CE 407 Notes
Single-stage absorption

Today's quotation: "I'm NOT eating the gravy and that's FINAL!!!"
Elroy Hutch, just after deciding not to eat the gravy

1. 120 m^3 of a 30 °C gas mixture with composition 96 mole percent air(3), 4 mole percent acetone(1) is contacted with 160 kg of 30 °C pure water(2). The vapor-liquid system is allowed to come to equilibrium isothermally at 30 °C at a constant pressure of 1.2 atm. What are the final compositions of the liquid and vapor phases? You should neglect dissolution of air in the liquid but you must account for evaporation of water. Thus, the vapor phase contains all three components, but the liquid phase contains only acetone(1) and water(2).

Data and assumptions: The vapor phase behaves as an ideal gas. Henry's law holds for acetone with Henry's law constant $k_1 = 1440$ mm Hg at 30 °C. Raoult's law holds for water. The saturated vapor pressure of water at 30 °C is 0.0419 atm.

2. (Simpler version of Problem **1** $\Rightarrow$ COOL man!) 120 m^3 of a 30 °C gas mixture with composition 96 mole percent air(3), 4 mole percent acetone(1) is contacted with 160 kg of 30 °C pure water(2). The vapor-liquid system is allowed to come to equilibrium isothermally at 30 °C at a constant pressure of 1.2 atm. What are the final compositions of the liquid and vapor phases? You should neglect both dissolution of air in the liquid and evaporation of water. Thus, the vapor phase contains only acetone(1) and air(3), and the liquid phase contains only acetone(1) and water(2).

Data and assumptions (Simpler version of the problem $\Rightarrow$ less data needed!): The vapor phase behaves as an ideal gas. Henry's law holds for acetone with Henry's law constant $k_1 = 1440$ mm Hg at 30 °C.

<u>3</u>. 10 m^3 of 25 °C contaminated air (composition 90 mole percent air, 10 mole percent benzene) is to be cleaned up by contact and equilibration with 400 mol of an absorption oil (which forms an ideal liquid solution with benzene) under isothermal conditions at atmospheric pressure. What is the composition of the final gas? How many moles of benzene are absorbed by the liquid?

Data and assumptions: Neglect any evaporation of oil as well as dissolution of air in the liquid. The vapor phase behaves as an ideal gas. The saturated vapor pressure of benzene at 25 °C is 95 mm Hg.

Problem 1 and 2 SOLUTION

For both versions, the total amount of acetone (1), water (2) and air (3) are the same.

Gas

$$n_1 + n_3 = \text{total moles of gas} \overset{\text{by ideal gas law}}{=} \frac{pV^t}{RT} = \frac{(1.2)(101325\ Pa)(120\ m^3)}{(8.314\ J/mol\,K)(303.15\ K)}$$

(1.2 atm; 30 °C)

$$= 5789\ mol$$

$$n_1 = (0.04)(5789) = 232\ mol\ \text{acetone}$$

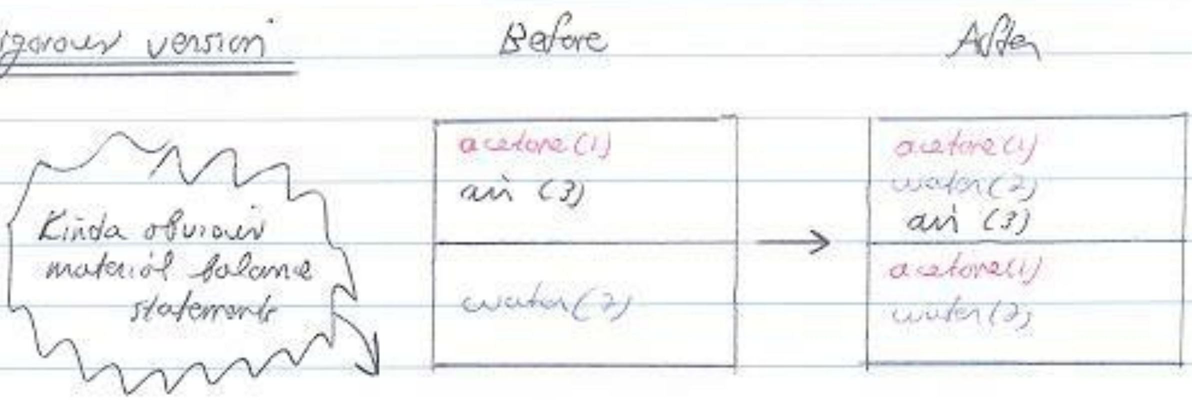
$$n_3 = (0.96)(5789) = 5557\ mol\ \text{air}$$

