Answer Sheet for CHE654 Homework Set #4
(100 Points)

Note: For all problems, submit a copy of your process flow diagram and a copy of your input summary of the process.

28. (25 points) ***Quick Property Analysis, II***

(a) The values of the retrieved binary parameters in °C for the 3 binary system are

Binary System	Interaction Parameters	Range of Temperature (°C)
Chloroform-Ethanol		
Water-Formic acid		
Isobutyl alcohol-Pinene		

If which pair has no interaction parameters, why:

_____

_____

(b) Classification:

Chloroform-Ethanol : ☐ Minimum ☐ Maximum boiling-point azeotrope

Water-Formic acid : ☐ Minimum ☐ Maximum boiling-point azeotrope Isobutyl

alcohol-Pinene : ☐ Minimum ☐ Maximum boiling-point azeotrope

(c) UNIQ-RK property method is not appropriate for the Water-Formic acid system

because _____

_____

Two alternate property methods better suited to predict the azeotrope for Water-Formic acid system are _____

UNIQ-RK property method is not appropriate for the Isobutyl alcohol-Pinene system because _____

_____

Two alternate property methods better suited to predict the azeotrope for Isobutyl alcohol-Pinene system are _____

Binary System	**Interaction Parameters**	**Range of Temperature (°C)**
Water-Formic acid		
Isobutyl alcohol-Pinene		

(d) Don't forget to submit the *T-x*y plots of each system!

Summary Table:

Binary System	**Azeo. Temp.**	**%Error**	**Azeo. *x***	**%Error**
Chloroform-Ethanol				
Water-Formic acid				
Isobutyl alcohol-Pinene				

(e) Don't forget to submit the vapor pressure profile (in psia) of all components as a function of T from 0 to 100 °C.

Rearrange the relative volatility in increasing order:

_____

29. (25 points) ***Choosing Appropriate Property Methods, I***

Consider the following mixtures at some given operating conditions. Choose an appropriate property method in ASPEN PLUS to calculate a desired property using any of the property features we learned such as Quick Property Analysis, Prop-Sets, and unit operation modules. Note that there is more than one choice but you are to pick one that gives high, if not best, accuracy. There is no need to save your work. Just write down the answers in the blank spaces below and tick if your property method uses Henry's Law.

(a) Activity coefficient γ of *n*-pentane in a liquid solution of 30 mol% *n*-pentane, 30 mol% acetone, and 40 mol% ethanol at 60 °F and 20 psia.

Property Method: _____ O With O Without Henry's Law

Activity coefficient of *n*-pentane = _____

(b) Solubility (in mole fraction) of water in the organic phase of a liquid solution with 30 mol% water, 30 mol% caprolactone, and 40 mol% 3-heptanone at 20 °C and 1 bar.

Property Method: _____ O With O Without Henry's Law

Solubility of water = _____

(c) Solubility of O_2 (mole ppm) in a mixed solvent of 45-45 mol% benzene and toluene at 70 °F and 10 psia (the remaining 10 mol% is oxygen. special note: you are not allowed to pick an equation of state for this problem).

Property Method: _____ O With O Without Henry's Law

Solubility of O_2 = _____ ppm

(d) Vapor fugacity coefficient of cyclopentane in a two-phase mixture of 25 mol% benzene, 25 mol% cyclohexane, 25 mol% *n*-hexane, and 25 mol% cyclopentane at 150 psia and with 50 mol% vapor (the remaining 50% is liquid).

Property Method: _____ O With O Without Henry's Law

Vapor fugacity coefficient of cyclopentane = _____

(e) Heat of mixing of an equimolar mixture of formic-acid and acetone at 50 °F and 20 psia.

Property Method: _____ O With O Without Henry's Law

Heat of mixing = _____ Btu/lbmol

(f) Liquid viscosity of a mixture of 40 mol% acetic-acid, 40 mol% methanol, and 20 mol% CO_2 at 100 °C and 50 bar.

Property Method: _____ O With O Without Henry's Law

Liquid viscosity = _____ cP

(g) Temperature in a 1-bar flash vessel needed to produce a vapor stream that contains 40 mol% ammonia from a feed mixture at 20 °C and 1 bar containing 30 mol% ammonia, 30 mol% methanol, 30 mol% ethanol, 5 mol% O_2, and 5 mol% N_2.

Property Method: _____ O With O Without Henry's Law

Flash temperature = _____ °C

(h) Pressure at which the heat of vaporization of water is equal to 9.0 kcal/gmol. Note that the heat of vaporization of water at 1 atm = 9.71 kcal/gmol.

Property Method: _____ O With O Without Henry's Law

Pressure = _____ atm

31. (25 points) ***Choosing Appropriate Property Methods, III***

Consider the following mixtures at some given operating conditions. Choose an appropriate property method in ASPEN PLUS to calculate a desired property using any of the property features we learned such as Quick Property Analysis, Prop-Sets, and unit operation modules. Note that there is more than one choice but you are to pick one that gives high, if not best, accuracy. There is no need to save your work. Just write down the answers in the blank spaces below and tick if your property method uses Henry's Law.

(a) Solubility (mole ppm) of N_2 in a two-phased mixture of 20 mole% N_2, 30 mole% water, 20 mole% methanol, and 30 mole% acetone at 1 atm and 30 °C.

Property Method: _____ O With O Without Henry's Law

Solubility of N_2 = _____ ppm

(b) Solubility (mass faction) of water in the organic phase of a two-liquid mixture with 50 mass% isoheptanol and 50 mass% water at 1 atm and 20 °C.

Property Method: _____ O With O Without Henry's Law

Solubility of water = _____

(c) Heat of mixing of a mixture of 30 mole% benzene, 30 mole% toluene, and 40 mole% para-xylene at 20 atm and 10 °C.

Property Method: _____ O With O Without Henry's Law

Heat of mixing = _____ Btu/lbmol

(d) Liquid fugacity coefficient of ethanol in a liquid mixture of 50 mole% ethanol and 20 mole% propane, and 30 mole% acetylene at 50 atm and 25 °C.

Property Method: _____ O With O Without Henry's Law

Liquid fugacity coefficient = _____

(e) Heat of vaporization of pure water at 80 °C.

Property Method: _____ O With O Without Henry's Law

Heat of vaporization = _____ Btu/lbmol

(f) Vapor enthalpy of a 2-phase mixture of 20 mole% ammonia, 30 mole% benzoic-acid, and 50 mole% *n*-butane at 1 atm and vapor fraction = 0.3.

Property Method: _____ O With O Without Henry's Law

Vapor enthalpy = _____ Btu/lbmol

(g) Which of the following 5 components has the 3rd highest volatility (i.e. 2 components are more volatile and 2 components are less volatile) at T = 100 °F: 1-hexene, 1,4-hexadiene, methanol, chloroform, and 3-methylcyclopentene?

Property Method: _____ O With O Without Henry's Law

Component with the 3rd highest volatility = _____

(h) Solubility (mole ppm) of O_2 in a two-phased mixture of 10 mole% O_2, 30 mole% ethanol, 30 mole% 1-propanol, and 30 mole% *n*-butanol at 14.7 psia and 100 °F.

Property Method: _____ O With O Without Henry's Law

Solubility of O_2 = _____ ppm

33. (25 points) ***Toluene-Benzene Recovery Process with Multiple Property Methods***

(a) Mole fraction of benzene in the 2nd-Column overhead stream: _____

Molar ratio toluene: hydrogen in reactor feed: _____

(b) Hydrogen molar feed flow rate: _____ gmol/min

Mole fraction of benzene in the 2nd-Column overhead stream: _____