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Model: NRTL

System: Water and N,N Dimethylacetamide.

### Lap report

By modified Raoult's law:-

$$p y_i = p_i^{\text{sat}} \gamma_i x_i$$

$$p y_1 = p_1^{\text{sat}} \gamma_1 x_1 \quad \text{--- (i)}$$

$$p y_2 = p_2^{\text{sat}} \gamma_2 x_2 \quad \text{--- (ii)}$$

(i)  $\rightarrow$  for water

(ii)  $\rightarrow$  for N,N-Dimethylacetamide

$y_i \rightarrow$  mole fraction of component  $i$   
in vapor phase

$x_i \rightarrow$  mole fraction of component  $i$   
in liquid phase.

$\gamma_i \rightarrow$  Activity coefficient of  $i^{\text{th}}$   
Component.

$p_i^{\text{sat}} \rightarrow$  vapor pressure of pure  $i^{\text{th}}$   
Component at temperature  $T$ .

$p \rightarrow$  total pressure

by eq. (i) and (ii)

after eliminating  $y_1, y_2, x_1$   
we get

$$p - p_1^{\text{sat}} (1 - x_2) \gamma_1 + (-p_2^{\text{sat}} \gamma_2 x_2) = 0 \quad \text{--- (iii)}$$

here  $p = 760 \text{ mm Hg}$

for  $p_1^{\text{sat}}, p_2^{\text{sat}}$  use Antoine's eqn.

$$\log [p_i^\circ] = A - \frac{B}{t+C}$$

A, B, c for water and N, N-Dimethylacetamide are given

for  $T_1, T_2$

$$\ln \gamma_1 = x_2^2 \left[ T_{21} \left( \frac{G_{21}}{x_1 + x_2 G_{21}} \right)^2 + \frac{T_{12} G_{12}}{(x_2 + x_1 G_{12})^2} \right]$$

$$\ln \gamma_2 = x_1^2 \left[ T_{12} \left( \frac{G_{12}}{x_2 + x_1 G_{12}} \right)^2 + \frac{T_{21} G_{21}}{(x_1 + x_2 G_{21})^2} \right]$$

$$G_{12} = \exp(-\alpha_{12} T_{12})$$

$$G_{21} = \exp(-\alpha_{21} T_{21})$$

$$\alpha_{12} = \alpha_{21} = 0.3009 \text{ (given)}$$

$$\gamma_1^\infty = 1.60, \gamma_2^\infty = 1.63$$

So we will find  $T_{12}, T_{21}$  by using these values, then  $G_{12}, G_{21}$  can be easily found.

$$\ln \gamma_1^\infty = T_{21} + T_{12} \exp(+\alpha T_{12}) \text{ (iv)}$$

$$\ln \gamma_2^\infty = T_{12} + T_{21} \exp(-\alpha T_{21}) \text{ (v)}$$



by using above two eqns and iterations, in excel sheet I find:-

$$T_{12} = 0.32, T_{21} = 0.18$$

$$\Rightarrow G_{12} = 0.908, G_{21} = 0.95 \\ \approx 0.91$$

now in eq. (iii)  
for a T value I have found  $x_2$  and by using  $x_2 = 1 - x_1$