Liquid

$$n_2 = 160\ kg\ \text{water} \times \frac{1000\ g}{1\ kg} \times \frac{1\ mol}{18.015\ g} = 8881\ mol\ \text{water}$$

Problem 1 SOLUTION

Rigorous version:



$$\begin{cases} n_1^l + n_1^v = n_1 \\ n_2^l + n_2^v = n_2 \\ 0 + n_3^v = n_3 \end{cases} \quad \text{or} \quad \begin{cases} n_1^v = n_1 - n_1^l \\ n_2^v = n_2 - n_2^l \\ n_3^v = n_3 \end{cases}$$

no dissolution of air in the liquid — a VERY good approx.

Two unknowns: n_1^l and n_2^l

Need to consider equilibrium relation for each distributed component (i.e., component present in both phases).

$$\begin{cases} y_1 P = k_1 x_1 & \text{Henry's law for acetone} \\ y_2 P = P_2^{sat} x_2 & \text{Raoult's law for water} \end{cases}$$

How do we apply these eqs.? Write all mole fractions in terms of mole numbers:

$$y_1 = \frac{n_1^v}{n_1^v + n_2^v + n_3^v} = \frac{n_1 - n_1^e}{n_1 - n_1^e + n_2 - n_2^e + n_3}$$

$$x_1 = \frac{n_1^e}{n_1^e + n_2^e + 0}$$

$$y_2 = \frac{n_2^v}{n_1^v + n_2^v + n_3^v} = \frac{n_2 - n_2^e}{n_1 - n_1^e + n_2 - n_2^e + n_3}$$

$$x_2 = \frac{n_2^e}{n_1^e + n_2^e + 0}$$

∴ get 2 eqs. in 2 unknowns:

$$\frac{n_1 - n_1^e}{n_1 - n_1^e + n_2 - n_2^e + n_3} = \left(\frac{k_1}{P}\right) \frac{n_1^e}{n_1^e + n_2^e} \qquad (1)$$

$$\frac{n_2 - n_2^e}{n_1 - n_1^e + n_2 - n_2^e + n_3} = \left(\frac{P_2^{sat}}{P}\right) \frac{n_2^e}{n_1^e + n_2^e} \qquad (2)$$

How to solve?

Method 1 (iterative method). Rewrite eqs. (1) and (2) as

$$n_1 (n_1^e + n_2^e) - n_1^e (n_1^e + n_2^e) = (k_1/P)\, n_1^e (n_1 - n_1^e + n_2 - n_2^e + n_3)$$

$$n_1 (n_1^e + n_2^e) = n_1^e (n_1^e + n_2^e) + (k_1/P)\, n_1^e (n_1 - n_1^e + n_2 - n_2^e + n_3)$$

$$n_1^e = \frac{n_1 (n_1^e + n_2^e)}{n_1^e + n_2^e + (k_1/P)(n_1 - n_1^e + n_2 - n_2^e + n_3)} \qquad (1')$$

and

$$n_2(n_1^e + n_2^e) - n_2^e(n_1^e + n_2^e) = (P_2^{sat}/P)(n_1 - n_1^e + n_2 - n_2^e + n_3)$$

$$n_2(n_1^e + n_2^e) = n_2^e(n_1^e + n_2^e) + (P_2^{sat}/P)(n_1 - n_1^e + n_2 - n_2^e + n_3)$$

$$n_2^e = \frac{n_2(n_1^e + n_2^e)}{n_1^e + n_2^e + (P_2^{sat}/P)(n_1 - n_1^e + n_2 - n_2^e + n_3)} \quad (2')$$

(0^{th} approx. $(n_1^e)_0$) (0^{th} approx. $(n_2^e)_0$)

As starting approx., set $n_1^e = 0$ and $n_2^e = n_2$ in right-hand sides. (Very approximately, amt. of acetone absorbed is neglected and evap. of water is also neglected.) This gives

1st approx. →

$$(n_1^e)_1 = \frac{232(0 + 8881)}{0 + 8881 + \frac{(1440)}{(1.2)(760)}(232 - 0 + 8881 - 8881 + 5557)} = 114 \text{ mol}$$

$$(n_2^e)_1 = \frac{8881(0 + 8881)}{0 + 8881 + \left(\frac{0.0419}{1.2}\right)(232 - 0 + 8881 - 8881 + 5557)} = 8883 \text{ mol}$$

Obtain improved approximation by substituting 1st approximation into right-hand sides:

$$(n_1^e)_2 = \frac{232(114 + 8883)}{114 + 8883 + \frac{1440}{(1.2)(760)}(232 - 114 + 8881 - 8883 + 5557)} = 113 \text{ mol}$$

$$(n_2^e)_2 = \frac{8881(114 + 8883)}{114 + 8883 + \left(\frac{0.0419}{1.2}\right)(232 - 114 + 8881 - 8883 + 5557)} = 8679 \text{ mol}$$

One more iteration gives essentially converged values:

converged answer for $n_1^e \approx (n_1^e)_3 = 113$ mol acetone

converged answer for $n_2^e \approx (n_2^e)_3 = 8678$ mol water

Method 2 (WHY NOT USE MAPLE?!)

