CHE221: Computational Assignment

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Introduction

To analyze our system, we apply Gibbs' Phase rule, given as

$$F = C - \pi + 2$$

The number of components as well as the number of phases are given to be 2, so We see that the degree of freedom is 2, meaning we need to specify two variables to get all the information required for the system. Given that we are working with an isobaric system, P is specified. We can assume x and solve further.

Procedure/Algorithm

1. First, we use the temperature explicit form of Antoine's equation to get initial values for T_i^{sat}, i = 1,2. Put P as P_{sat}. P = 101.325 kPa (Given).

$$T_i^{sat} = \frac{B_i}{A_i - lnP} - C_i$$

   $A_1 = 8.11220, B_1 = 1592.864, C_1 = 226.184 A_2 = 8.07131, B_2 = 1730.630, C_2 = 233.426$

2. As an initial guess value, we take T to be equal to the weighted mean of T_1^{sat} and T_2^{sat}, with the weights being equal to the molar fractions of the two components, i.e. x_1 and x_2.

3. Once we have this value of temperature, we can calculate the activity coefficients γ_1 and γ_2 using the Wilson model, as well as the saturation pressures P_1^{sat} and P_2^{sat}. Now, we can get an estimate of P_1^{sat}, by using the values of γ_1 and γ_2.

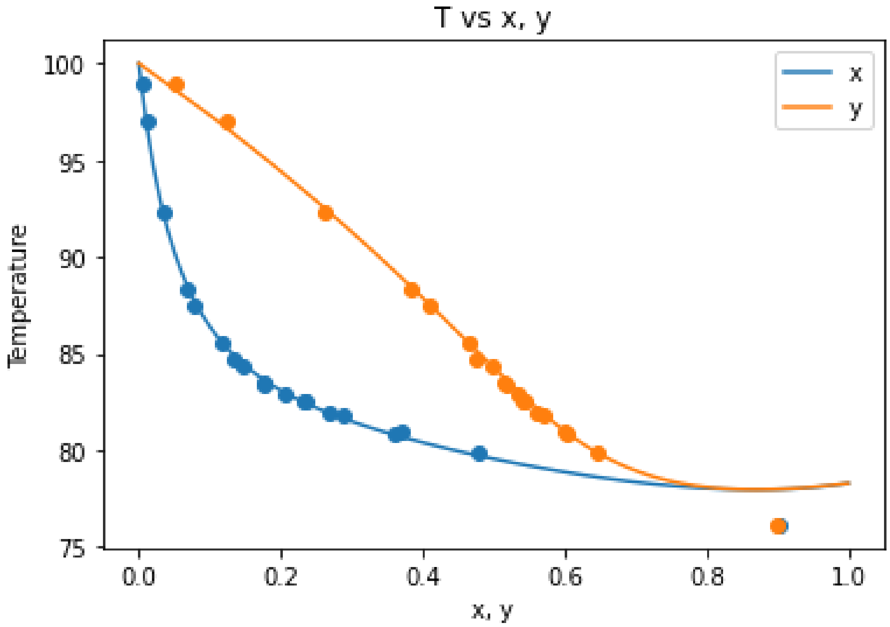
4. Using this value of P_1^{sat}, temperature can be calculated using the the Antoine's equation. We have to iterate and repeat Step 3 till T converges. What we have employed here is the Fixed Point Iteration Method.

5. Once we have found the value of Temperature, and consequently P_1^{sat}, we can calculate the value of y given by the following relation.

$$y_1 = \frac{x_1 * \gamma_1 * P_1^{sat}}{P}$$

Plotting the Graph

Since we have to find the temperature for a range of x_1s, 100 equally spaced values of x_1 are chosen. The corresponding values of T and y_1 are calculated using the algorithm described above. A graph is plotted with T on the y-axis and x and y on the x-axis. The experimental data (provided with the problem statement) is also plotted on the same graph as points. Since the points lie on the curve, this confirms that the model has been implemented correctly.



For the second part of the problem, a y vs x graph is plotted. Once again, the experimental data is plotted on the same graph as points and the points lying on the curve confirms the correctness of the model.