Single Stage Absorption – "Rigorous" case versus "Usual Assumptions" case

1) 90 m^3 of a 35 C gas mixture with composition 96 mole percent air (3), 4 mole percent toluene (1) is contacted with 1500 kg of 35 C pure n-decane (2). The vapor-liquid system is allowed to come to equilibrium isothermally at 35 C at a constant pressure of 1.0 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 the evaporation of n-decane. Thus, the vapor phase contains all three components, but the liquid phase contains only toluene (1) and n-decane (2).

   Assume that the vapor phase behaves as an ideal gas and the Raoult's law holds for both toluene and n-decane.

For both Problems 1 and 2:

The total amounts of toluene (1), n-decane (2), and air (3) are the same for both Problem 1 and Problem 2:

Vapor Phase – Originally contains $\mathbf{n_1}$ moles toluene and $\mathbf{n_3}$ moles air. The Total moles can be calculated using the Ideal Gas Law

$$n_T = n_1 + n_3 = \frac{PV}{RT} = \frac{1\ atm * 90\ m^3}{8.2057 * 10^{-5}\ \frac{m^3\ atm}{K\ mol} * 308.15\ K} = 3559.3\ total\ moles$$

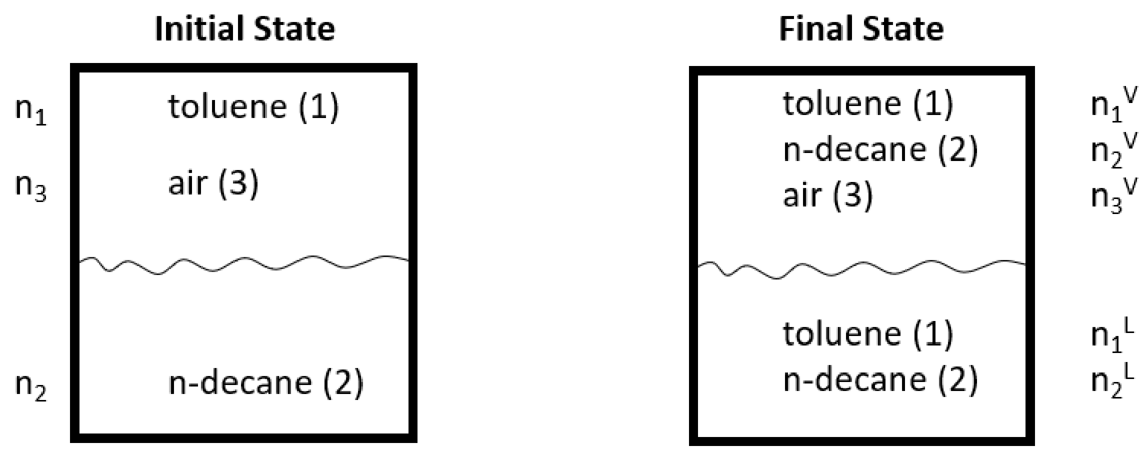
$$n_1 = 0.04 * n_T = 142.37\ mol\ toluene$$

$$n_3 = 0.96 * n_T = 3416.9\ mol\ air$$

Liquid Phase –

$$n_2 = 1500\ kg\ n - decane * \frac{1000\ g}{kg} * \frac{1\ mol\ n - decane}{142.286\ g}$$
$$= 10,542.15\ mol\ n - decane$$

Problem 1



Mass Balance (neglects dissolution of air in n-decane)

$$n_1^L + n_1^V = n_1 \quad \rightarrow \quad n_1^V = n_1 - n_1^L$$

$$n_2^L + n_2^V = n_2 \quad \rightarrow \quad n_2^V = n_2 - n_2^L$$

$$0 + n_3^V = n_3 \quad \rightarrow \quad n_3^V = n_3$$

Equilibrium Relationships (assumes Raoult's Law)

$$y_1 P = x_1 P_1^{sat}$$

$$y_2 P = x_2 P_2^{sat}$$

Using Antoine's Equation (constants and Matlab code available on Computer Code Tab)

$$P_1^{sat} = 46.79\ mm\ Hg\ for\ Toluene\ (1)$$

$$P_2^{sat} = 2.580\ mm\ Hg\ for\ n - Decane\ (2)$$

Now we need to express the mole fractions in terms of the numbers of moles

$$y_1 = \frac{n_1^V}{n_1^V + n_2^V + n_3^V} = \frac{n_1 - n_1^L}{(n_1 - n_1^L) + (n_2 - n_2^L) + n_3}$$