Attached maple code gives the same answer (not surprisingly).

Now can compute mole fraction

gas composition:

$$y_1 = \frac{232 - 113}{232 - 113 + 8881 - 8678 + 5557} = 0.0202$$

$$y_2 = \frac{8881 - 8678}{232 - 113 + 8881 - 8678 + 5557} = 0.0345$$

$$y_3 = 1 - y_1 - y_2 = 0.9453 \qquad = 0.9453$$

liquid composition:

$$x_1 = \frac{113}{113 + 8678} = 0.0129$$

$$x_2 = \frac{8678}{113 + 8678} = 0.9871$$

$$x_3 = \qquad = 0 \quad \text{(by assumption)}$$

Problem 2 SOLUTION

Approximate version

Before	After
acetone (1), air (3)	acetone (1), air (3)
water (2)	acetone (1), water (2)

Obvious material balance statements:

$$\begin{cases} n_1^{\ell} + n_1^{v} = n_1 \\ n_2^{\ell} + 0 = n_2 \\ 0 + n_3^{v} = n_3 \end{cases} \quad \text{or} \quad \begin{cases} n_1^{v} = n_1 - n_1^{\ell} \\ n_2^{\ell} = n_2 \\ n_3^{v} = n_3 \end{cases}$$

Only one unknown n_1^{ℓ}

5

```
> # The two unknowns are n11 and n21
  #
  # Equation (1) can be written as f1(n11,n21) = 0,
  # where f1(n11,n21) is the function
  #
  f1 := (n11,n21) -> (232 - n11)
          / (232 - n11 + 8881 - n21 + 5557)
          - 1440 / 1.2 / 760 * n11 / (n11 + n21);
```

$$f1 := (n1l, n2l) \to \frac{232 - n1l}{14670 - n1l - n2l} - \frac{1.578947368\, n1l}{n1l + n2l}$$

```
> #
  # Equation (2) can be written as f2(n11,n21) = 0,
  # where f2(n11,n21) is the function
  #
  f2 := (n11,n21) -> (8881 - n21)
          / (232 - n11 + 8881 - n21 + 5557)
          - 0.0419 / 1.2 * n21 / (n11 + n21);
```

$$f2 := (n1l, n2l) \to \frac{8881 - n2l}{14670 - n1l - n2l} - \frac{.03491666667\, n2l}{n1l + n2l}$$

```
> #
  # Solve the two equations simultaneously for the
  # two unknowns
  #
  fsolve({f1(n11,n21) = 0, f2(n11,n21) = 0},
          {n11,n21},
          {n11 = 0..232, n21 = 0..8881});
```

$$\{n1l = 112.8481606,\ n2l = 8678.367352\}$$

```
> #
  # What fun!!
  #
> 
```

Consider equil. relation for the only distributed component, acetone:

$$y_1 P = k_1 x_1 \qquad \text{(Henry's law)}$$

(Simpler) expressions for mole fractions are

$$y_1 = \frac{n_1 - n_1^e}{n_1 - n_1^e + 0 + n_3}$$

$$x_1 = \frac{n_1^e}{n_1^e + n_2}$$

Get equation

$$\boxed{\frac{n_1 - n_1^e}{n_1 - n_1^e + n_3} = \left(\frac{k_1}{P}\right) \frac{n_1^e}{n_1^e + n_2}}$$

Solve: $(n_1 - n_1^e)(n_1^e + n_2) = \left(\frac{k_1}{P}\right) n_1^e (n_1 - n_1^e + n_3)$

or $n_1 n_1^e + n_1 n_2 - (n_1^e)^2 - n_2 n_1^e$

$$= \left(\frac{k_1}{P}\right)\left[n_1 n_1^e - (n_1^e)^2 + n_1^e n_3\right]$$

or

$$(n_1^e)^2 \underbrace{\left(\frac{k_1}{P} - 1\right)}_{0.5789 \,\equiv A} + n_1^e \underbrace{\left[n_1 - n_2 - \left(\frac{k_1}{P}\right)(n_1 + n_3)\right]}_{-1.779 \times 10^4 \,\equiv B} + \underbrace{n_1 n_2}_{2060 \times 10^6 \,\equiv C} = 0$$

Happy quadratic equation $\Rightarrow$

$$n_1^e = \frac{-B \pm \sqrt{B^2 - 4AC}}{2A} = (\sout{3.061 \times 10^4} \text{ or } 116) \text{ mol acetone}$$

NO!

