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Design Calculations of the TXY Data and drawing of the Equilibrium Curve (X-Y) Diagram of a Binary Distillation Column using Excel

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ABSTRACT: *The importance of the equilibrium (x-y) curve in the design of a binary distillation column was explained. The two ways to do distillation design calculations of a binary distillation column by McCabe Thiele method were considered. One is the graphical method and other way is by using any other commercial simulation software. The Ms Excel software that can easily be gotten and not so expensive was used in this study. All the two ways were used to calculate the TXY data and draw or plot the equilibrium (x-y) curve. The study showed that the TXY data obtained are the same when approximated to 2 decimal places for the two ways to do distillation design calculations of a binary distillation column by McCabe Thiele method. The equilibrium (x-y) curve is also the same in shape and size, when the same scale was used. The study also showed that the calculation and the graphical method using hand is time and energy consuming whereas the calculations and the plot using Ms Excel is less time and energy consuming. Another problem was observed when a similar new design is to be carried out. The calculations and drawing will be started all over again with the hand method but it was not so with MS Excel. As you input the necessary values, all other values will change as well since the formulars are already stored in the MS Excel memory.*
KEYWORDS: *design, equilibrium curve, Binary, distillation, Excel.*

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I. INTRODUCTION

Distillation is one of the oldest unit operations and is the most widely used separation technique in process industry. Distillation is a separation process used to separate two or more components into an overhead distillate and bottoms where the bottoms product is liquid, and the distillate may be liquid or a vapor or both [11; 12; 13; 14]. Distillation is based on the fact that the vapor of a boiling mixture will be richer in the components that have lower boiling points. There are many types of distillation columns, each one of them is designed to be used in specific kind of separation. Depending on how they are operated they can be classified to: Continuous or Batch distillation columns [1; 2]. Binary distillation is a special distillation process. It is a multistage process for separating a mixture of two components [5; 8; 9]. The separation process requires that (i) a second phase be formed so that both vapor and liquid phases can contact each other on each stage within a separation column, (ii) the components have different volatilities so that they will partition between the two phases to different extents, and (iii) the two phases can be separated by gravity or other mechanical means [16]. A binary distillation column is shown in Figure 1. Ideally, the more volatile component is separated as vapor and flows out from top. The less volatile component flows out at bottom as liquid. The product for a binary distillation process is a pure component, or technically a purer component. The component can be obtained by collecting the vapor flow or the liquid flow. There are two ways to do distillation calculations by McCabe Thiele method. One is graphical method and other way is by using any other commercial simulation software. The graphical method is by hand and is time consuming. The use of the commercial simulation software though is costly and requires license is the best especially when different mixtures are involved. In this paper, Ms –Excel is used to calculate and draw the equilibrium curve diagram of a binary distillation column.

The McCabe Thiele's equations are given elsewhere [3; 11; 12; 13; 14; 19].

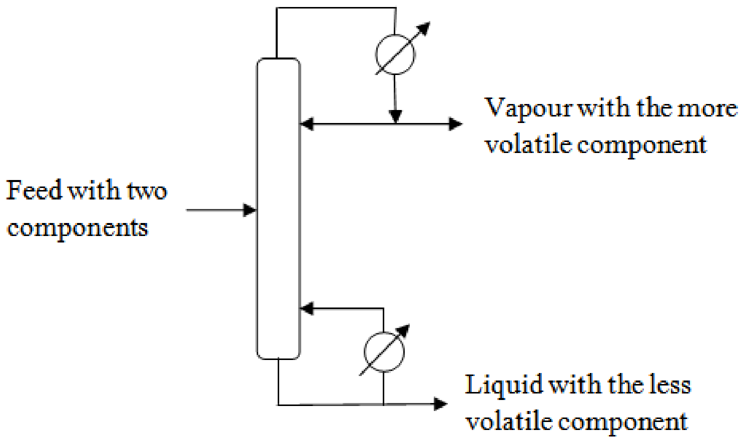


Figure 1. A binary distillation column

II. METHODOLOGY

2.1 The Design Procedure

McCabe and Thiele method uses the equilibrium curve diagram to determine the number of theoretical stages (trays) required to achieve a desired degree of separation. It assumes constant molar overflow and this implies that: (i) molal heats of vaporization of the components are roughly the same; (ii) heat effects are negligible. The information required for the systematic calculation are the vapour liquid equilibrium (VLE) data, feed condition (temperature, composition), distillate and bottom compositions; and the reflux ratio, which is defined as the ratio of reflux liquid over the distillate product. Figure 1 is usually separated into the top section and bottom section of the binary distillation column. The detail procedures for the McCabe and Thiele Method are shown elsewhere [1; 3; 5; 7; 9; 16; 19].

2.2 The Design specifications

Suppose, we are going to design a distillation column to separate benzene-toluene mixture with feed flow rate 3000Kmole/hr, the feed is saturated liquid, the feed has 60% mol fraction of benzene and the over head product has 0.95 mol fraction of benzene and the bottom product contain 0.05 mol fraction of benzene. The system operates in partial reboiler and total condenser modes. The distillation column also operates at atmospheric pressure (p= 1atm) and the operating reflux ratio is 2. The design specifications are shown in table 1. The variables in table 1 that are not found in the design problem can be obtained from literatures [3; 10; 11; 12; 13; 14; 19].

Table 1: Design specifications

Feed rate	3000 Kmole/hr
Feed composition	60% benzene, 40% toluene
Column operating pressure	Atmospheric (1atm)
Column reboiler	Partial
Column condenser	Total
Distillate composition, x_d	95% benzene
Bottom composition, x_b	95% toluene
Relative volatility of benzene to toluene	2.3
Reflux ratio	2
Molecular weight of benzene, MW_{lk}	78.114 kg/kmol
Molecular weight of toluene, MW_{Hk}	92.141 kg/kmol
Boiling point of benzene	80.1 ^{0}C
Boiling point of toluene	110.6 ^{0}C
Vapour density of benzene	2.77kg/m^3
Vapou density of toluene	876kg/m^3
Plate or tray spacing	0.5m

2.3 Assumptions made during the design

The McCabe-Thiele method of column design is used with the following assumptions inherent in the calculation:

- Constant vapor and liquid flow rates in any given section of the tower.
- The latent heat of evaporation is approximately constant with composition and also does not vary much as we proceed from tray to tray.

- The system is non-foaming and non corrosive, and thus we can use carbon steel rather than stainless steel as our material of construction.

2.4 Design steps

Though our concern in this study is the design calculations of the TXY data and drawing of the equilibrium curve (X-Y) diagram of the binary distillation column, the following steps should be followed in the binary distillation column design [8; 13; 14; 15]:

i. Determine the vapor-liquid equilibrium curve (x-y diagram) from Antoine data.
ii. Obtain the physical data of benzene and toluene required for the design.
iii. Calculate the flow rate of various stream through the column
iv. Calculate the minimum reflux ratio and the minimum number of trays required.
v. Using the physical data and flow rates calculate the reboiler and condenser duties.
vi. Calculate maximum and minimum liquid and vapor flow rates.
vii. To start the iteration, select reasonable plate spacing and using the trial plate spacing calculate the column diameter.
viii. Select a trial plate layout, select down-comer area, active, area and size, weir height and length.
ix. From this data check that the weeping rate is satisfactory.
x. Calculate the plate pressure drop.
xi. Check that the down-comer area backup is acceptable.
xii. If at any stage some of the values are too high or low select new trial values and repeat the iterations above.

2.5 Design Calculations of the TXY data and drawing the equilibrium curve (XY) diagram of a binary distillation column:

2.5.1 Calculation and drawing the graph with hand (manually)

Step1: use the Antoine equation (1) to calculate the vapor pressure of benzene and toluene with temperature range for boiling points of benzene and toluene [19]:

$$\mathrm{Log}P_{vap}^{0} = a - \frac{b}{T+c} \tag{1}$$

P_{vap}^{0} for benzene is P_b^0 and for toluene is P_t^0. T is the boiling point temperatures for benzene and toluene. The Boiling point Temperature for benzene = $BP_{lk} = T_{Benzene}^{Bp} = 80.1℃$ and Boiling point Temperature for toluene = $BP_{Hk} = T_{Toluene}^{Bp} = 110.6℃$

The constants a, b and c of the Antoine equation (1) are shown in table 2 [4; 11, 17; 18**]**.

Table 2. The constants a, b, c for the Antoine equation

Compound	A	B	C
Benzene	6.90565	1211.033	220.79
Toluene	6.95334	1343.943	219.377

Calculation of vapour at 80.1℃

For Benzene: $\mathrm{Log}P_b^0 = a - \frac{b}{T+c} = 6.90565 - \frac{1211.033}{80.1+220.79} = 2.88081$

$P_b^0 = 760 \text{ mmHg}$

For Toluene: $\mathrm{Log}P_t^0 = a - \frac{b}{T+c} = 6.95334 - \frac{1343.943}{80.1+219.377} = 2.46571$

$P_t^0 = 292.2 \text{ mmHg}$

Appling the above steps for the other temperature between (80.1- 110.6) we obtained the following results, listed in table 2.

Step2: Calculation of x_A using equation (2) as given by [19]

$$x_A = \frac{P-P_B}{P_A-P_B} \tag{2}$$

Where

x_A = moles of component A (Benzene) in the liquid = x_b

P = 1atm = 760 mmHg

P_B = Vapour pressure of component B (Toluene) = P_t = 292.2 mmHg

P_A = Vapour pressure of component A (Benzene) = P_b= 760 mmHg

Therefore, $x_b = \frac{P-P_t}{P_b-P_t} \frac{760-292.2}{760-292.2} = 1$

Step3: Calculation of y_B using equation (3) as given by [19]

$$y_b = \frac{\alpha x_b}{1+x_b(\alpha-1)} \tag{3}$$

Relative volatility is given as 2.3 and so

$$y_b = \frac{\alpha x_b}{1+x_b(\alpha-1)} = \frac{2.3(1)}{1+1(2.3-1)} = \frac{2.3}{2.3} = 1$$

Appling the above steps for the other temperature between (80.1- 110.6), we obtained the following TXY data for benzene and toluene as listed in table 3.

Table 3. TXY data for benzene and toluene

Temp. (^{0}C)	P_b^0 (mmHg)	P_t^0 (mmHg)	x_b	y_b
80.1	760.0	292.2	1.00	1.00
82	805.5	311.9	0.91	0.96
84	855.7	333.7	0.82	0.91
86	908.3	356.8	0.73	0.86
88	963.3	381.1	0.65	0.81
90	1021.0	406.7	0.58	0.76
92	1081.3	433.7	0.50	0.70
94	1144.3	462.1	0.44	0.64
96	1210.1	492.0	0.37	0.58
98	1278.8	523.4	0.31	0.51
100	1350.5	556.3	0.26	0.44
102	1425.2	590.9	0.20	0.37
104	1503.1	627.2	0.15	0.29
106	1584.2	665.2	0.10	0.21
108	1668.6	704.9	0.06	0.12
110	1756.4	746.6	0.01	0.03
110.6255	1784.5	760	0.00	0.00

Step4: from data in table 3, Plot $y_b$versus x_b in a graph using hand as in figure 2.

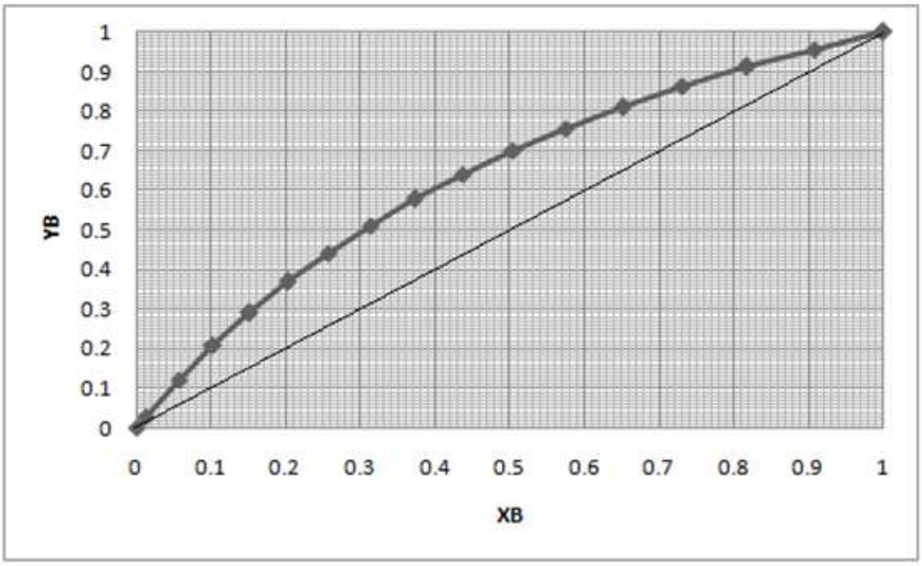


Figure 2. Equilibrium curve (y-x) diagrame

2.5.2 Calculation and drawing the graph with MS Excel

If $\text{Log}P_{vap}^0 = a - \frac{b}{T+c}$ as in equation (1)

