Lab Session 6

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AIM

The goal of the laboratory session is to understand vapor/liquid equilibrium, plot P-x-y for a binary mixture of CH_3OH and CO_2 with pressure on the y-axis and mole fraction of CH_3OH on the x-axis, plot T-x-y of this mixture, and determine the state of the binary mixture containing 40 mole% CH_3OH at 78 bar and 210 ^oC.

METHOD

Plotting P-x-y graph:

Approach 1: Using Antoine equation, P^{vap} of CH_3OH and CO_2 is calculated at a temperature of 483 K with values of coefficients already obtained from previous lab.

Approach 2: Calculation of P_{bubble} is done by using the below equation,

$$P_{bubble} = (P^{vap})_{CH3OH}*x_1 + (P^{vap})_{CO2}*(1-x_1)$$

Approach 3: Using P_{bubble}, we calculated mole fraction of CH_3OH in vapor phase using the below equation,

$$y1 = P^{vap} *x_1/ P_{bubble}$$

Approach 4: Now, using the values of x_1, y_1, and P_{bubble}, the plot of P-x-y is obtained as shown in results.

Plotting T-x-y graph:

Approach 1: First, we will calculate dew point temperature using below equation,

$$\frac{y1}{K1} + \frac{y2}{K2} = 1$$

Approach 2: K1 and K2 can be expressed as shown below,

$$K1 = \frac{P1vap}{P}$$

$$K2 = \frac{P2vap}{P}$$

Approach 3: Then using Raoult's law we can calculate mole fraction of CH_3OH in liquid phase.

Plotting contour illustrating R^3_{CH3OH}, R^3_{H2O}, R^2_{CO2} and R^2_{H2} as a function of temperature and pressure of stream 1a:

Approach 1: First, we iterate pressure from 1 bar to 78 bar, and then iterate temperature from 273K to 500K.

Approach 2: For every value of temperature, we calculate P^{vap} for CH_3OH, H_2O, CO_2, and H_2.

Approach 3: Using value of P^{vap}, we calculate bubble pressure P_b and dew pressure P_d.

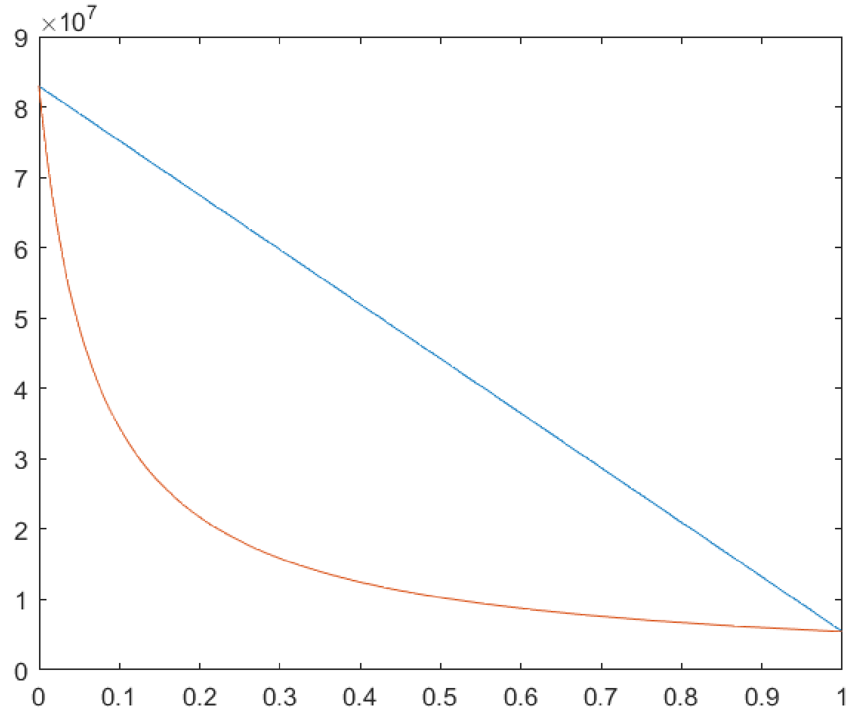
Approach 4: We then compare pressure value to decide whether only vapor phase is obtained or only liquid phase is obtained, or a mixture is obtained.

Approach 5: Then we calculate V, L and mole fraction in liquid phase as x and mole fraction in vapor phase as y.

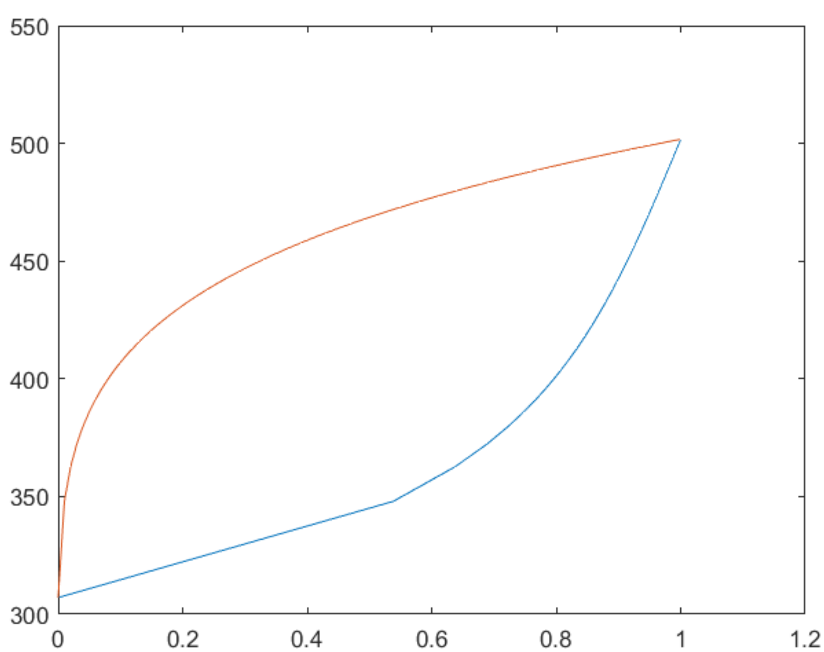
Approach 6: Using molar flow rates V, L and F and mole fraction x, y and z, recovery of each component is obtained.

RESULTS AND ANALYSIS

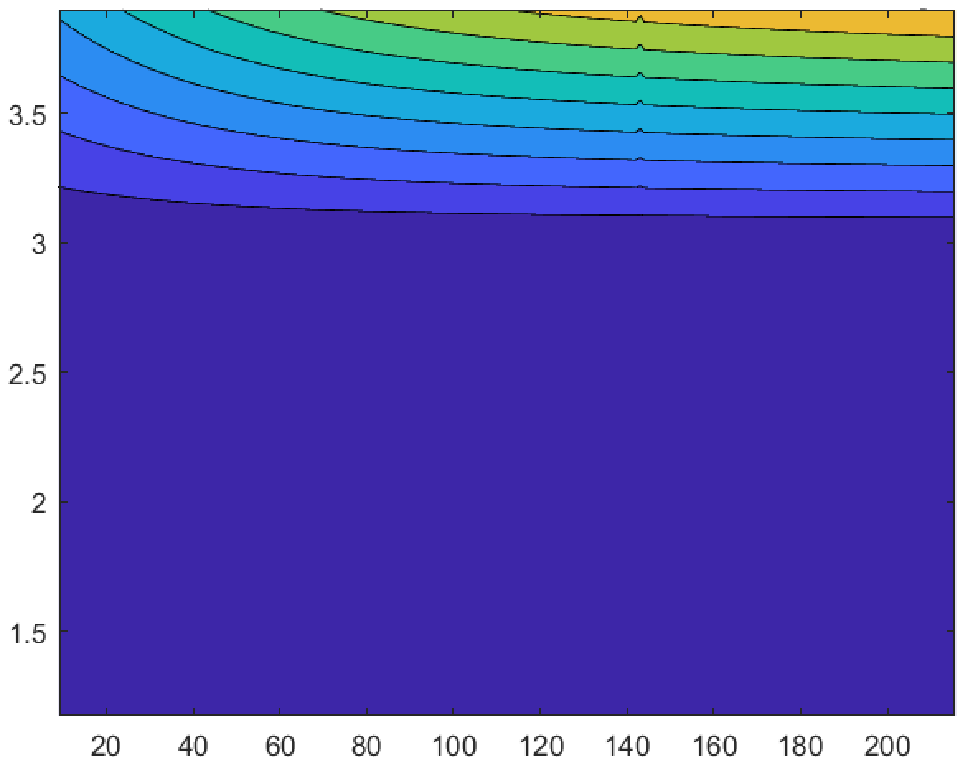
The following P-x-y graph is obtained,



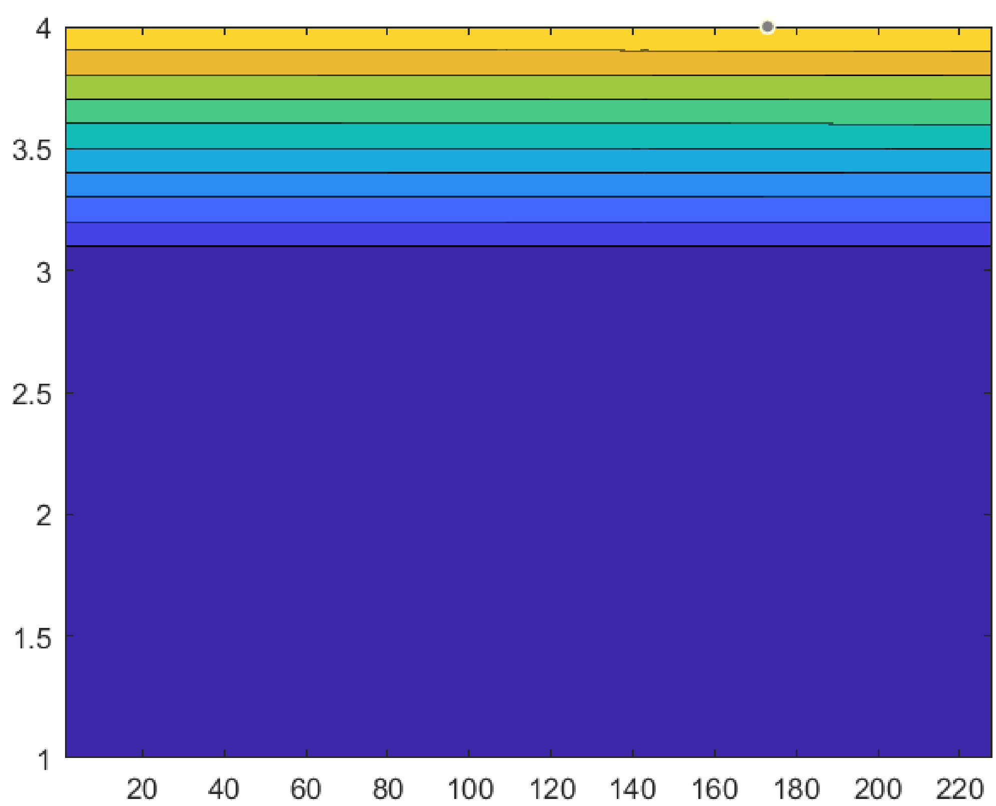
The following T-x-y graph is obtained,



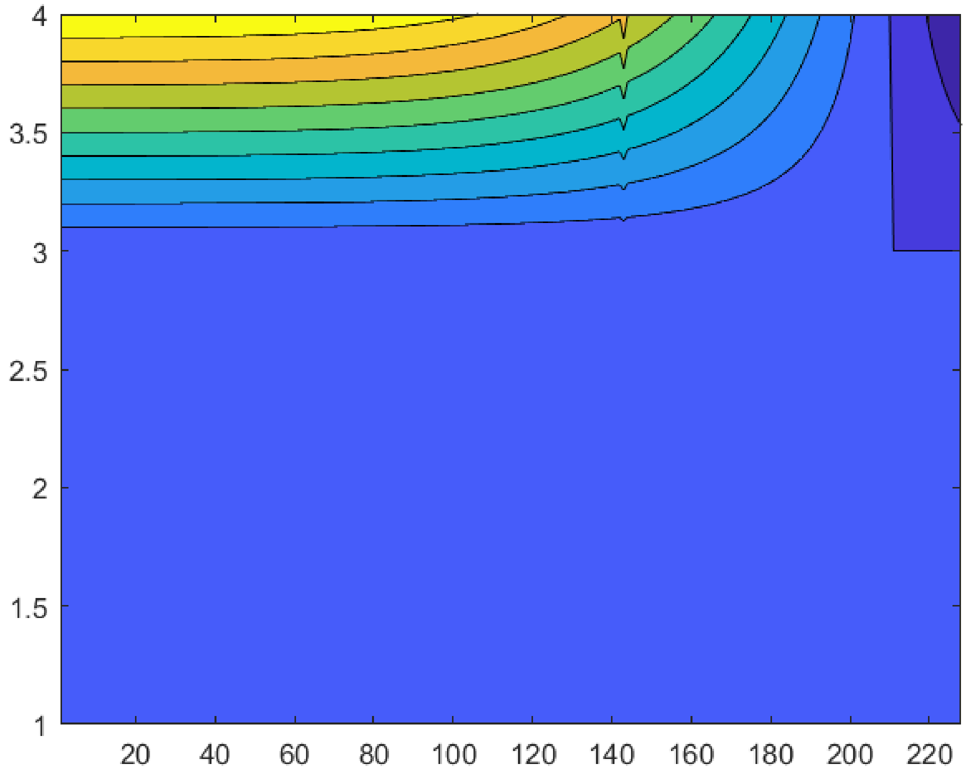
The following contour graph is obtained for CO_2,



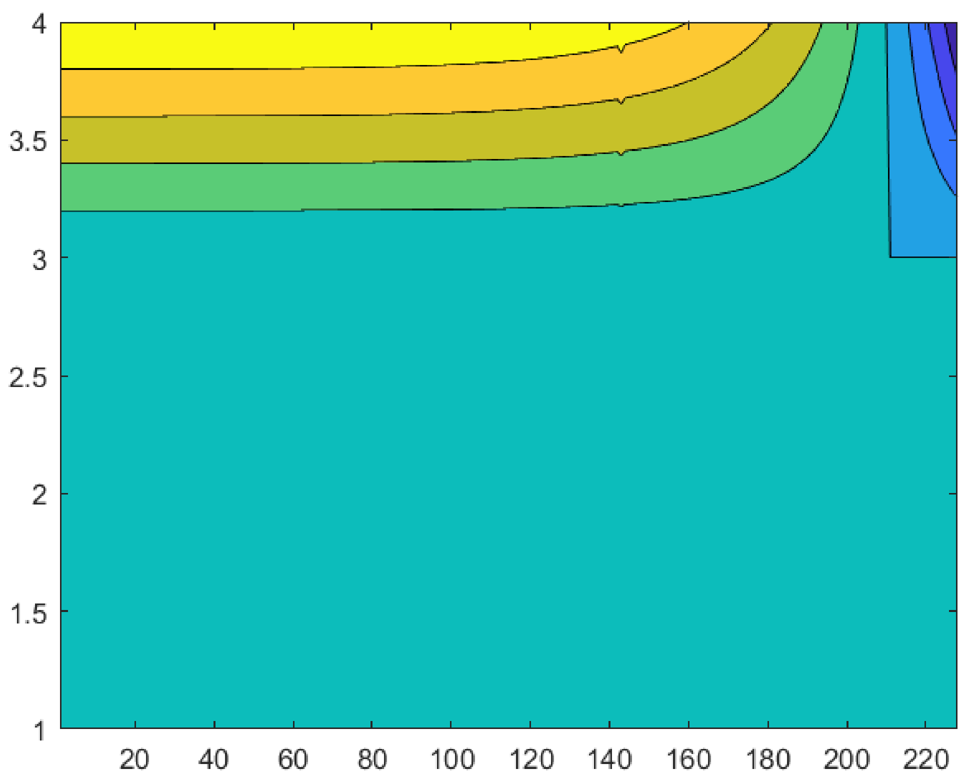
The following contour graph is obtained for H_2,