$n_1^e = 116$ mol acetone

Compute mole fractions

gas composition

$$y_1 = \frac{232-116}{232-116+5557} = 0.0204$$

$$y_2 = 0 \quad \text{(by assumption)}$$

$$y_3 = 1 - y_1 = 0.9796$$

liquid composition

$$x_1 = \frac{116}{116 + 8881} = 0.0129$$

$$x_2 = 1 - x_1 = 0.9871$$

$$x_3 = 0 \quad \text{(by assumption)}$$

Comparison

	Rigorous	Approx.	Elroy's evaluation
y_1	0.0202	0.0204	Wow!
y_2	0.0345	0 (by assumption)	all wrong
x_1	0.0129	0.0129	Wow!

Problem 3 SOLUTION

(i) Preliminaries

$$10 \text{ m}^3 \text{ gas} \times \frac{101325 \text{ Pa}}{(8.314 \text{ J/mol K})(298.15 \text{ K})} = 408.8 \text{ mol gas}$$

$$V_{air} = (408.8 \text{ mol})(0.90) = 367.9 \text{ mol air}$$

$$(V_{benz})_{before} = (408.8 \text{ mol})(0.10) = 40.9 \text{ mol benzene}$$

$$L_{oil} = 400 \text{ mol oil}$$

$$(L_{benz})_{before} = 0 \text{ mol benzene}$$

(ii) Material balance

$$(V_{benz})_{before} + (L_{benz})_{before} = (V_{benz})_{after} + (L_{benz})_{after}$$

or

$$40.9 \text{ mol} + 0 \text{ mol} = (V_{benz})_{after} + (L_{benz})_{after}$$

or

$$(L_{benz})_{after} = 40.9 \text{ mol} - (V_{benz})_{after}$$

(iii) Definition of mole fractions

In the final ("after") state

$$y = y_{benz} = \frac{(V_{benz})_{after}}{V_{air} + (V_{benz})_{after}} = \frac{(V_{benz})_{after}}{367.9 \text{ mol} + (V_{benz})_{after}}$$

$$x = x_{benz} = \frac{(L_{benz})_{after}}{L_{oil} + (L_{benz})_{after}}$$

$$= \frac{40.9 \text{ mol} - (V_{benz})_{after}}{400 \text{ mol} + 40.9 \text{ mol} - (V_{benz})_{after}}$$

$$= \frac{40.9 \text{ mol} - (V_{benz})_{after}}{440.9 \text{ mol} - (V_{benz})_{after}}$$

Note that both x and y are expressible in terms of the single unknown $(V_{benz})_{after}$

(iv) Equilibrium relation

Ideal gas + ideal solution behavior ⟹ Raoult's law valid. ∴ in final equil. state $yP = xP^{sat}_{benz}$

or $y = \left(\frac{P^{sat}_{benz}}{P}\right)x = \left(\frac{95}{760}\right)x$

because $P = 1\text{ atm} = 760\text{ mmHg}$ and $P^{sat}_{benz} = 95\text{ mmHg}$ @ the temp. (25°C) of the problem.

(v) Put things together

$$\underbrace{\frac{(N_{benz})_{after}}{367.9\text{ mol} + (N_{benz})_{after}}}_{y} = \left(\frac{95}{760}\right)\underbrace{\frac{40.9\text{ mol} - (N_{benz})_{after}}{440.9\text{ mol} - (N_{benz})_{after}}}_{x}$$

or

$$(N_{benz})_{after}\left[440.9\text{ mol} - (N_{benz})_{after}\right] = \left(\frac{95}{760}\right)\left[367.9\text{ mol} + (N_{benz})_{after}\right]\left[40.9\text{ mol} - (N_{benz})_{after}\right]$$

or ...

or $(0.875)(N_{benz})^2_{after} - (481.775\text{ mol})(N_{benz})_{after} + 1880.89\text{ mol}^2 = 0$

Solve by quadratic formula:

$$(N_{benz})_{after} = \frac{481.775 \pm \sqrt{(481.775)^2 - 4(0.875)(1880.89)}}{2(0.875)}\text{ mol}$$

$$= \frac{481.775 \pm 474.894}{1.75}$$

$= \sout{956.7\text{ mol}}$ (+ root) bigger than the original amount of benzene!

