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SYSTEM – Methanol - Water

Activity Coefficient Model – VAN LAAR

In this assignment, we will use modified Raoult's law with activity coefficients given by van laar equation using Matlab . We will use Antoine's equation to compute saturated pressure.

AIM- To compute -(a) isobaric T vs x, y diagram , (b) y vs x diagram (c) Comparison with the experimental results provided.

Given:-

```
P=760 mm hg;
A1=8.08097
A2=8.07131
B1=1582.271
B2=1730.630
C1=239.726
C2=233.426
A12=0.7715
A21=0.5775
T (in degree celcius)
P1sat, P2sat (vapour pressure of pure components 1 and 2 in mm
Hg)
```

$\ln\gamma_1$=(A12)*((A21*x2)/(A12*x1+A21*x2))*((A21*x2)/(A12*x1+A21*x2))

$\ln\gamma_2$=(A21)*((A12*x1)/(A12*x1+A21*x2))*((A12*x1)/(A12*x1+A21*x2))

Antoine's equation:-

```
log P1sat= A1-(B1/(T+C1))

log P2sat= A2-(B2/(T+C2))

 x2=1-x1

 y2=1-y1
```

$P = P1sat*x1*\gamma_1 + P2sat*(1-x1)*\gamma_2$ ……(1)

Modified Raoults Law:-

$y1=P1sat*x1*\gamma 1\ /P$ …… (2)

$y2=P2sat*x2*\gamma 2\ /P$

DEGREE OF FREEEDOM ANALYSIS

We have two equations (i.e (1) and (2)) but 3 unknowns(T ,x1,y1) so we have to specify 2 variables , out of which one is given P=760 mm of Hg.

So we need to specify one more variable(T or x1 or y1) to solve the system of equations.

T-X-Y Data(Given)

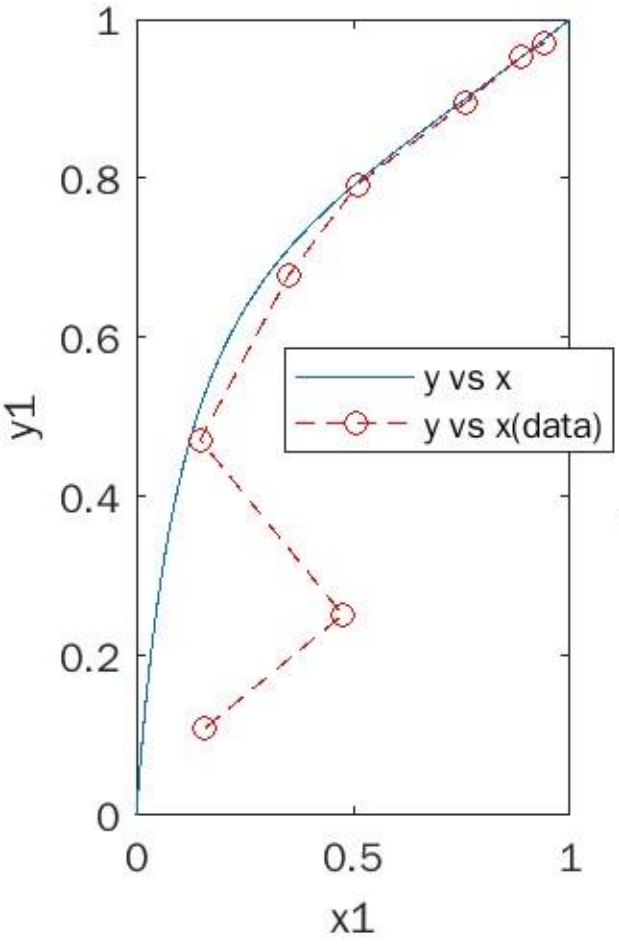
T	X1	Y1
96.70	0.0159	0.1100
92.70	0.0476	0.2521
84.60	0.1475	0.4716
77.10	0.3515	0.6786
73.20	0.5097	0.7923
68.60	0.7595	0.8953
66.70	0.8889	0.9536
66.30	0.9408	0.9702