(Substituted # of vapor moles for total moles minus liquid moles as per the mass balance)

$$x_1 = \frac{n_1^L}{n_1^L + n_2^L + n_3^L} = \frac{n_1^L}{n_1^L + n_2^L}$$

$$y_2 = \frac{n_2^V}{n_1^V + n_2^V + n_3^V} = \frac{n_2 - n_2^L}{(n_1 - n_1^L) + (n_2 - n_2^L) + n_3}$$

$$x_2 = \frac{n_2^L}{n_1^L + n_2^L + n_3^L} = \frac{n_2^L}{n_1^L + n_2^L}$$

We have two equations (the equilibrium relationships for toluene and for n-Decane) and originally had five unknowns ($n_1^V, n_2^V, n_3^V, n_1^L, \text{and } n_2^L$). By using the mass balances, we reduce that to two unknowns ($n_1^L, \text{and } n_2^L$).

Substitute the mole fraction expressions into the equilibrium relationships:

Equation 1

$$\frac{n_1 - n_1^L}{(n_1 - n_1^L) + (n_2 - n_2^L) + n_3} = \frac{P_1^{sat}}{P} * \frac{n_1^L}{n_1^L + n_2^L}$$

Equation 2

$$\frac{n_2 - n_2^L}{(n_1 - n_1^L) + (n_2 - n_2^L) + n_3} = \frac{P_2^{sat}}{P} * \frac{n_2^L}{n_1^L + n_2^L}$$

Two equations and two unknowns, but not trivial to solve!

Method 1 Iterative Method

Rearrange Equation 1

$$(n_1 - n_1^L)(n_1^L + n_2^L) = \frac{P_1^{sat}}{P}\left((n_1 - n_1^L) + (n_2 - n_2^L) + n_3\right)$$

$$n_1(n_1^L + n_2^L) = n_1^L\left[n_1^L + n_2^L + \frac{P_1^{sat}}{P}\left((n_1 - n_1^L) + (n_2 - n_2^L) + n_3\right)\right]$$

Equation 1’

$$n_1^L = \frac{n_1(n_1^L + n_2^L)}{n_1^L + n_2^L + \frac{P_1^{sat}}{P}\left((n_1 - n_1^L) + (n_2 - n_2^L) + n_3\right)}$$

Similarly, **Equation 2'**

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

Note that n_1^L occurs on both sides of Equation 1' and that n_2^L occurs on both sides of Equation 2' so the equations cannot be solved directly.

Substitute in the values calculated earlier:

Equation 1'

$$n_1^L = \frac{142.37(n_1^L + n_2^L)}{n_1^L + n_2^L + \frac{46.79}{760}\left((142.37 - n_1^L) + (10{,}542.15 - n_2^L) + 3416.9\right)}$$

Similarly, **Equation 2'**

$$n_2^L = \frac{10{,}542.15\,(n_1^L + n_2^L)}{n_1^L + n_2^L + \frac{2.580}{760}\left((142.37 - n_1^L) + (10{,}542.15 - n_2^L) + 3416.9\right)}$$

We will now solve iteratively, start with guess of $n_1^L = 0$ and $n_2^L = n_2 = 10{,}542.15$. Place these values into the Right-Hand Side of the equations 1' and 2' and see if the values calculated as the Left-Hand Side of the equations match the guesses. If the values calculated do not match the guesses used then take the calculated values and use them as the next set of guesses. Continue until the calculated values match the inputted values for that iteration. This could also be solved using MatLab. I used Excel to run the iterations. We can see that after three iterations the solution has converged:

B7 =B$1*(B6+C6)/(B6+C6+E$1/E$3*(B$1-B6+B$2-C6+B$3))

	A	B	C	D	E	F	G	H
1	n1=	142.37		P1sat=	46.79			
2	n2=	10542.15		P2sat=	2.58			
3	n3=	3416.9		P=	760			
4								
5	Iteration	n1L	n2L					
6	0	0	10542.15		Delta 1	Delta 2		
7	1	139.471	10530.08105		139.471	-12.069		
8	2	139.6054	10530.65138		0.134484	0.570332		
9	3	139.6062	10530.6545		0.000736	0.003117		
10	4	139.6062	10530.65451		4.02E-06	1.7E-05		
11	5	139.6062	10530.65451		2.2E-08	9.32E-08		
12	6	139.6062	10530.65451		1.2E-10	5.09E-10		
13	7	139.6062	10530.65451		6.82E-13	0		

The solution is that:

$$\boldsymbol{n_1^L = 139.6062\ moles\ Toluene}$$

$$\boldsymbol{n_2^L = 10,530.6545\ moles\ n - Decane}$$

One can also use MatLab to solve the two equations.

Now we can calculate the mole fractions:

$$\boldsymbol{y_1 = \frac{n_1 - n_1^L}{(n_1 - n_1^L) + (n_2 - n_2^L) + n_3}}$$

$$\boldsymbol{= \frac{142.37 - 139.6062}{(142.37 - 139.6062) + (10542.15 - 10,530.6545) + 3416.9} = 0.000806}$$

$$\boldsymbol{x_1 = \frac{n_1^L}{n_1^L + n_2^L}}$$

$$\boldsymbol{= \frac{139.6062}{139.6062 + 10530.6545} = 0.013084}$$

$$y_2 = \frac{n_2 - n_2^L}{(n_1 - n_1^L) + (n_2 - n_2^L) + n_3}$$

$$= \frac{10542.15 - 10530.6545}{(142.37 - 139.6062) + (10542.15 - 10{,}530.6545) + 3416.9} = 0.00335$$

$$x_2 = \frac{n_2^L}{n_1^L + n_2^L}$$

$$= \frac{10530.6545}{139.6062 + 10530.6545} = 0.986916$$

$$y_3 = 1 - y_1 - y_2 = 0.995844$$

$x_3 = 0$ by assumption

Summary:

Vapor:

$y_1 = 0.000806$

$y_2 = 0.00335$

$y_3 = 0.995844$

Liquid:

$x_1 = 0.013084$

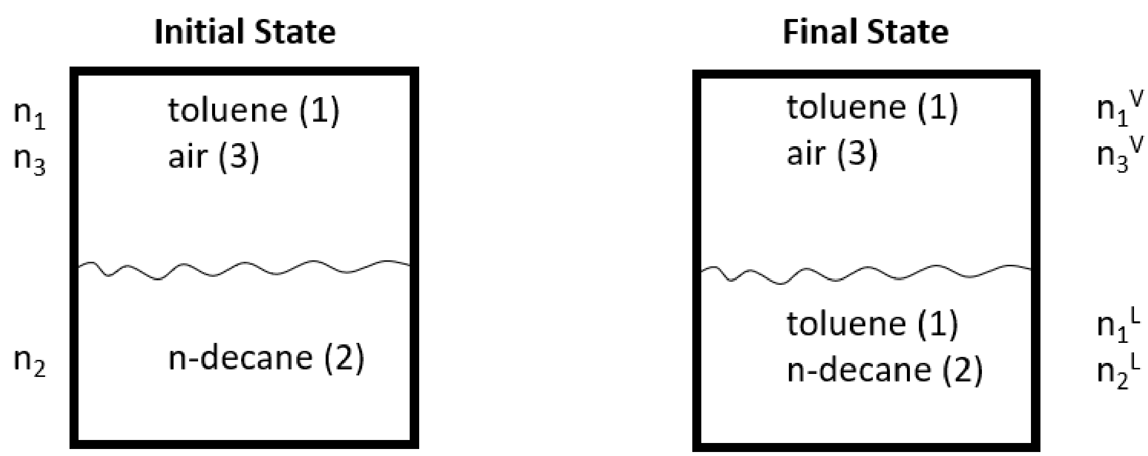
$x_2 = 0.986916$

$x_3 = 0$

Problem 2

2) (Simpler version of Problem 1) 90 m^3 of a 35 C gas mixture with composition 96 mole percent air (3), 4 mole percent toluene (1) is contacted with 1500 kg of 35 C pure n-decane (2). The vapor-liquid system is allowed to come to equilibrium isothermally at 35 C at a constant pressure of 1.0 atm. **What are the final compositions of the liquid and vapor phases?** You should neglect both dissolution of air in the liquid as well as evaporation of n-decane. Thus, the vapor phase contains only toluene (1) and air (3), and the liquid phase contains only toluene (1) and n-decane (2).

Assume that the vapor phase behaves as an ideal gas and the Raoult's law holds for both toluene (1) and n-decane (2).



From Problem 1:

Vapor Phase –

$$n_T = 3559.3 \; total\; moles$$

$$n_1 = 142.37 \; mol\; toluene$$

$$n_3 = 3416.9 \; mol\; air$$

Liquid Phase –

$$n_2 = 10,542.15 \; mol\; n - decane$$

$$P_1^{sat} = 46.79 \; mm\; Hg\; for\; Toluene\; (1)$$

Mass Balance (neglects dissolution of air in n-decane and evaporation of n-decane into air)

$$n_1^L + n_1^V = n_1 \quad \rightarrow \quad n_1^V = n_1 - n_1^L$$

$$n_2^L + 0 = n_2 \quad \rightarrow \quad n_2^L = n_2$$

$$0 + n_3^V = n_3 \quad \rightarrow \quad n_3^V = n_3$$

$$n_3^L = n_2^V = 0$$

With the assumptions of Problem 2, we only have one Equilibrium Relationship (assumes Raoult's Law):

$$y_1 P = x_1 P_1^{sat}$$

$$y_1 = \frac{n_1^V}{n_1^V + n_2^V + n_3^V} = \frac{n_1 - n_1^L}{n_1 - n_1^L + 0 + n_3}$$

$$x_1 = \frac{n_1^L}{n_1^L + n_2^L + n_3^L} = \frac{n_1^L}{n_1^L + n_2}$$

Substitute Mole Fraction expressions into Equilibrium Relationship:

$$\frac{n_1 - n_1^L}{n_1 - n_1^L + n_3} = \frac{P_1^{sat}}{P} * \frac{n_1^L}{n_1^L + n_2}$$

$$(n_1 - n_1^L)(n_1^L + n_2) = \frac{P_1^{sat}}{P} n_1^L (n_1 - n_1^L + n_3)$$

$$n_1 n_1^L + n_1 n_2 - (n_1^L)^2 - n_1^L n_2 = \frac{P_1^{sat}}{P}\left[n_1 n_1^L - (n_1^L)^2 + n_1^L n_3\right]$$

$$\left(\frac{P_1^{sat}}{P} - 1\right)(n_1^L)^2 + \left[n_1 - n_2 - \frac{P_1^{sat}}{P}(n_1 + n_3)\right] n_1^L + n_1 n_2 = 0$$

This is a Quadratic Equation with the solution:

$$n_1^L = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

With the coefficients:

$$a = \left(\frac{P_1^{sat}}{P} - 1\right) = \frac{46.79}{760} - 1 = -0.93843$$

$$b = n_1 - n_2 - \frac{P_1^{sat}}{P}(n_1 + n_3)$$

$$= 142.37 - 10542.15 - \frac{46.79}{760} * \ (142.37 + 3416.9)$$

$$= -10,618.91$$

$$c = n_1 n_2 = \ 142.37 * \ 10542.15 = 1,500,885.9$$

$$n_1^L = \frac{-(-10,618.91) \pm \sqrt{(-10,618.91)^2 - 4(-0.93843)1,500,885.9}}{2(-0.93843)}$$

$$n_1^L = \ -11,455.2 \text{ or } 139.6182$$

Obviously, the negative solution does not have any meaning

$$n_1^L = \ 139.6182$$

Now we calculate the mole fractions:

$$y_1 = \frac{n_1 - \ n_1^L}{n_1 - \ n_1^L + n_3} = \frac{142.37 - \ 139.6182}{142.37 - \ 139.6182 + 3416.9} = 0.000805$$

$y_2 = 0$ by assumption

$$y_3 = 1 - y_1 = 0.999195$$

$$x_1 = \frac{n_1^L}{n_1^L + n_2} = \frac{139.6182}{139.6182 + 10542.15} = 0.013071$$

$$x_2 = 1 - x_1 = 0.986929$$

$x_3 = 0$ by assumption

Comparison of Results (not required)

Component	More Rigorous	"Usual Assumptions"
y_1	0.000806	0.000805
y_2	0.00335	0
y_3	0.995844	0.999195
x_1	0.013084	0.013071
x_2	0.986916	0.986929
x_3	0	0

Note that the results in both phases for Toluene are essentially the same whether we use the more rigorous version or not. Using the "usual assumptions" leads to vapor results for n-decane that are way off, but that was the simplification made. It is important to note that the more rigorous result for n-decane vapor is still a *very* small mole fraction.