or

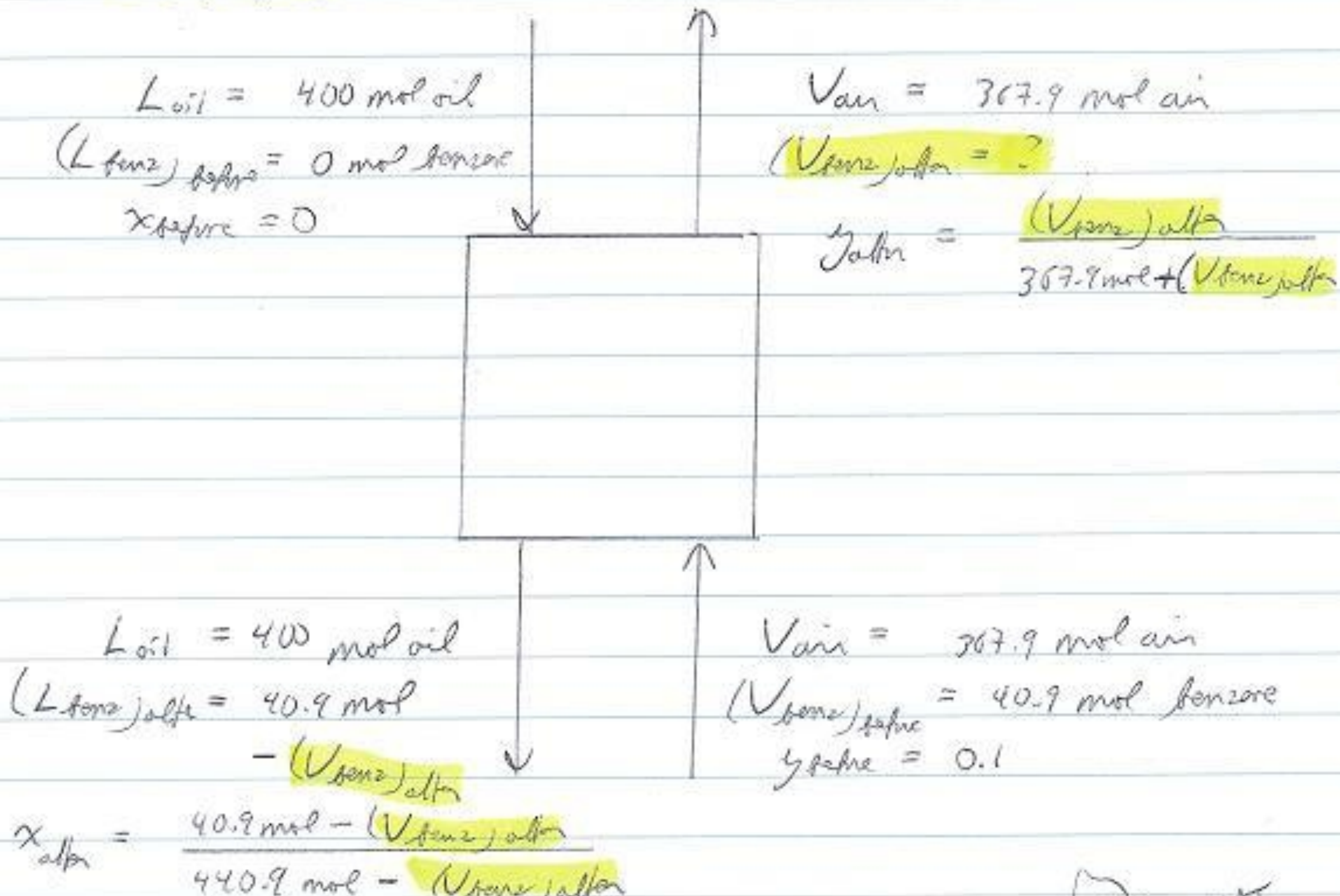
3.9 mol (− root)

Then $y = \frac{3.9}{367.9 + 3.9} = 0.0105$

$$x = \frac{40.9 - 3.9}{440.9 - 3.9} = 0.0847$$

(vi) Summary

In the following flowsheet $(V_{benz})_{after}$ came out to be 3.9 mol



(vii) List of answers

Composition of final gas

$y = y_{benzene} = 0.0105$ (1.05 mole % benzene)

Moles benzene absorbed by liquid is $40.9 - 3.9 = 37$ mol

(viii) Not required: