Computational Assignment Report

CHE221

ARMEET SINGH LUTHRA,200185

System: 2-Butanol & 1,3,5-TrimethylBenzene

Activity Coefficient Model – Wilson

Pressure- 760mm Hg

Formulas Used:

1) For getting activity coefficient

Wilson [8]	$\lambda_{12}-\lambda_{11}$ 1)	$-\ln(x_1+\Lambda_{12}x_2)+x_2\left(\frac{\Lambda_{12}}{x_1+\Lambda_{12}x_2}-\frac{\Lambda_{21}}{\Lambda_{21}x_1+x_2}\right)$ (30a)
	$\lambda_{21}-\lambda_{22}$	$-\ln(x_2+\Lambda_{21}x_1)-x_1\left(\frac{\Lambda_{12}}{x_1+\Lambda_{12}x_2}-\frac{\Lambda_{21}}{\Lambda_{21}x_1+x_2}\right)$ (30b)

1) $\Lambda_{12}=\frac{V_2^L}{V_1^L}\exp-\frac{\lambda_{12}-\lambda_{11}}{RT}$ $\qquad$ $\Lambda_{21}=\frac{V_1^L}{V_2^L}\exp-\frac{\lambda_{21}-\lambda_{22}}{RT}$

V_i^L molar volume of pure liquid component i. For values of V_i^L see Appendix A.

λ_{ij} interaction energy between components i and j $\lambda_{ij}=\lambda_{ji}$

2) For getting $P_{sat}(T)$.

2. Antoine Vapor Pressure Equation

The Antoine vapor pressure equation is used in the following form:

$$\log[p_i^0]=A-\frac{B}{t+C}$$

with $[p_i^0]$ vapor pressure of pure component i in mm Hg

t temperature in degrees Celsius (° C)

Code Logic

- Find T_1^{sat} and T_2^{sat} at P=760mm.
- Enter loop, vary x from 0 to 1 with increment of 0.01
- Loop starts
- Assume T' as the equilibrium temperature of the mixture
- $T' = x * T_1^{sat} + (1-x) * T_2^{sat}$
- Use the equation:

  At equilibrium:

  $P = P_1^{sat}(T)*x*gamma1(x,T)+P_2^{sat}(T)*(1-x)*gamma2(x,T)$

  $P_2^{sat}(T) = P/((1-x)*gamma2(x,T)+(P_1^{sat}(T)/P_2^{sat}(T))*x*gamma1(x,T))$

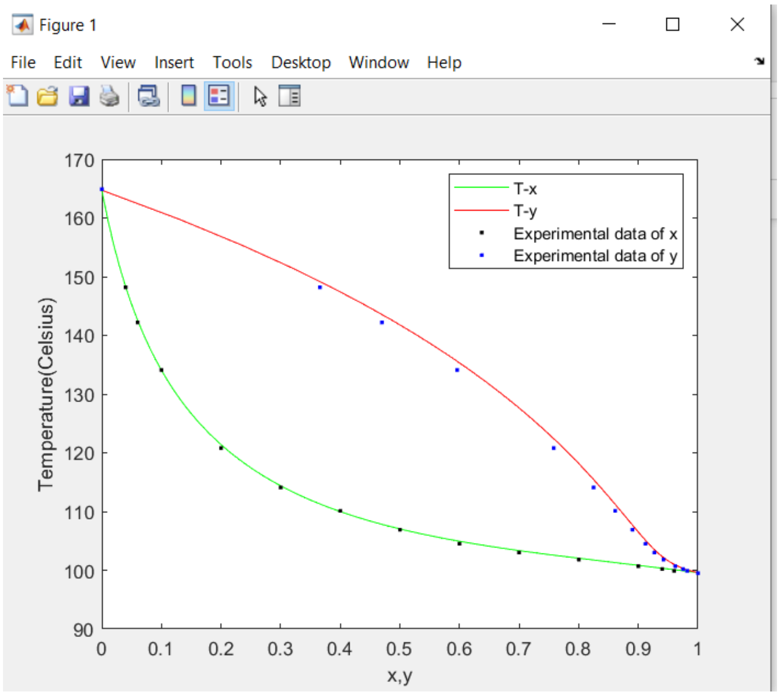
  We use fixed point iteration method to find the Equilibrium Temperature, starting with initial $T_o=T'$.

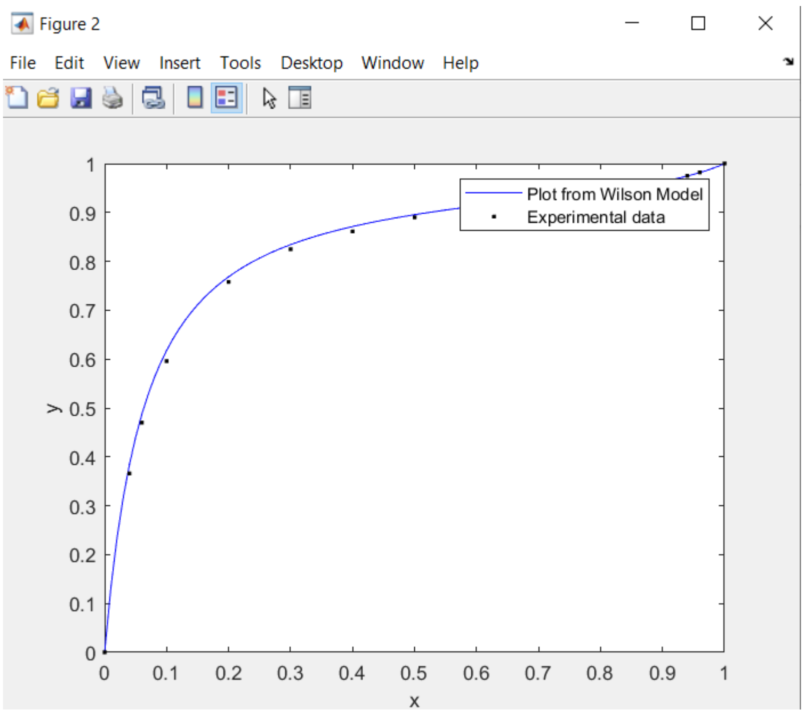
  $P_2^{sat}(T_n)=P/((1-x)*gamma2(x,T_{n-1})+(P_1^{sat}(T_{n-1})/P_2^{sat}(T_{n-1}))*x*gamma1(x,T_{n-1}))$

  Get T_1 from $P_2^{sat}(T_1)$ using Antoinne's equation.
  Iterate till you get a Temperature such that there is negligible difference in value for the next iteration.
- Calculate y from equation:

  $P(1-y)=(1-x)*gamma2*P_2^{sat}(T);$
- Loop ends
- Output the plots,

PLOTS





Output

- T_2^{sat} =164.7161° Celsius at P=760mm, Pure 1,3,5-TrimethylBenzene
- T_1^{sat} = 99.5955° Celsius at P=760mm, Pure 2-Butanol

```
At P=760mm Hg, Pure component T2sat= 164.716100 Celsius ,
T1sat= 99.595500 Celsius
The relative error(in %) from experimental data for y
 NaN
 4.877647
 3.584777
 3.631280
 1.373884
 1.123431
 1.191737
 0.616620
 0.156843
 0.169359
 0.185455
 0.145834
 0.037839
 0.039290
 0.000000
The relative error(in %) from experimental data for
Equilibrium Temperature
0.111535
0.035574
0.261024
0.035132
0.484000
0.242874
0.103589
0.122054
0.410634
0.331683
0.239394
0.126077
0.136006
0.188989
0.095946
```