Modified Raoult's Law for 2 Butanol and 1 butanol System

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Modified Raoult's law to properly evaluate the activity coefficient γi, and thus take into account liquid-phase deviations from ideal solution behavior, produces a much more reasonable and broadly applicable description of VLE behavior:

$$yiP = xi\ \gamma iPi\ sat\ (i = 1, 2, \ldots, N)$$

This equation provides for an entirely satisfactory representation of the VLE behavior of a great variety of systems at low to moderate pressures. Because ∑ yi = 1, maybe summed over all species to yield:

$$P = \sum xi\ \gamma iPi\ sat$$

An alternative may be solved for xi, in which case summing overall species yields:

$$P = 1 / \sum\ yi/\gamma i\ Pi\ sat$$

For calculating Activity Coefficient, Here I used **Margules**

ln $\gamma 1=[A_{12}+2(A_{21}-A_{12})x1]*(x2*x2)$

ln $\gamma 2=[A_{21}+2(A_{12}-A_{21})x2]*(x1*x2)$

For Calculating **Psat(saturation pressure) ,**Here I used **Antoine Equation**

Log_{10}(Psat)=A-(B/(T+C))

Psat --- Vapour pressure of pure component in mmHg

T ---- Temperature in (deg C)

Steps of the Algorithm:

1. I take a data (from provided data)of x1 and T store its value in an array.
2. I calculate γ1 and γ2 for every x1 corresponding Temperature.
3. I calculate Psat1 and Psat2 for these corresponding x1 and T
4. Then finally I calculate y1 and y2 and compare then y1 with experiment yexp (given)
5. Plot a graph between y1 and x1
6. Plot a graph between T and x1,y1

Matlab Code:

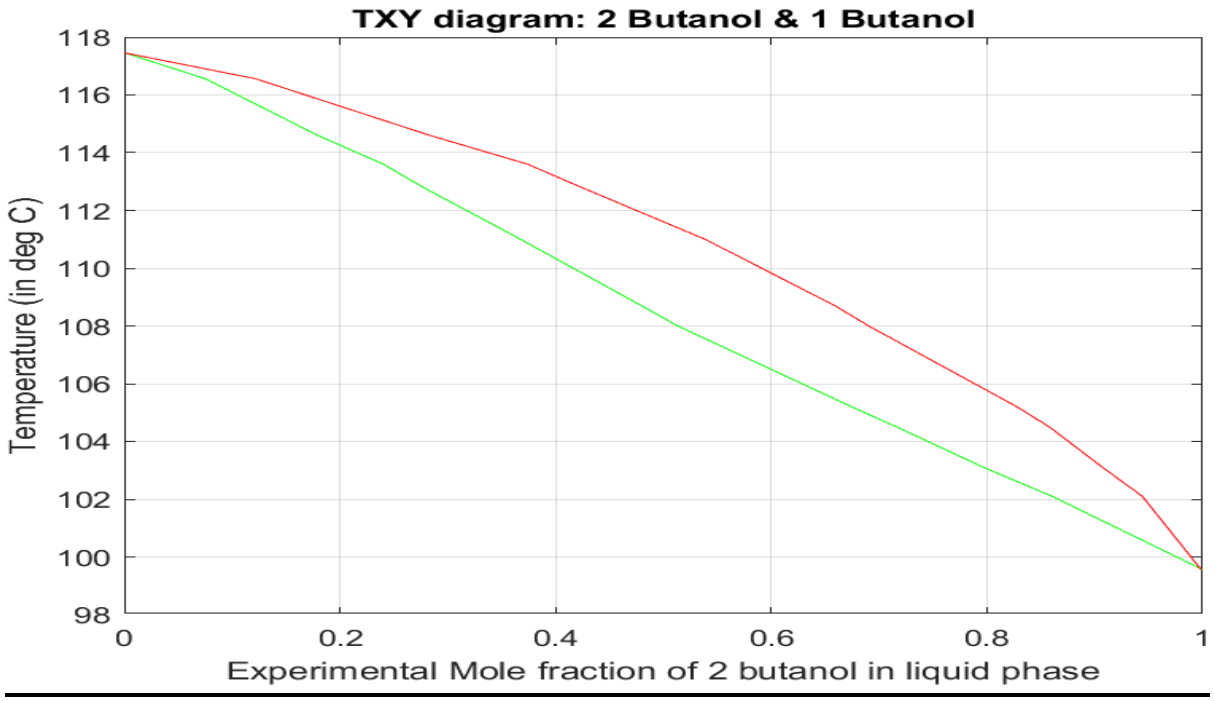
```
clc
clear
A12=-0.1464;
A21=-0.0259;
%Given experimental value T (deg C) & Mol fraction of 2 butanol
x1=[0.0000 0.0752 0.1793 0.2403 0.2771 0.3675 0.47960 0.5132 0.6744 0.7164 0.7962
0.8603 1.0000];
T=[117.46 116.56 114.60 113.60 112.80 111.00 108.70 108.00 105.20 104.50 103.11
102.10 99.56];
%Given constant
A=7.47429;
B=1314.188;
C=186.500;
A2=7.83800;
B2=1558.190;
C2=196.881;
Ptotal=760.00;
x2=1-x1;
%calculation of gamma1 and gamma2
for k=1:13
if x1(k)==0.0000
    l1(k)=0.86;
    l2(k)=exp((A21+2*(A12-A21)*x2(k))*(x1(k)^2));
elseif x1(k)==1.0000
     l1(k)=exp((A12+2*(A21-A12)*x1(k))*(x2(k)^2));
    l2(k)=0.97;

else
l1(k)=exp((A12+2*(A21-A12)*x1(k))*(x2(k)^2));
l2(k)=exp((A21+2*(A12-A21)*x2(k))*(x1(k)^2));
end

Psat1(k)=10^(A-(B/(T(k)+C)));
Psat2(k)=10^(A2-(B2/(T(k)+C2)));
y1(k)=(Psat1(k)*l1(k)*x1(k))/Ptotal;
y2(k)=(Psat2(k)*l2(k)*x2(k))/Ptotal;
end

yexp=[0.0000 0.1146 0.2770 0.3615 0.4077 0.5152 0.6270 0.6580 0.7900 0.8247 0.8780
0.9180 1.0000];

%percentage error calculation
```

```
for k=1:13
    err(k)=(abs(y1(k)-yexp(k))/y1(k))*100;
end
```

```
figure
plot(x1,y1,'b',x1,y1+y2,'r')  % red line in this graph show y1+y2 value that
should be equal to 1
hold on
grid on;
title('Y1X1 diagram: 2 Butanol & 1 Butanol');
xlabel('Experimental Mole fraction of 2 Butanol in liquid phase');
ylabel('Calculated Mole fraction of 2 Butanol in vapour phase');
```

```
figure
plot(x1,T,'g',y1,T,'r')
hold on
grid on;
title('TXY diagram: 2 Butanol & 1 Butanol');
xlabel('Experimental Mole fraction of 2 butanol in liquid phase');
ylabel('Temperature (in deg C)');
```

Txy Graph of 2Butanol and 1 Butanol system



X-Y graph (mole fraction of 2 Butanol in liquid and vapour phase respectively)