Then, $P_{vap}^0 = 10^{\left(a-\frac{b}{T+c}\right)}$ or

$$P_b^0 = 10^{\left(a-\frac{b}{T+c}\right)} \text{ and } P_t^0 = 10^{\left(a-\frac{b}{T+c}\right)} \tag{4}$$

Where P_b^0 and P_t^0 are the vapour pressure of benzene and toluene respectively

The Excel code for equation (4) is

$$P_b^0 = 10^{\wedge[a-(b)*(T+c)^\wedge-1]} \text{ and } P_t^0 = 10^{\wedge[a-(b)*(T+c)^\wedge-1]} \tag{5}$$

Excel code 1

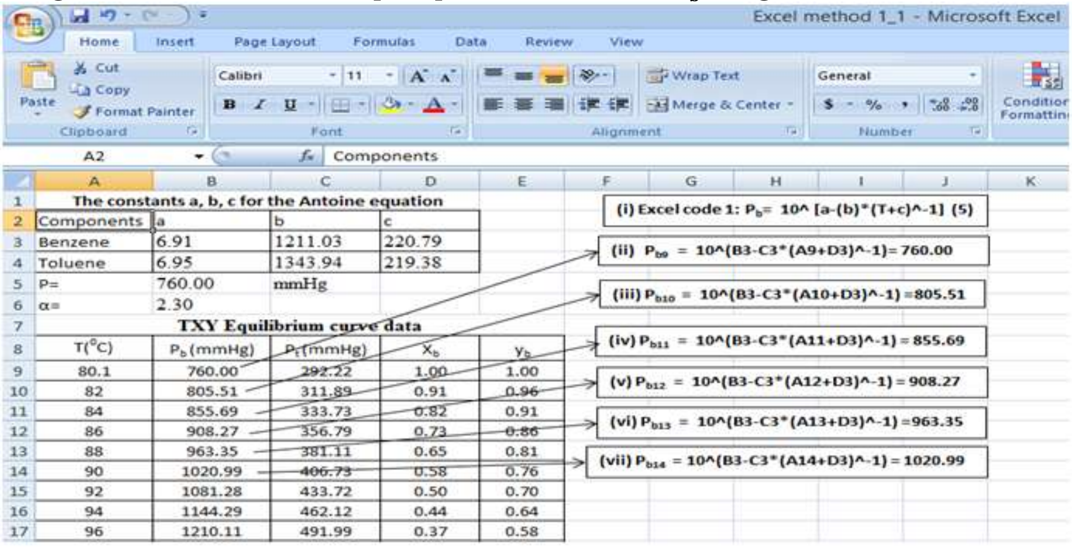
$$P_b^0 = 10^{\wedge[a-(b)*(T+c)^{\wedge}-1]} \qquad (5)$$

Excel code 2

$$P_t^0 = 10^{\wedge[a-(b)*(T+c)^{\wedge}-1]} \qquad (6)$$

The excel code 1 in (5) is used to calculate the value of the vapour pressure of butane, $\mathbf{P_b^0}$ and the excel code 2 in (6) is used to calculate the vapour pressure of toluene, $\mathbf{P_t^0}$ using Ms Excel user interface as shown in figure 3 and figure 4 respectively.

Figure 3. Calculation of the vapour pressure of benzene, P_b^0 using Ms Excel user interface.



