THC & Water Solution

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Prompt

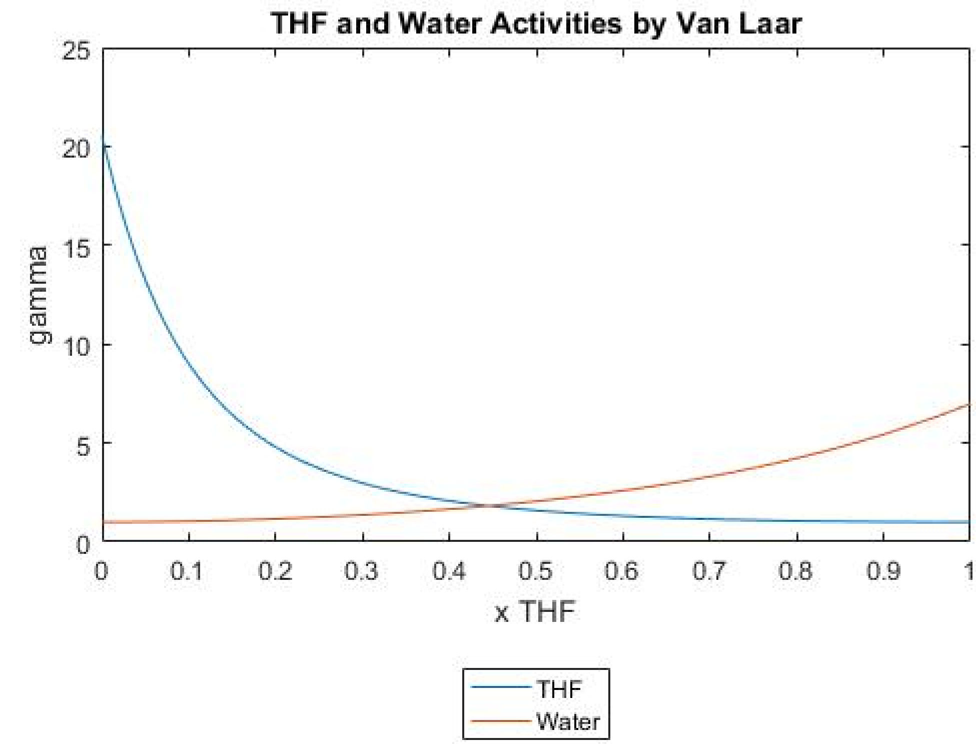
The past decade has witnessed significant research on clathrate hydrates. Clathrate hydrates have found applications in the storage and transportation of various gases, and can be also be used in CO2 sequestration. Tetrahydrofuran (THF) is a heterocyclic ether which is readily miscible with water, and stands out as a potential material for hydrate formation. To understand the conditions that lead to the formation of hydrates, it is imperative to investigate the thermodynamics of a THF-water mixture. Under the assumption that van Laar correlations apply to the non-ideality of a THF-water mixture, plot the (a) P vs x, y and (b) T vs x, y diagram at room temperature and pressure. Use the van Laar equation for activity coefficients.

