Strategy to solve story problems in homework and tests

The goal of this class is to introduce and develop computational skills, using ***Mathcad***, to solve Chemical Engineering problems. Therefore, the assessment puts emphasis on how you use ***Mathcad*** to solve the *mathematical* parts of the problems more than how you understand the chemical-engineering settings in the story that may eventually come to you later in the future.

The settings presented in the problems are definitely essential to provide you useful general ideas of how ***Mathcad*** can be applied in Chemical Engineering. However, they must not hinder you from using ***Mathcad*** in solving the problem because all variables and equations needed are explicitly given in the problem statement.

In this short note, a strategy comprising of a few steps can be very useful in avoiding confusion between mathematical issues to be solved and engineering stuff that flows as the background story. Remember, the former is particularly of our interest for success in this class.

Let us take problem 6 in chapter 2 as our example, but the strategy applies for any story problem throughout the textbook, and tests, of course.

Preparation: using scrap paper as needed

Step 1: Make a list of equations given in the problem. Determine their meaning without worrying about the theory or derivation that leads to them. Look also at the hierarchy of the equations because a higher-rank equation will need some information from lower one(s).

In problem 6: We have 3 equations with an order from higher to lower ranks.

$$\frac{P}{\rho RT} = 1 + B\rho \qquad (1)$$

$$B = b_0\lambda^3\left(1 - \frac{\lambda^3 - 1}{\lambda^3}\exp\frac{\varepsilon}{kT}\right) \qquad (2)$$

$$b_0 = \tfrac{2}{3}\pi N_A\sigma^3 \qquad (3)$$

Step 2: Make a list of variables (including those with constant values) involving in the equations. Determine also their meaning. The variables and their meaning are usually described in the text or even table-like enlisted.

In problem 6: The variables are enlisted in the problem statement: b_0, σ, ε, λ, k, N_A, and described in the text: P, T, ρ, R, B, along with their meaning.

Step 3: Understand the questions/tasks. Determine what variable is the unknown in each question/task (it is called the dependent variable). Make a list of the other variables (they are called independent variables), the values of which are available for solving the question/task.

In problem 6: (a) The unknown is B. The independent variables are T (200 K $\le T \le$ 1200 K), σ (= 3.917 Å), λ (= 1.83), ε/k (= 119.0 K). The task is to make a graph B vs. T.

(b) The same as (a), but with different values of independent variables: σ (= 3.40 Å), λ (= 1.85), ε/k (= 88.8 K)

(c) The unknown is ρ. The independent variables are T (= 680 K) and P (= 40 bar). The task is to calculate ρ in a unit of mol/cm^3.

(d) The unknown is ρ, and the independent variables are T (400 K $\le T \le$ 700 K) and P = 60 bar for the first plot, and P ($0 \le P \le$ 60 bar) and T = 400 K for the second plot. The task is to make plots of ρ vs. T and ρ vs. P. Along with those plots we are also to plot the ideal-gas density, which is given in the text as the ideal-gas equation: $P/\rho RT = 1$.

Writing program: on MathCad worksheet

Step 4: Write all known constant values on your worksheet. In ***Mathcad*** you need to write all these values before writing anything else because you will call them in any later parts of your program.

In problem 6: We have constant values of R, N_A, and the properties of CO_2 and CH_4 molecules (σ, ε/k, λ). Because we have two types of molecules you may want to write their properties as arrays, say, with index 1 for CO_2 and index 2 for CH_4. Values of R and N_A can be obtained from any reference books.

Step 5: Explicitly write the dependent variables as a functions of independent variables, starting from the lowest-rank equation. These functions are the equations you will use both for calculations and plotting graphs.

In problem 6: The lowest rank is Eq (3) where the dependent variable is b_0 and the independent variable is σ, therefore, the function we need to define is b_0 as a function of σ.

$$b_0(\sigma) := \tfrac{2}{3}\pi N_A \sigma^3 \qquad (4)$$

The next higher rank is Eq (2) where the dependent variable is B and the independent variables are the molecule properties (σ, ε/k, λ) and temperature T. Be sure to write b_0 on the right-hand side as $b_0(\sigma)$ as described above.

$$B(\sigma,\lambda,\frac{\varepsilon}{k},T) := b_0(\sigma)\lambda^3\left(1-\frac{\lambda^3-1}{\lambda^3}\exp\frac{\varepsilon/k}{T}\right) \qquad (5)$$

The highest rank is Eq (1) that is not written as an explicit equation of a dependent variable in terms of independent variables. Therefore, we delay this issue until we need Eq (1) to solve for ρ in tasks (c) and (d).

Note: If you use arrays to define the molecule properties, then you must also have arrays for both b_0 and B. To get the arrays, vectorize the right-hand side of the equations, though you don't need to for Eq (1) (why?).

Step 6: Pick the equations that are needed to solve the question/task in hand. Define also all the known independent variables that are not included as constant value in step 4.

In problem 6: (a) and (b) need Eq (2), and consequently Eq (3) in the background. The independent variable to be defined here is the temperature: 200 K $\le T \le$ 1200 K. Write the temperature range on the worksheet, and then make the plots of B vs. T.

(c) and (d) need Eq (1), and consequently Eq (2) and Eq (3) in the background. The dependent variable is ρ with independent variables T and P. To solve for ρ, we have options, for example whether we use the "solve" command or the "root" command. In both cases we must write ρ as a function of T and P, $\rho(T,P)$. In using these commands, Eq (1) needs to be rearranged as:

$$\frac{P}{\rho RT} - 1 - B\rho = 0 \qquad (6)$$

If using "solve" command:

$$\rho(P,T) := \frac{P}{\rho RT} - 1 - B(\sigma,\lambda,\frac{\varepsilon}{k},T)\rho \text{ solve}, \rho \rightarrow$$

This command will give you all possible solutions, including complex values if they exist. Therefore, $\rho\,(P,T)$ is an array here from which we need to pick the physical value (that has the physical meaning) as our solution. Use this physical solution in the plots you are asked to make in (d). Of course, you need to define the range of T or P before plotting.

If using "root" command, you need an initial-guess value for ρ. This is an important step, because guesses could give you wrong answer (***Mathcad*** converges to another unphysical solution) or even no answer (***Mathcad*** fails to converge). For this particular problem, as we deal with gases, the ideal-gas density will be good used as a guess. From the ideal-gas equation we can write:

$$\rho := \frac{P}{RT}$$

and then write:

$$\rho(P,T) := \text{root}\left(\frac{P}{\rho RT} - 1 - B(\sigma,\lambda,\frac{\varepsilon}{k},T)\rho, \rho\right)$$

Note: In this final step, you may use other options to solve this problem, such as "polyroots" command recalling that Eq (1) can be rearranged as a polynomial equation, or "Find" with "Given" block that is commonly used to solve simultaneous equations.