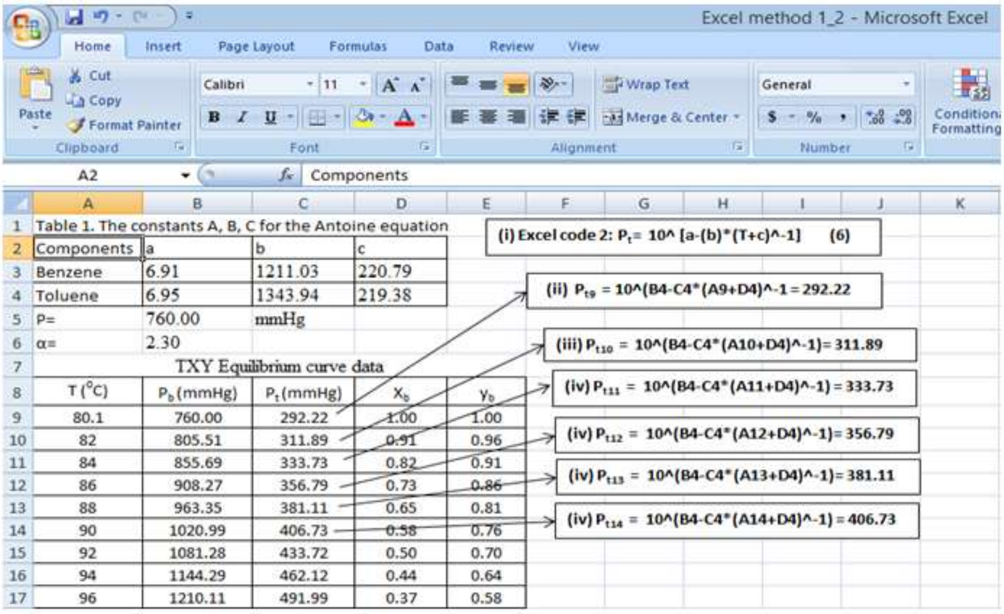


Figure 4. Calculation of the vapour pressure of toluene, P_t^0 using Ms Excel user interface.

2.5.3 Using Figure 3 to explain calculations in Ms excel

Excel stores its values in columns (denoted by A to z) and rows (from 1 to infinity).

In figure 3:

(i) Shows the excel code 1: $\mathbf{P_b^0 = 10^{\wedge[a-(b)*(T+c)^\wedge-1]}}$ as shown in (5)
(ii) Shows $\mathbf{P_{b9}}$ = **10^(B3-C3*(A9+D3)^-1) = 760.00 mmHg**
(iii) Shows $\mathbf{P_{b10}}$ = **10^(B3-C3*(A10+D3)^-1) =805.51 mmHg**
(iv) Shows $\mathbf{P_{b11}}$ = **10^(B3-C3*(A11+D3)^-1) = 855.69 mmHg**
(v) Shows $\mathbf{P_{b12}}$ = **10^(B3-C3*(A12+D3)^-1) = 908.27 mmHg**
(vi) Shows $\mathbf{P_{b13}}$ = **10^(B3-C3*(A13+D3)^-1) =963.35 mmHg**
(vii) Shows $\mathbf{P_{b14}}$ = **10^(B3-C3*(A14+D3)^-1) = 1020.99 mmHg**

Where
$\mathbf{P_{b9}}$ → the value of the vapour pressure of benzene in row 9 = 760.00 mmHg
B3 →means the value in column B row 3 = 6.91
C3 →means the value in column C row 3 = 1211.03
A9 →means the value in column A row 9 = 80.1 ^{0}C
^ →means raised to
***** →means multiplication
$\mathbf{P_{b10}}$ → the value of the vapour pressure of benzene in row 10 = 805.51 mmHg
A10 →means the value in column A row 10 = 82 ^{0}C
$\mathbf{P_{b11}}$ → the value of the vapour pressure of benzene in row 11 = 855.69 mmHg
A11 →means the value in column A row 11 = 84 ^{0}C
$\mathbf{P_{b12}}$ → the value of the vapour pressure of benzene in row 12 = 908.27 mmHg
A12 →means the value in column A row 12 = 86 ^{0}C
$\mathbf{P_{b13}}$ → the value of the vapour pressure of benzene in row 13 = 963.35 mmHg
A13 →means the value in column A row 13 = 88 ^{0}C
$\mathbf{P_{b14}}$ → the value of the vapour pressure of benzene in row 14 = 1029.99 mmHg
A14 →means the value in column A row 14 = 90 ^{0}C

This is how excel works and is applicable to all other figures. A detail explanation of how excel is used to solve problems is found elsewhere [6].