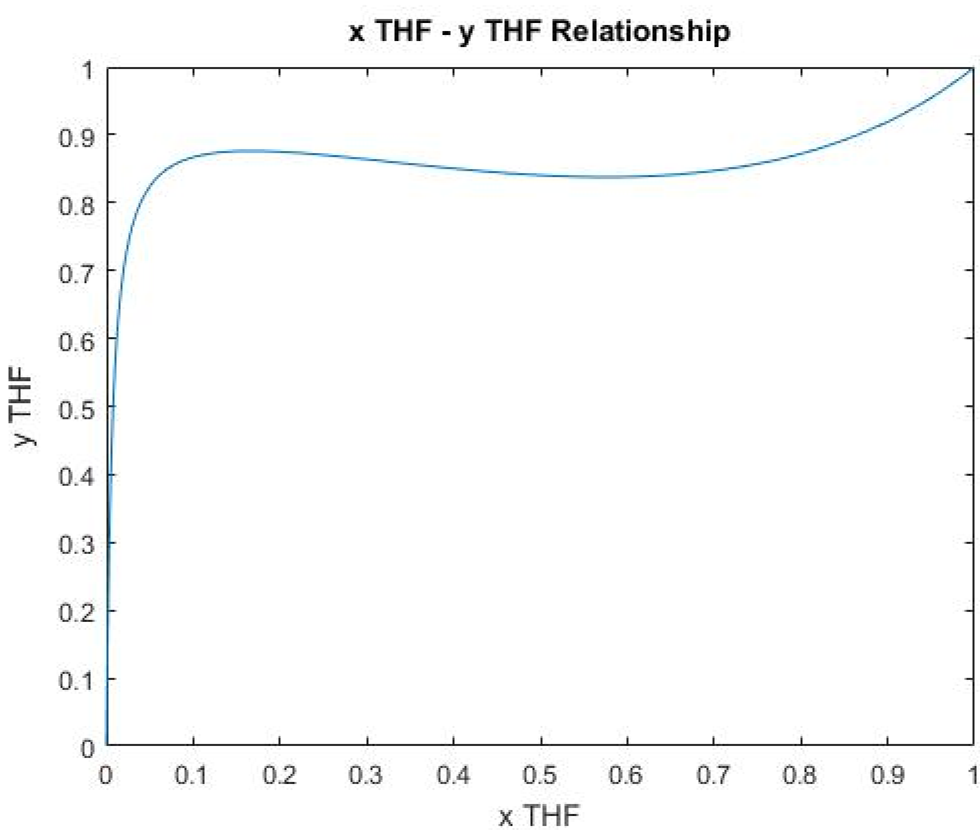
All of the plots will be at the end of the code for each section. Tables with all the values will be presented at the end of the last problem (end of the file).

