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Project: Vapor-Liquid Equilibrium

1. Degrees of Freedom

$df = 2 - \# \text{ phases} + \# \text{ species} - \text{reactions} - \text{special}$

Phases: Gas & Liquid

Species: Water, ethanol, acetone, acetic acid

$df = 2 - 2 + 4 - 0 - 0$

$df = 4$

2. Ideal Gas and Liquid System

Given: liquid composition = 40% water, 24% ethanol, 13% acetone, and 23% acetic acid

pressure = 1 atm

Find: bubblepoint temperature, first bubble composition

MATLAB command window:

```
ITERATION 6268
Bubble Point Calculation Ideal
T(K) = 359.950
y(water) = 0.246
y(ethanol) = 0.337
y(acetone) = 0.335
y(acetic acid) = 0.081
error = -5.964e-04
P(atm) = 1.000
```

Given: gas composition = 40% water, 24% ethanol, 13% acetone, and 23% acetic acid

pressure = 1 atm

Find: dewpoint temperature, first liquid droplet composition

MATLAB command window:

```
ITERATION 6614
Dew Point Calculation Ideal
T(K) = 371.550
x(water) = 0.421
x(ethanol) = 0.112
x(acetone) = 0.037
x(acetic acid) = 0.430
error = -7.336e-04
P(atm) = 1.000
```

3. Real Gas and Liquid System

Given: liquid composition = 40% water, 24% ethanol, 13% acetone, and 23% acetic acid

pressure = 1 atm

Find: bubblepoint temperature, first bubble composition

MATLAB command window:

```
ITERATION 998
Bubble Point Calculation Real
T(K) = 350.850
y(water) = 0.275
y(ethanol) = 0.287
y(acetone) = 0.384
y(acetic acid) = 0.055
error = 4.690e-04
P(atm) = 1.000
```

Given: gas composition = 40% water, 24% ethanol, 13% acetone, and 23% acetic acid

pressure = 1 atm

Find: dewpoint temperature, first liquid droplet composition

MATLAB command window:

```
ITERATION 1096
Dew Point Calculation Real
T(K) = 365.750
x(water) = 0.336
x(ethanol) = 0.121
x(acetone) = 0.034
x(acetic acid) = 0.509
error = 2.572e-04
P(atm) = 1.000
```