The following contour graph is obtained for CH_3OH,



The following contour graph is obtained for H_2O,



CONCLUSION

The P-x-y graph obtained is linear with mole fraction of CH_3OH in liquid phase while it has non-linear relation with mole fraction of vapor phase.

The enclosed area of T-x-y graph shows that CO_2 and CH_3OH are in mixture form.

APPENDIX

The MATLAB code to solve the problem is as follows:

```
A= [24.89 24.70 22.36];
B= [4525.8 4941.25 1992.9];
z = [0.12 0.12 0.25 0.51];
T=483;
P=78e5;

% P-x-y
p1 = exp(A(1)-(B(1)/T));
p2 = exp(A(3)-(B(3)/T));
x1=linspace(0,1,100);
P_total = (p1.*x1)+ p2.*(1-x1);
y1=(p1.*x1)./P_total;

% T-x-y
Temp=[];
count=0;
y2=[];
x2=[];
for i=0:0.01:1
    count=count+1;
    y2(count)=i;
    f = @(T1)[(i/(exp(A(1)-(B(1)/T1))/P))+((1-i)/(exp(A(3)-(B(3)/T1))/P))-1];
    Temp(count)=fsolve(f,483);
    p1_vap = exp(A_ch3oh-(B_ch3oh/Temp(count)));
    x2(count)= (y2(count)*P)/p1_vap;
end


F=100;
V=0;
L=0;
CO2_rec=[];
H2_rec=[];
CH3OH_rec=[];
H2O_rec=[];
p=[];
tt=[];
for i=1:78
    p(i)=i*10^5;
    pp=i*10^5;
    x=[];
    y=[];
    cnt=0;
    for t=273:500
        cnt=cnt+1;
        tt(cnt)=t;
        P_vap=[];
        P_b=0;
        P_d=0;
```

```
        for i=1:3
            P_vap(i)=exp(A(i)-(B(i)/t));
        end
        P_vap(4)=1.44e9;
        for i=1:4
            P_b=P_b+z(i)*P_vap(i);
        end
        for i=1:4
            P_d=P_d+z(i)/P_vap(i);
        end
        if pp>P_b
            x=z; y=0; V=0; L=F;
        elseif(pp<P_d)
            y=z; x=0; V=F; L=0;
        elseif(P_d<=pp && pp<=P_b)
            K= P_vap./pp;
            shi_func = @(s)[(z(1)*(1-K(1))/(1+s*(K(1)-1)))+ (z(2)*(1-K(2))/(1+s*(K(2)-1)))
+(z(3)*(1-K(3))/(1+s*(K(3)-1))) + (z(4)*(1-K(4))/(1+s*(K(4)-1)))];
            shi = fsolve(shi_func,0.8);
            V=F*shi;
            L=F-V;
            x=z./(1+shi.*(K-1));
            y=K.*x;
        end
        CO2_rec(i,cnt) = (y(3)*V)/(z(3)*F);
        H2_rec(i,cnt) = (y(4)*V)/(z(4)*F);
        CH3OH_rec(i,cnt) = (x(1)*L)/(z(1)*F);
        H2O_rec(i,cnt) = (x(2)*L)/(z(2)*F);
    end
end
% plotting graph
figure
plot(x2,Temp, y2,Temp);
figure
plot(x1,P_total,y1,P_total);
figure
contourf(CO2_rec);
figure
contourf(H2_rec);
figure
contourf(CH3OH_rec);
figure
contourf(H2O_rec);
```