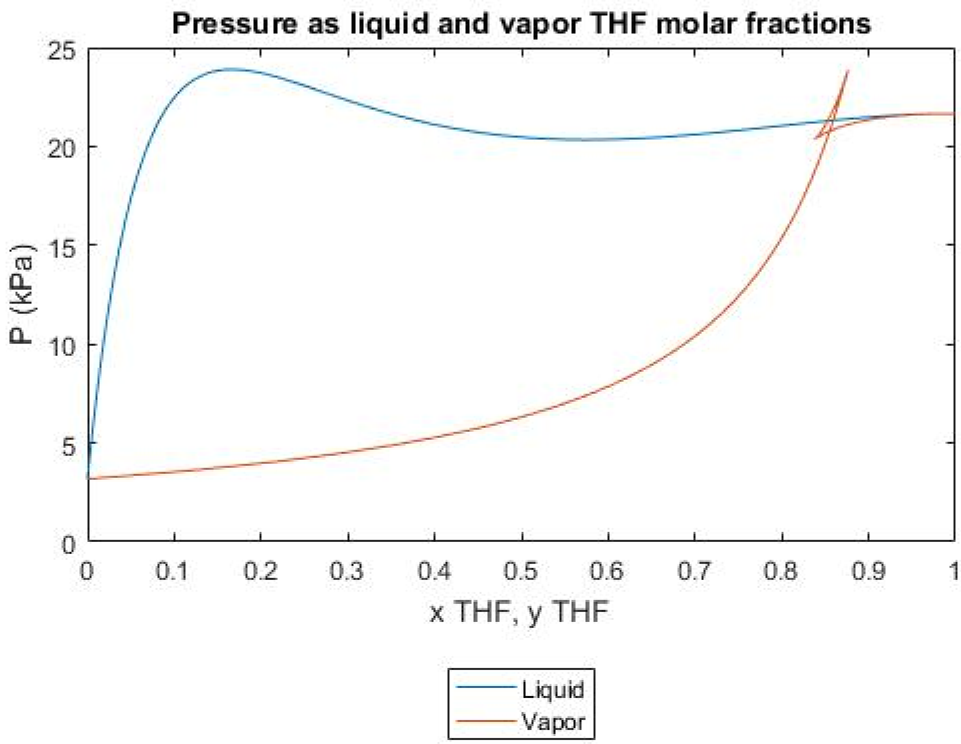
P-xy Diagram

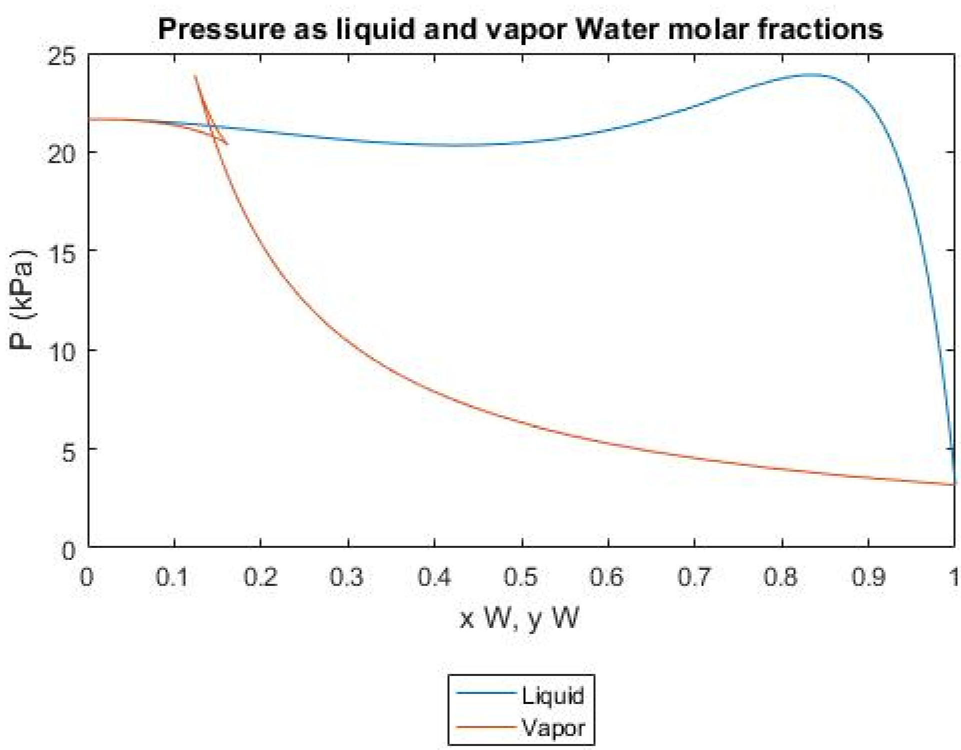
```
% First, we define the liquid molar fraction of THF and water as a
 linearly-spaced, 1000-element vector from 0 to 1.

    xTHF = linspace(0,1,1000);
    xW = 1 - xTHF;

% From Perry's Handbook, we find the Van Laar coeffiecients for a THF
 and water solution, and the vapor preassure for both components at
 room temperature.

% <https://accessengineeringlibrary.com/browse/perrys-chemical-
engineers-handbook-eighth-edition/p200139d899713_6001>

    alpha = 3.0216;
    beta = 1.9436;

    VpTHF = 21.65; % in kPA
    VpW = 3.18;

% With these values, we find the Van Laar activity coefficients for
 both components. The activity of THF and water is plotted against the
 liquid molar fraction of THF.

    gammaTHF = exp(alpha./(1+alpha.*xTHF./beta./xW).^2);
    gammaW = exp(beta./(1+beta.*xW./alpha./xTHF).^2);

    figure
    plot(xTHF,gammaTHF,xTHF,gammaW)
    title('THF and Water Activities by Van Laar')
    xlabel('x_ THF')
```

```
    ylabel('gamma')
    legend('THF','Water','Location', 'southoutside')

% We define the total pressure as the sum of partial pressures, as by
 Dalton's Law of Partial Pressures, and use Raoult's Law to express
 the partial pressures as the activity times the vapor pressure.

    P = VpTHF.*gammaTHF.*xTHF + VpW.*gammaW.*xW;

% We then define the vapor molar fraction of THF as the fraction
 of partial pressure of THF and the toal pressure. The relationship
 between the liquid and vapor molar fractions is plotted.

    yTHF = VpTHF.*gammaTHF.*xTHF./P;

    figure
    plot(xTHF,yTHF)
    title('x_ THF - y_ THF Relationship')
    xlabel('x_ THF')
    ylabel('y_ THF')

% In this section we will generate Pressure diagrams for both
 components.

    figure
    plot(xTHF, P, yTHF, P)
    title('Pressure as liquid and vapor THF molar fractions')
    xlabel('x_ THF, y_ THF')
    ylabel('P (kPa)')
    legend('Liquid','Vapor','Location', 'southoutside')
    figure
    plot(xW, P, 1-yTHF, P)
    title('Pressure as liquid and vapor Water molar fractions')
    xlabel('x_ W, y_ W')
    ylabel('P (kPa)')
    legend('Liquid','Vapor','Location', 'southoutside')
```