1f $x_A = \frac{P-P_B}{P_A-P_B}$ or $x_b = \frac{P-P_t}{P_b-P_t}$ for benzene in (2), then $x_b = (P-P_t)/(P_b-P_t)$ (7)

Where P = is the atmospheric pressure, P_b and P_t are the vapour pressures of benzene and toluene respectively and x_A = moles of component A (Benzene) in the liquid = x_b

The Excel code for (7) is

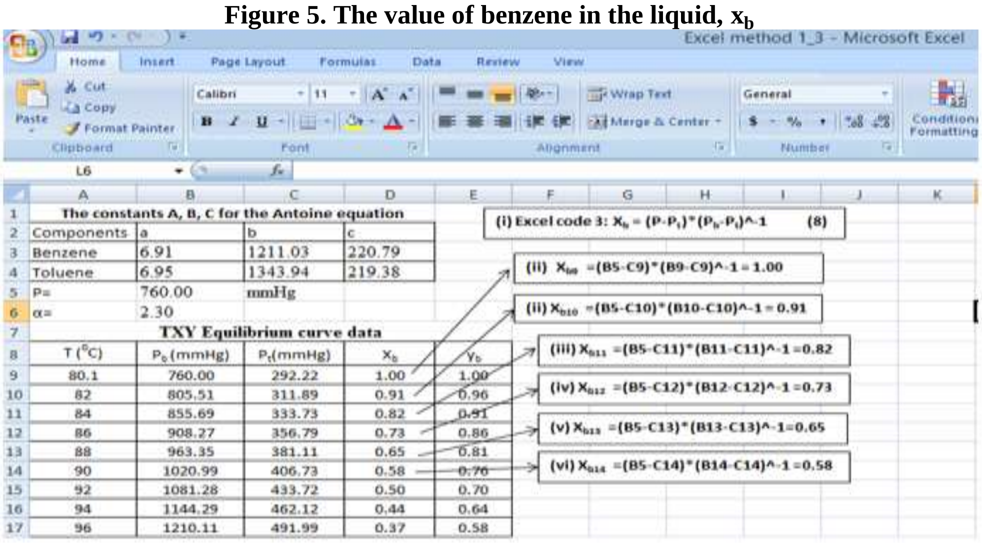
$$x_b = (P-P_t)*(P_b-P_t)^{\wedge-1} \quad (8)$$

Excel code 3

$$x_b = (P - P_t) * (P_b - P_t)^{\wedge-1} \quad (8)$$

The excel code 3 in (8) is used to calculate the value of benzene in the liquid, $\mathbf{x_b}$ as shown in figure 5.

Figure 5. The value of benzene in the liquid, $\mathbf{x_b}$



The constants A, B, C for the Antoine equation

Components	a	b	c
Benzene	6.91	1211.03	220.79
Toluene	6.95	1343.94	219.38
P=	760.00	mmHg	
α=	2.30		

TXY Equilibrium curve data

T (^{0}C)	P_b (mmHg)	P_t(mmHg)	X_b	Y_b
80.1	760.00	292.22	1.00	1.00
82	805.51	311.89	0.91	0.96
84	855.69	333.73	0.82	0.91
86	908.27	356.79	0.73	0.86
88	963.35	381.11	0.65	0.81
90	1020.99	406.73	0.58	0.76
92	1081.28	433.72	0.50	0.70
94	1144.29	462.12	0.44	0.64
96	1210.11	491.99	0.37	0.58

If $y_b = \frac{\alpha x_b}{1+x_b(\alpha-1)}$ in (3), then $y_b = a(x_b)/[1+x_b(\alpha-1)]$ (9)

Where y_b = moles of benzene in the gas or vapour, x_b = moles of benzene in the liquid and α is the relative volatility

