CHE221A

ASSIGNMENT 07

MODEL SOLUTION

1. From the given S_O, S_H & S_M values it can be considered that

$$S_O \approx S_H \approx S_M$$

Therefore, we can use Raoult's law to determine Bubble pt. & Dew pt. temperature.

(a) Bubble point temperature:-

Given,

$$x_o = 0.3, \; x_h = 0.3 \; \& \; x_M = 0.4, \; P = 1\,bar$$

Using Raoult's law;

$$x_i P_i^{sat} = y_i P$$

$$\therefore \quad P = x_o P_o^{sat} + x_h P_h^{sat} + x_M P_M^{sat}$$

$$1 = (0.3)\exp\left(10.422 - \frac{26719}{\left(\frac{8.314}{1000}\right)T}\right) + (0.3)\exp\left(10.456 - \frac{29676}{RT}\right)$$

$$+ (0.4)\exp\left(11.431 - \frac{35200}{\left(\frac{8.314}{1000}\right)T}\right)$$

→ From excel solver;

$$\boxed{T_{bubble} = 333.9\ K}$$

[b] Dew point temperature :-

Given;

$y_o = 0.3,\ y_h = 0.3,\ y_m = 0.4$

$P = 1\ bar$

→ Using Rault's law;

$$x_i P_i^{sat} = y_i P$$

$$\therefore x_o + x_h + x_M = 1$$

$$\therefore \frac{y_o P}{P_o^{sat}} + \frac{y_h P}{P_h^{sat}} + \frac{y_m P}{P_M^{sat}} = 1$$

$$\therefore \frac{0.3}{\exp\left(10.422 - \frac{26799}{\frac{8.314 T}{1000}}\right)} + \frac{0.3}{\exp\left(10.456 - \frac{29676}{\frac{8.314 T}{1000}}\right)} + \frac{0.4}{\exp\left(11.431 - \frac{35200}{\frac{8.314 T}{1000}}\right)} = 1$$

→ Using excel solver :-

$$\boxed{T_{dew} = 352.9\ K}$$

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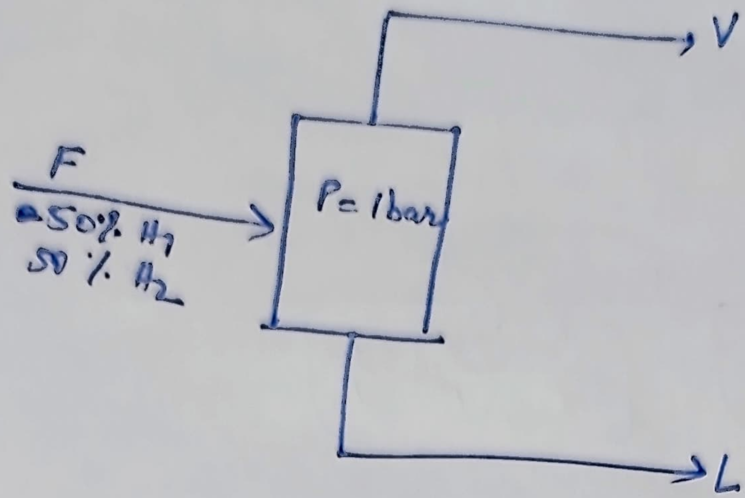

→ Given;

$$L = 0.6F$$

$$\therefore V = 0.4F \qquad [\because F = L + V]$$

Let Basis : $F = 100$ moles

$\therefore x_{1,f} = 50$ moles

$\therefore x_{2,f} = 50$ moles

$\therefore L = 60$ moles, $V = 40$ moles

→ Mass balance over component Hi gives;

$$x_{i,f} \cdot F = y_i V + x_i L \quad — (1)$$

Using raoult's law we get;

$$x_{1,f} = x_1 \left[\frac{P_1^{sat}}{P} \left(\frac{V}{F}\right) + \frac{L}{F} \right]$$

Similiarly;

$$x_{2,f} = x_2 \left[\frac{P_2^{sat}}{P} \left(\frac{V}{F}\right) + \frac{L}{F} \right]$$

As we know;

$$x_1 + x_2 = 1$$

$$\therefore \frac{x_1 f}{\left[\frac{P_1^{sat}}{P}\left(\frac{V}{F}\right) + \frac{L}{F}\right]} + \frac{x_2 f}{\left[\frac{P_2^{sat}}{P}\left(\frac{V}{F}\right) + \frac{L}{F}\right]} = 1$$

→ Substituting appropiate values and using excel solver;

$$\boxed{\begin{array}{c} T = -6.597\,°C \\ \text{or} \\ T = 266.40\,K \end{array}} \Rightarrow \text{Temperature of ash unit}$$

→ To get composition Liquid & vapor streams;

$$x_i P_i^{sat} = y_i P \quad - (2)$$

Solving eq (1) & (2) leads to;

$x_1 = 0.543$	$y_1 = 0.434$
$x_2 = 0.457$	$y_2 = 0.566$

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→ To obtain the values of A_{12}, A_{21} & C we have to fit experimental values of $\frac{G^E}{RT}$ by given correlation:-

$$\frac{G^E}{RT} = \left(A_{21} x + A_{12} x_2 - C x_1 x_2\right) x_1 x_2 \quad \text{—— (1)}$$

→ To obtain experimental G^E/RT we use the following:-

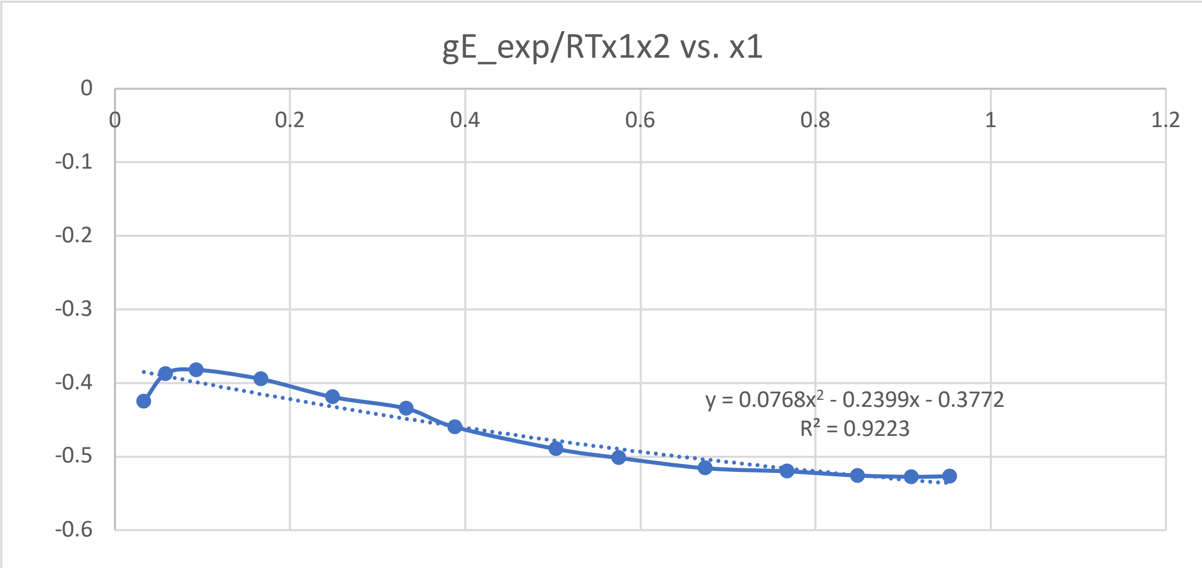
$$\frac{G^E}{RT} = \cancel{A_{21} x_1}\; x_1 \ln \gamma_1 + x_2 \ln \gamma_2$$

where $\gamma_i = \dfrac{y_i P_i^{sat}}{x_i P}$ (Modified Raoult's law)

$$\therefore \boxed{\frac{G^E}{RT} = x_1 \ln\left(\frac{y_1 P_1^{sat}}{x_1 P}\right) + x_2 \ln\left(\frac{y_2 P_2^{sat}}{x_2 P}\right)}$$

→ Now, from the values obtained a plot of $\frac{G^E}{RT x_1 x_2}$ vs. x_1 is made and subsequently curve fitting is carried out using eq (1) in terms of x_1 only.

- The following plot shows the curve fitting to obtain constants C, A_{12} and A_{21}



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$$\boxed{\frac{G^E}{RT x_1 x_2} = C x_1^2 + (A_{21} - A_{12} - C)x_1 + A_{12}}$$ as Fitting function

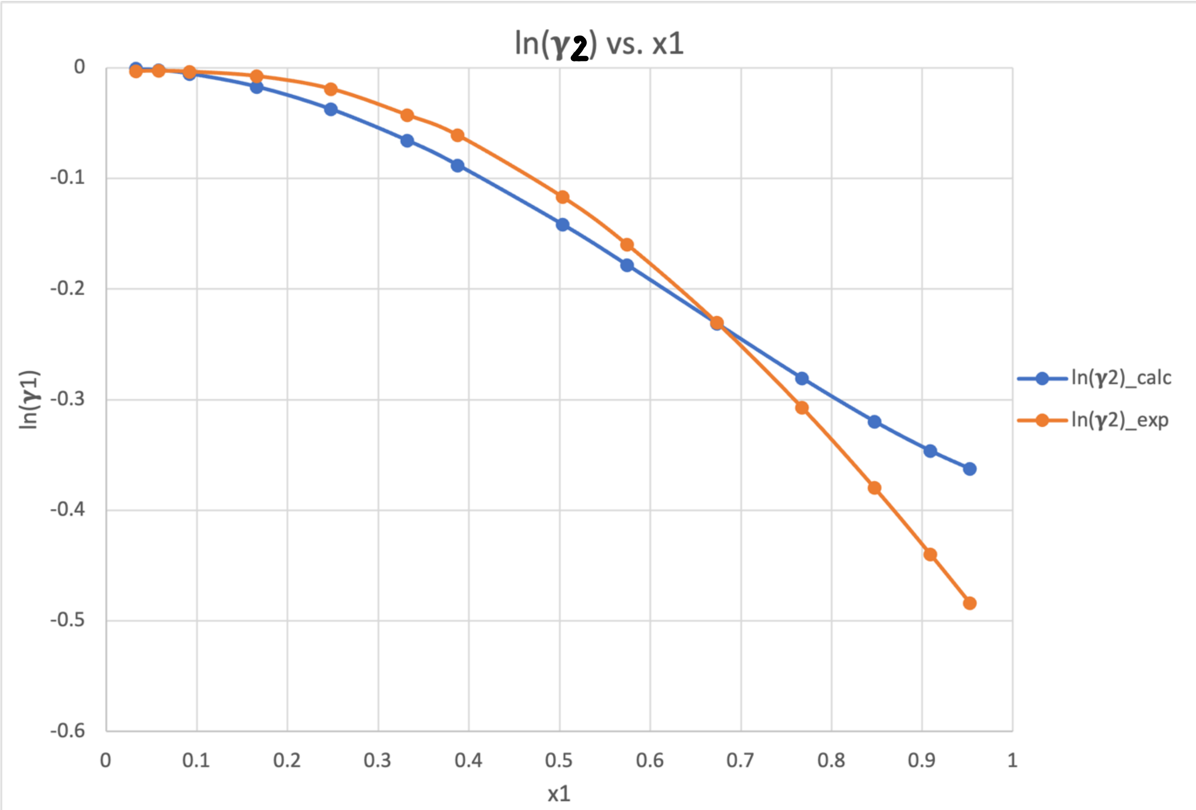
→ This leads to values of constants as below:–

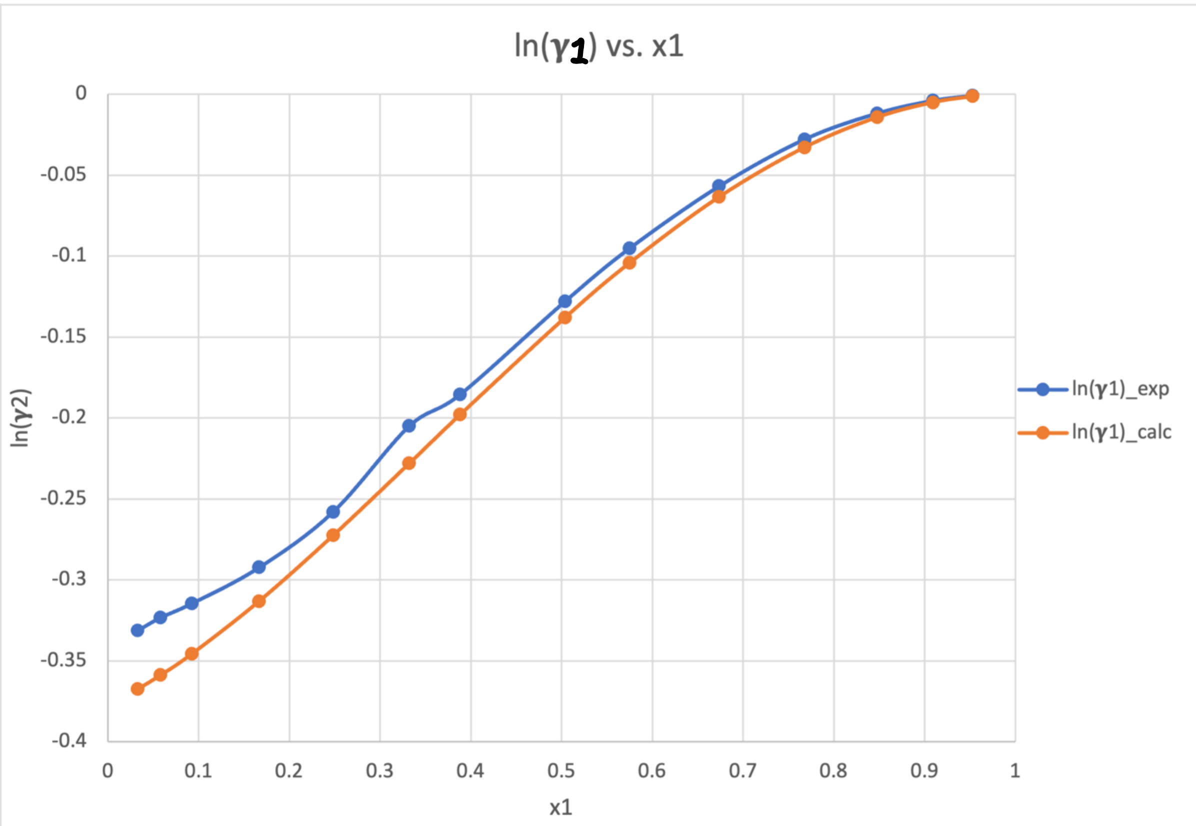
$C = 0.0768$

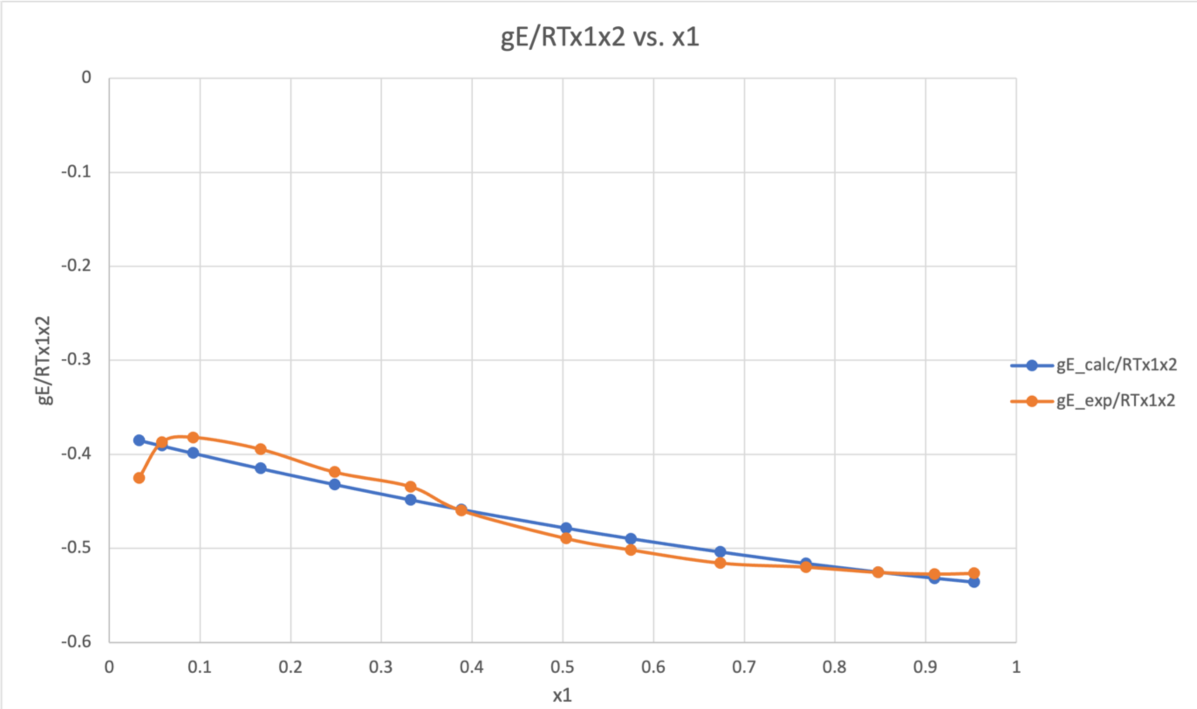
$A_{12} = -0.3772$

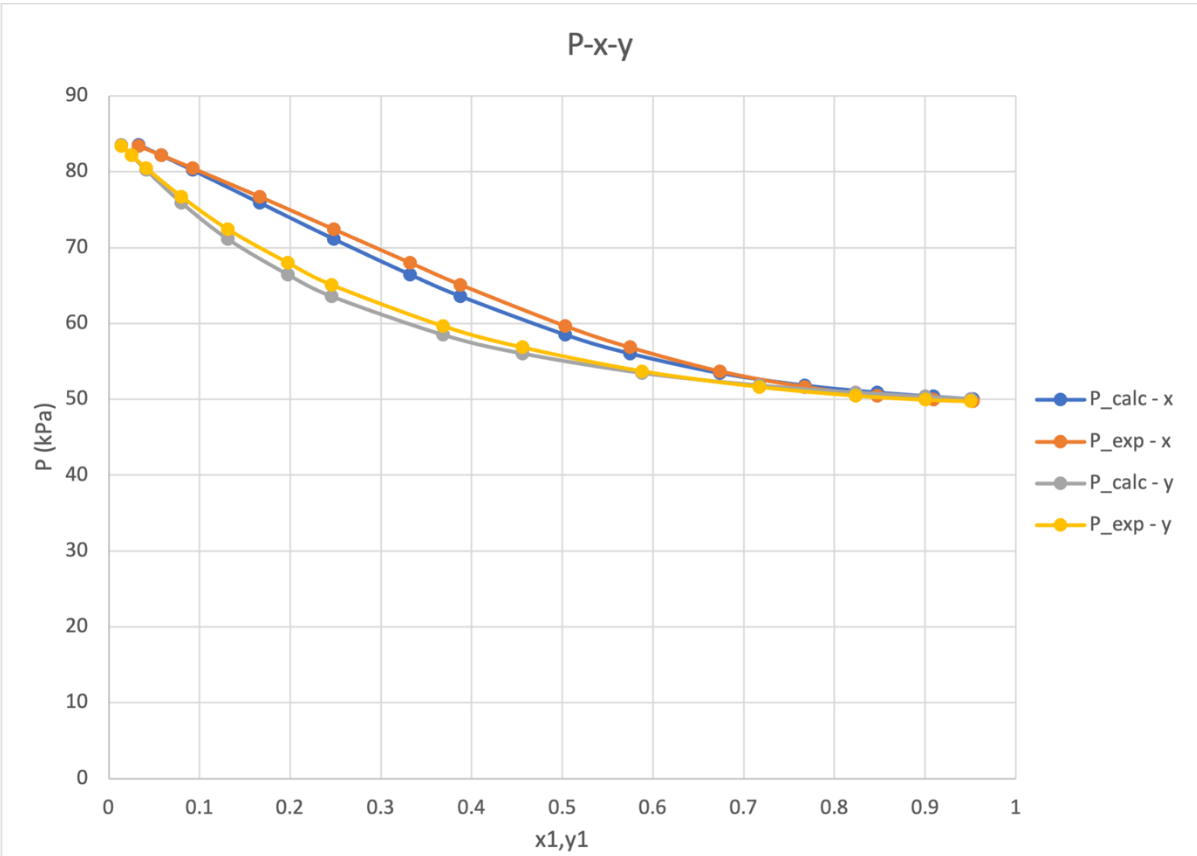
$A_{21} = -0.5403$

→ Using these values and given eqn of $\ln \gamma_1$ & $\ln \gamma_2$, calculated / correlated values are obtained and plotted as follows:–


ln(γ2) vs. x1
0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
ln(γ1)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x1
ln(γ2)_calc
ln(γ2)_exp


ln(γ1) vs. x1
0
-0.05
-0.1
-0.15
-0.2
-0.25
-0.3
-0.35
-0.4
ln(γ2)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x1
ln(γ1)_exp
ln(γ1)_calc


gE/RTx1x2 vs. x1
0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
gE/RTx1x2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x1
gE_calc/RTx1x2
gE_exp/RTx1x2


P-x-y
90
80
70
60
50
40
30
20
10
0
P (kPa)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x1,y1
P_calc - x
P_exp - x
P_calc - y
P_exp - y