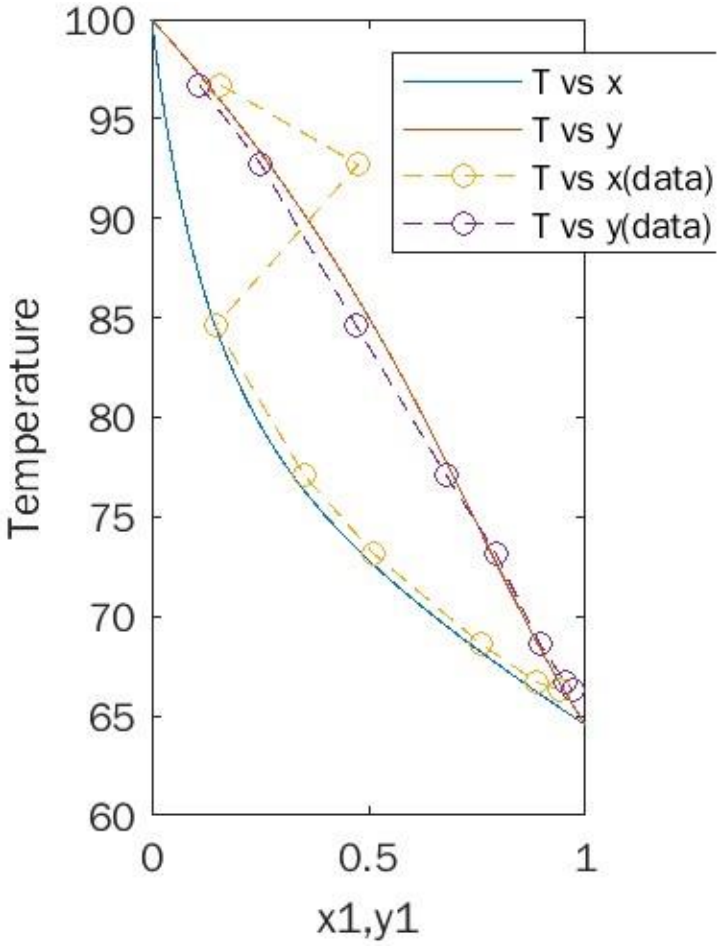
Matlab code

```
P=760;

A1=8.08097;A2=8.07131;

B1=1582.271;
B2=1730.630;
C1=239.726;
C2=233.426;
A12=0.7715;
A21=0.5775;
T=linspace(50,100,51);
x1=zeros(size(T)); %Mole fraction in liquid phase of methanol
x2=zeros(size(T)); %Mole fraction in liquid phase of water
y1=zeros(size(T)); %Mole fraction in vapour phase of methanol
y2=zeros(size(T)); %Mole fraction in vapour phase of water
G1=zeros(size(T)); %activity coefficient of methanol
G2=zeros(size(T)); %activity coefficient of water
```

```
P1sat=zeros(size(T));
P2sat=zeros(size(T));
for i=1:51
P1sat(i)=10^(A1-(B1/(T(i)+C1))); P2sat(i)=10^(A2-(B2/(T(i)+C2)));
eqn=@(x1) 760-P1sat(i)*x1*exp((A12)*((A21*(1-x1))/(A12*x1+A21*(1-
x1)))*((A21*(1x1))/(A12*x1+A21*(1-x1))))-P2sat(i)*(1-
x1)*exp((A21)*((A12*x1)/(A12*x1+A21*(1x1)))*((A12*x1)/(A12*x1+A21*(1-x1))));
x1(i)=fzero(eqn,0);
x2(i)=1-x1(i);

G1(i)=exp((A12)*((A21*x2(i))/(A12*x1(i)+A21*x2(i)))*((A21*x2(i))/(A12*x1(i)+A21*x2
(i))));
G2(i)=exp((A21)*((A12*x1(i))/(A12*x1(i)+A21*x2(i)))*((A12*x1(i))/(A12*x1(i)+A21*x2
(i))));
y1(i)=P1sat(i)*x1(i)*G1(i)/P;
y2(i)=P2sat(i)*x2(i)*G2(i)/P;
end

%% Graph plotting and  comparison from the given data
Tpoints=[96.70,92.70,84.60,77.10,73.20,68.60,66.70,66.30];
xpoints=[0.159,0.476,0.1475,0.3515,0.5097,0.7595,0.8889,0.9408];
ypoints=[0.1100,0.2521,0.4716,0.6786,0.7923,0.8953,0.9536,0.9702];
tiledlayout(1,2);
nexttile;
plot(x1,y1);
hold on
plot(xpoints,ypoints,'--or');
hold off
xlim([0,1])
ylim([0,1])
nexttile;
plot(x1,T);
hold on
plot(y1,T);
hold on
plot(xpoints,Tpoints,'--or')
hold on
plot(ypoints,Tpoints,'--or')
hold off
xlim([0,1])
```

Results-


y1
x1
y vs x
y vs x(data)
0
0.2
0.4
0.6
0.8
1
0
0.5
1


Temperature
x1,y1
T vs x
T vs y
T vs x(data)
T vs y(data)
60
65
70
75
80
85
90
95
100
0
0.5
1