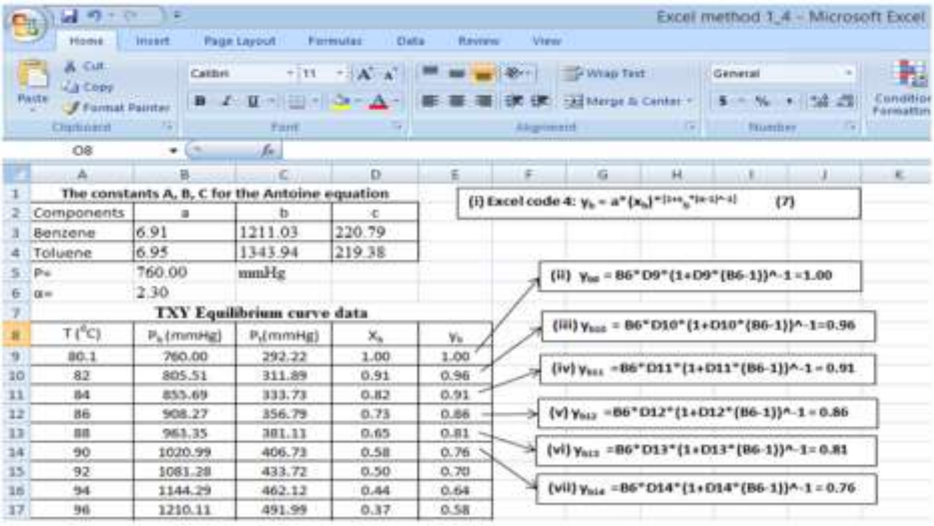
The Excel code for (9) is

$$y_b = a*(x_b)*^{[1+x_b*(\alpha-1)]^{\wedge-1}} \qquad (10)$$

Excel code 4	
$y_b = a*(x_b)*^{[1+x_b*(\alpha-1)]^{\wedge-1}}$	(10)

The excel code 4 in (10) is used to calculate the value of benzene in the liquid, x_b as shown in figure 6.

Figure 6. The value of benzene in the vapour or gas, y_b



So, applying the above steps for the other temperature between (80.1- 110.6), we obtained the TXY data for benzene and toluene as listed in table 3. How to obtain the equilibrium curve is shown in figure7

Table 3. TXY data from MS EXCEL user Interface

T (°C)	P_b (mmHg)	P_t(mmHg)	X_b	Y_b
80.1	760.00	292.22	1.00	1.00
82	805.51	311.89	0.91	0.96
84	855.69	333.73	0.82	0.91
86	908.27	356.79	0.73	0.86
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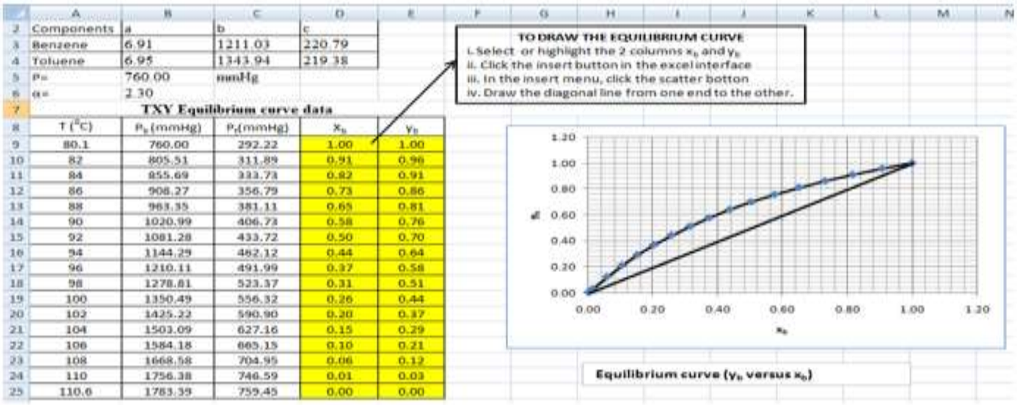
106	1584.18	665.15	0.10	0.21
108	1668.58	704.95	0.06	0.12
110	1756.38	746.59	0.01	0.03
110.6	1783.39	759.45	0.00	0.00



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110	1756.38	746.59	0.01	0.03
110.6	1783.39	759.45	0.00	0.00

Figure 7. How to obtain the equilibrium curve with excel

III. DISCUSSION AND CONCLUSION

Section 2.4.1 briefly shows the use of hand to calculate the TXY data and the use of hand to draw or plot the equilibrium curve with a graph sheet while section 2.4.2 shows the use of MS Excel to calculate the TXY data and the use of MS Excel to draw or plot the equilibrium curve. A careful comparison shows that the calculated values using hand and Ms Excel are the same when approximated to 2 decimal places. Also, the equilibrium curve plotted in both cases appears the same. The problem is that the calculation and the graphical method using hand is time and energy consuming whereas the calculations and the plot using Ms Excel is less time and energy consuming. Another problem was observed when a similar new design is to be carried out. The calculations and drawing will be started all over again with the hand method but it was not so with MS Excel. As you input the necessary values, all other values will change as well since the formulars are already stored in the MS Excel memory. Further work will be comparing the calculations and plot of the equilibrium curve using Ms Excel and other commercial simulation softwares, though they are costly and requires license.

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