i have found out  $x_1$ , (this work is in matlab)  
after that by using

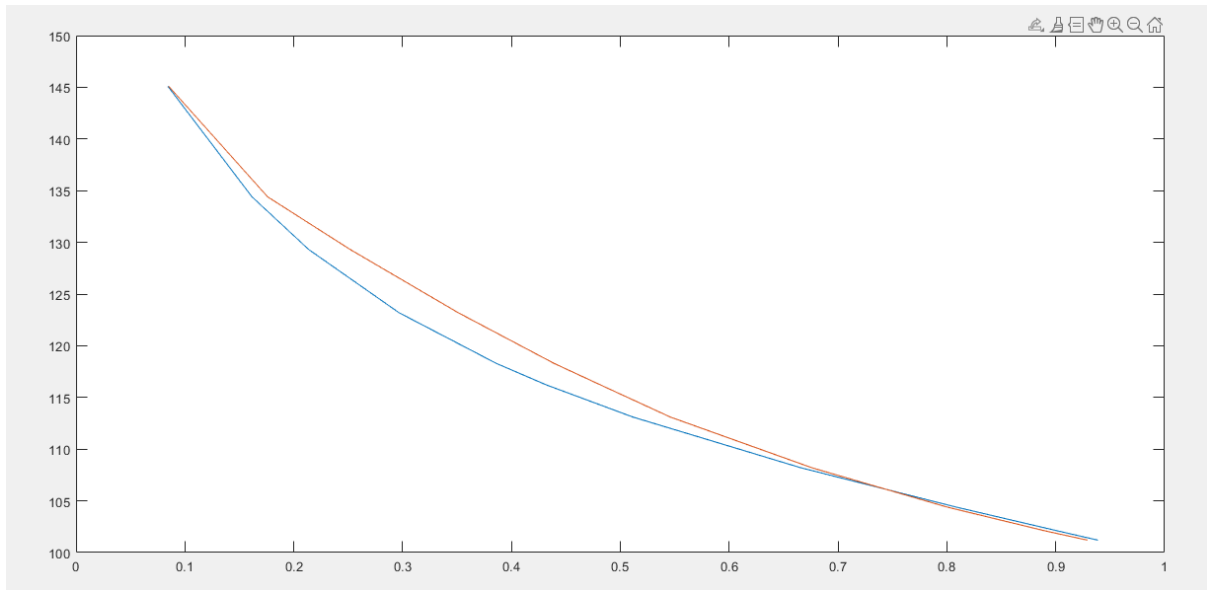
$$P y_1 = P_1^{sat} T_1 x_1$$

$$\Rightarrow y_1 - \frac{P_1^{sat} T_1 x_1}{P} = 0$$

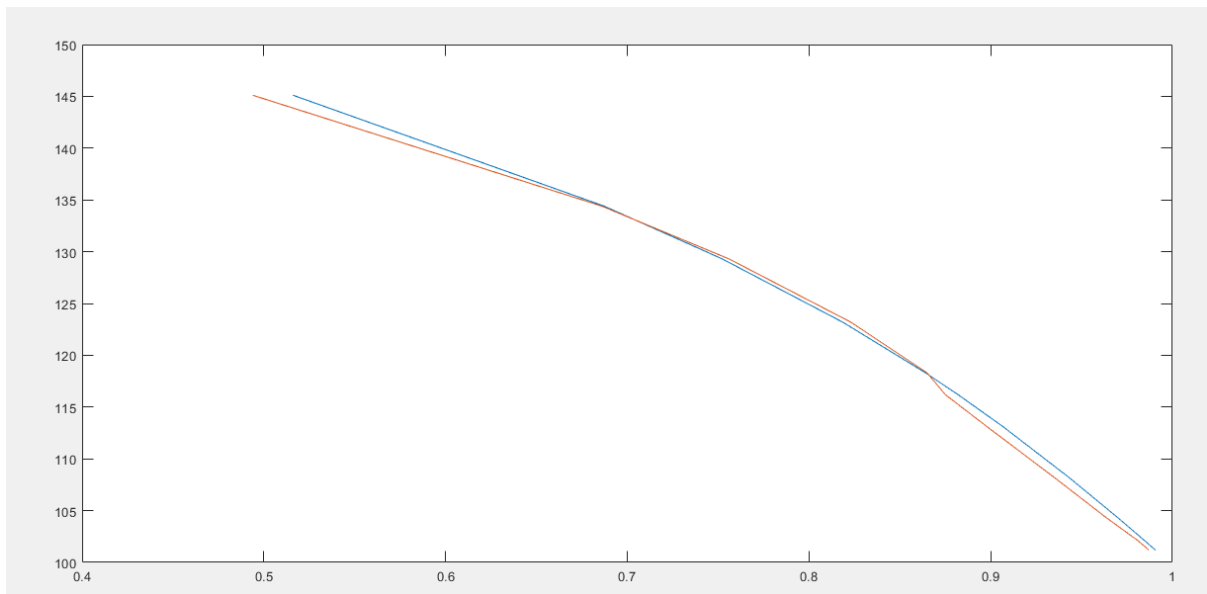
i have solved this eqn in matlab  
and found  $y_1$ .

After that i have found  $y_1, x_1$   
I have drawn graph between T and  $x_1$ , T and  $y_1$  and last  $y$  and  $x$

Plot for T vs X (both theoretical and experimental)



Plot for T vs Y (both theoretical and experimental)



Plot for Y vs X (both theoretical and experimental)