THF and Water Activities by Van Laar
gamma
x THF
0
5
10
15
20
25
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
THF
Water


x THF - y THF Relationship
y THF
x THF
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

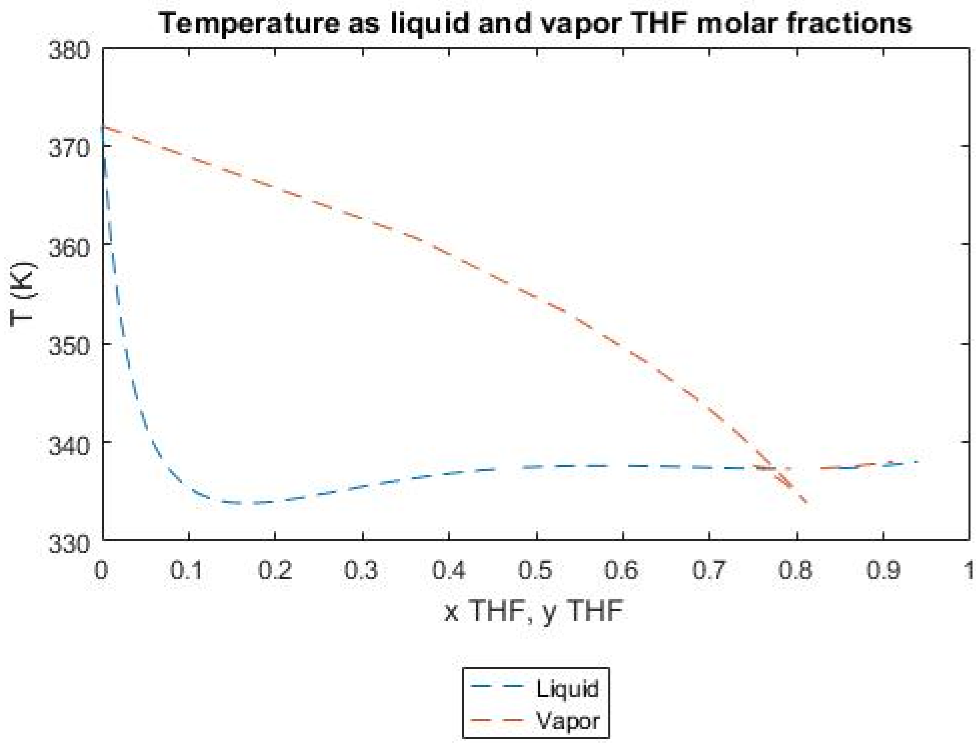

Pressure as liquid and vapor THF molar fractions
P (kPa)
x THF, y THF
Liquid
Vapor
0
5
10
15
20
25
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

