Distillation Column Design

Assignment 1

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System: Ethanol and Water
Activity Coefficient Model: Van Laar

Question 1

For your selected binary system, assuming it is an ideal system (i.e. Raoult’s law is directly valid, and there is no deviation from ideal behavior), Plot the y v/s x (Vapour-Liquid equilibrium) curve in MATLAB.

We selected the mixture of ethanol and water as an azeotropic binary system. Ethanol forms a constant-boiling mixture, or azeotrope, with water that contains 95% ethanol and 5% water and that boils at 78.15°C.

Then we used Raoult’s law for vapor-liquid equilibrium(VLE).

Raoult’s Law

Raoult's law states that the vapor pressure of each component in a liquid solution equals its pure component vapor pressure at system temperature, multiplied by that component's mole fraction in the liquid phase.

$$y_1 P = x_1 P_1^{sat}(T)$$

$$y_2 P = x_2 P_2^{sat}(T)$$

Code for plotting y vs x in MATLAB.

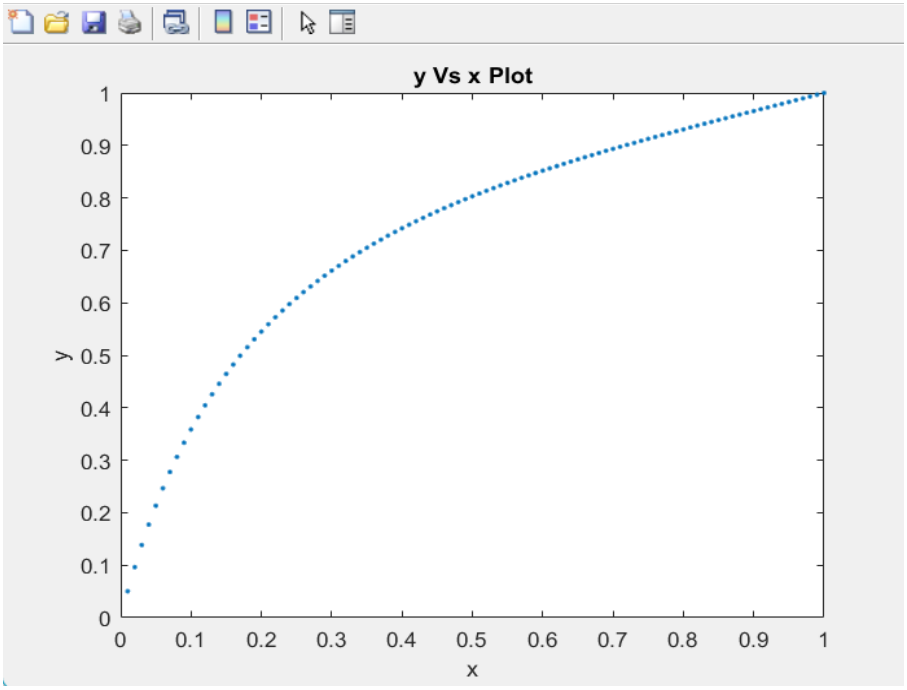
```
T = zeros(100,1);  % temperature
T1sat = Tsat(4.9231,1432.526,-61.819,760); %Calculating Saturated temperature using Antoine Equations
T2sat = Tsat(3.55959,643.748,-198.043,760);
for i = 1:100
    x1 = x(i);
    x2 = 1-x(i);
    T(i) = x(i)*T1sat + (x2)*T2sat;
    P1sat = Antoine(4.9231,1432.526,-61.819,T(i));
    P2sat = Antoine(3.55959,643.748,-198.043,T(i));
    P = x1*P1sat + x2*P2sat;  %Using Rault's Law yP=x*Psat

    y1 = (x1*P1sat)/P;  % Calculating mole fraction in Vapor Phase
    y(i) = y1;
end
```

```
%% Plotting y Vs x
figure
plot(x,y,'.');
xlim([0,1]);
xlabel('x');
ylabel('y');
title('y Vs x Plot');
```

```
%% function to calculate Psat using Antoine equation
function [psat] = Antoine(a,b,c,T)
    psat = 10.^((a-(b/(c+(T)))));
end
```

```
%% function to Calculate Tsat
function [T] = Tsat(a,b,c,p)
    T=(b/(a-log10(p)))-c;
end
```

Plot Of y VS x



Question 2

Plot y v/s x (vapor liquid equilibrium) curve in MATLAB for the same, taking into consideration the activity and fugacity coefficient in Raoult's Law (state all assumptions that you have taken).