Ideal/Real Analysis

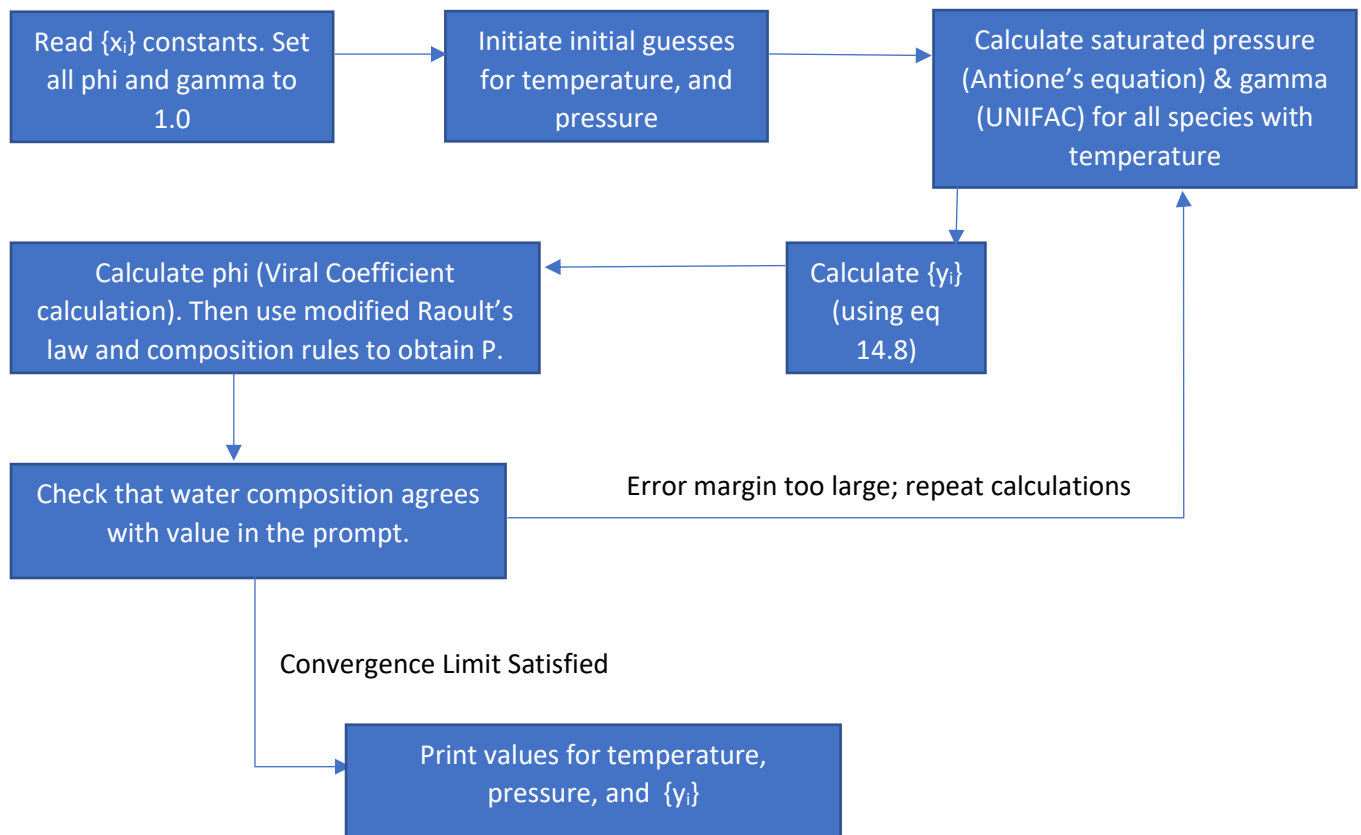
The ideal assumption of ideal gas was good for part 2. The ϕ values for the real dew and bubble point calculations were [0.9973, 1.0170, 1.0493, 0.9803] and [0.9912, 0.9993, 1.0276, 0.9692] respectively with water, ethanol, acetone, and acetic acid as the order of species. Since the ϕ values were close to 1, the gas compositions behaved close to ideal conditions. This physical phenomenon is reasonable since real gas behave closely to ideal behavior at low pressures which than minimizes interparticle interactions – a force assumed to be zero in the ideal conditions.

On the other hand, the ideal liquid solution assumption was not as robust. The γ values for the real dew and bubble point calculations were [1.5470, 1.1630, 1.3208, 1.0144] and [1.5860, 1.2096, 1.5293, 0.9254]. Since the values significantly deviate from 1, the ideal liquid solution assumption is not accurate and is the largest contributor to the discrepancy of the calculated temperatures and

composition between the ideal and real conditions. The mixture composition may be nonideal because the chemical species involved are of different chemical subgroups.

The ideal gas assumption would definitely not apply for high pressures and low temperature conditions. At high pressures, the proximity of molecules increases molecule interaction energy. Meanwhile low temperature means that a significant contributor to the overall energy in the system is the molecule interaction energy. The ideal liquid solution assumption would definitely not be valid for chemical species of drastically varying chemistry like ethanol and cyclohexane or acetone and benzene. Those molecule interactions would show positive deviations from Raoult's law. A mixture of similar weight saturated hydrocarbons would exhibit ideal liquid behavior since the molecules would be of similar chemistry.

4. Real Gas and Liquid System – Find Pressure, Temperature & Vapor Phase Composition



Given: liquid composition = 40% water, 24% ethanol, 13% acetone, and 23% acetic acid

gas composition = 20% water

MATLAB command window:

```
ITERATION 1007  
Composition of Vapor Phase, Temperature, and Pressure Calculation Real  
T(K) = 301.300  
y(water) = 0.200  
y(ethanol) = 0.224  
y(acetone) = 0.537  
y(acetic acid) = 0.042  
error = 8.243e-06  
P(atm) = 0.122
```