flash distil a feed that is 55.0 mol% ethane and 45.0 mol% n-pentane. The drum operates $p_{drum} = 700.0$ kPa and $T_{drum} = 30°C$. Feed flow rate is 100,000 kg/h.
   a. Find V/F, V, L, liquid mole fraction, and vapor mole fraction.
   b. Find the dimensions in metric units required for a vertical flash drum. Assume the vapor is an ideal gas to calculate vapor densities. Use DePriester chart for VLE. Be careful of units. Arbitrarily pick $h_{total}/D = 4$. $MW_{ethane} = 30.07$, $MW_{pentane} = 72.15$. Liquid densities are $\rho_E = 0.54$ g/ml (estimated), $\rho_P = 0.63$ g/ml.