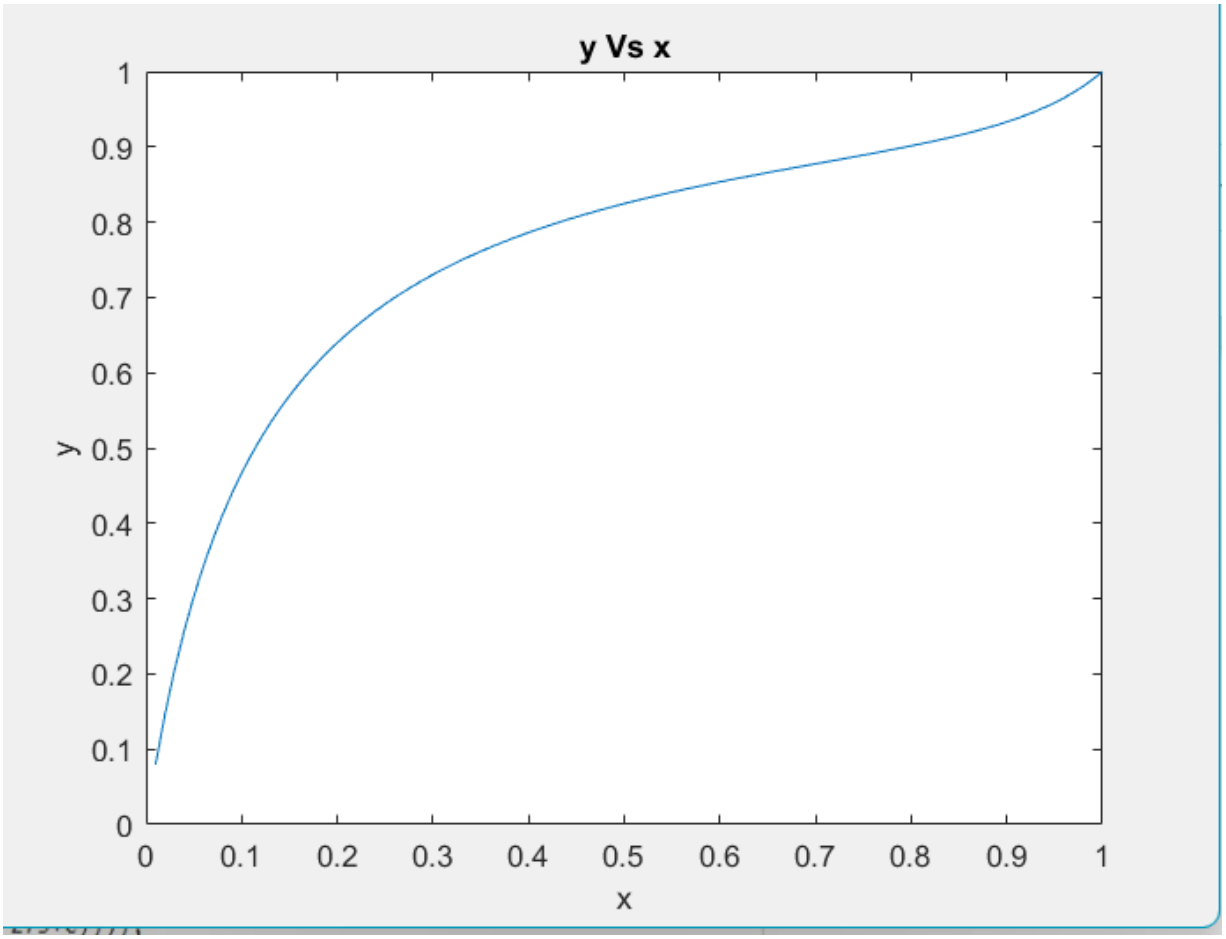
We have used Van Laar activity coefficient model for calculating $\boldsymbol{\gamma}$.

Van Laar Activity Coefficient Model

$$\begin{cases} \ln \gamma_1 = A_{12}\left(\dfrac{A_{21}X_2}{A_{12}X_1 + A_{21}X_2}\right)^2 \\ \ln \gamma_2 = A_{21}\left(\dfrac{A_{12}X_1}{A_{12}X_1 + A_{21}X_2}\right)^2 \end{cases}$$

```
y=zeros(100,1);                                 % mole fraction of ethanol in vapor phase
T=zeros(100,1);
x=zeros(100,1);                                 % mole fraction of ethanol in liquid phase
x(1)=0.01;
for i=2:100
    x(i)=x(i-1)+0.01;
end
t2=temp(3.55959,643.748,-198.043,760);          % saturation temperature for water
t1=temp(4.92531,1432.526,-61.819,760);          % saturation temperature for ethanol
for i=1:100
    g1=gamma1(x(i));
    g2=gamma2(x(i));
    T(i)=t1*x(i)+t2*(1-x(i));
    p2=pressure(3.55959,643.748,-198.043,T(i));   %saturation pressure for water at T(i)
    p1=pressure(4.92531,1432.526,-61.819,T(i));   %saturation pressure for ethanol at T(i)
    p=p1*g1*x(i)+p2*g2*(1-x(i));
    y(i)=p1*g1*x(i)/p;
end
% Plotting y vs x curve
figure
plot(x,y);
xlim([0,1]);
hold on;
xlabel('x');
ylabel('y');
hold off;

function [t]=temp(A,B,C,P)
    t=(B/(A-log10(P)))-C+273;
end
function [g1]=gamma1(x)
    g1=exp(0.4883*((1.1504*(1-x))/((0.4883*x)+1.1504*(1-x)))^(2));
end
function [g2]=gamma2(x)
    g2=exp(1.1504*((0.4883*x)/((0.4883*x)+1.1504*(1-x)))^(2));
end
function [p]=pressure(A,B,C,t)
    p=(10^(A-(B/(t-273+C))));
end
```

Plot of y Vs x


y Vs x
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
y
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x