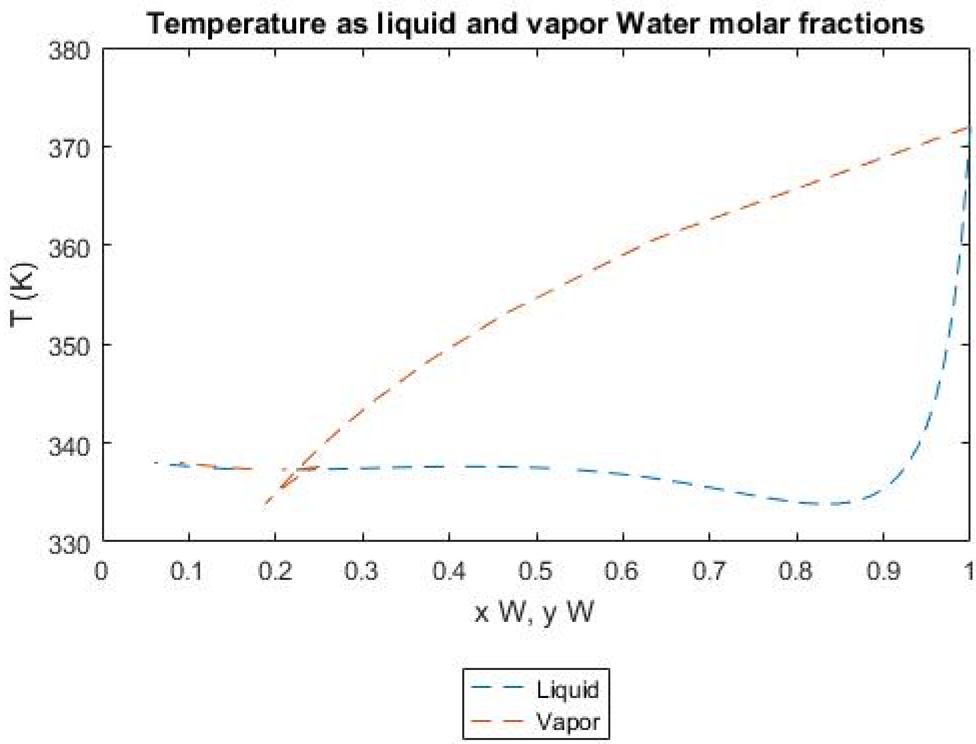

Pressure as liquid and vapor Water molar fractions
P (kPa)
x W, y W
Liquid
Vapor
0
5
10
15
20
25
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

T-xy Diagram

```
% From the NIST website, we find the Antoine's coeffiecients for both
 THF and water. We also set the total pressure to the room pressure,
 in bars.

% <http://webbook.nist.gov/cgi/cbook.cgi?
ID=C109999&Mask=4&Type=ANTOINE&Plot=on#ANTOINE>
% <http://webbook.nist.gov/cgi/cbook.cgi?
ID=C7732185&Mask=4&Type=ANTOINE&Plot=on>

    At = 4.12118;
    Bt = 1202.942;
    Ct = -46.818;
    Aw = 6.20963;
    Bw = 2354.731;
    Cw = 7.559;

    P2 = 1.01325; % bar

% We define a MATLAB system for T (we let T be a symbolic variable).
 We then use Antoine's equation to find the vapor pressures of THF and
 water.

    syms T
    Pt = 10.^(At-Bt./(T+Ct));
    Pw = 10.^(Aw-Bw./(T+Cw));

% We create two empty vectors to keep track of all of the temperatures
 and vapor molar fractions.

    allT = [];
    yTHF2 = [];

% In this section we solve for the temperature as a function of the
 liquid molar fraction of THF, and we find the vapor molar fraction of
 both components. We then plot all of the data.

% We create a loop that will iterate through the liquid molar fraction
 of THF, in 100 steps. For each molar fraction value, we find the
 corresponding activity (by Van Laars equation), and use the 'solve'
 function to find the temperature. We also calculate the corresponding
 vapor molar fraction at that temperature.

    warning('off','all') % to avoid 'solve' warning messages
    for xTHF2 = linspace(0,1,100)
    xW = 1 - xTHF2;
    gammaTHF = exp(alpha./(1+alpha.*xTHF2./beta./xW).^2);
    gammaW = exp(beta./(1+beta.*xW./alpha./xTHF2).^2);
    allT = [allT eval(solve(xTHF2 ==(-Pw.*gammaW+P2)./(Pt.*gammaTHF-
Pw.*gammaW),T))];
    yTHF2 = [yTHF2 (10.^(At-Bt./(allT(end)+Ct)).*gammaTHF.*xTHF2./
P2)];
```

```
    end
    warning('on','all')

    xTHF2 = linspace(0,1,100);
    xW2 = 1 - xTHF2;

    figure
    plot(xTHF2,allT,'--',yTHF2,allT,'--') % with '--' to hide plot
gaps
    title('Temperature as liquid and vapor THF molar fractions')
    xlim([0 1])
    xlabel('x_ THF, y_ THF')
    ylabel('T (K)')
    legend('Liquid','Vapor','Location', 'southoutside')
    figure
    plot(xW2, allT,'--', 1-yTHF2, allT,'--')
    title('Temperature as liquid and vapor Water molar fractions')
    xlim([0 1])
    xlabel('x_ W, y_ W')
    ylabel('T (K)')
    legend('Liquid','Vapor','Location', 'southoutside')
```





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