CE 329 Fall 2015

MATLAB Assignment 1

The purpose of this assignment is to ensure that you know how to solve a set of non-linear equations numerically using MATLAB. You are strongly encouraged to do this by modifying the template file SolvNonDif.m from AFCoKaRE. The equations you will solve are the same as those that need to be solved for regular homework Assignment 3. Since the purpose here is only to test your ability to ***solve*** the equations, not your ability to set them up, the equations are being provided to you.

Your code should define variables and assign values to them for the initial moles of CO (1), the initial moles of H_2O (3), the pressure (P = 1 atm), the equilibrium constant for the water-gas shift (K_1 = 69.5) and the equilibrium constant for methanol synthesis (K_3 = 0.0014).

Your code also should define a variable for the total initial moles and calculate a value for it.

Your code should then solve the following two equations for the values of ξ_1 and ξ_3:

$$K_1 = \frac{\left(\xi_1\right)\left(\xi_1 - 2\xi_3\right)}{\left(n^0_{CO} - \xi_1 - \xi_3\right)\left(n^0_{H_2O} - \xi_1\right)}$$

$$K_3 = \frac{\left(\xi_3\right)\left(n^0_{total} - 2\xi_3\right)^2}{\left(n^0_{CO} - \xi_1 - \xi_3\right)\left(\xi_1 - 2\xi_3\right)^2}\left(\frac{1\text{ atm}}{P}\right)^2$$

Finally your code should use those results to calculate and *report* the partial pressure of methanol and the percent conversion of CO using the following equations:

$$P_{CH_3OH,eq} = \frac{\left(\xi_3\right)P}{\left(n^0_{total} - 2\xi_3\right)}$$

$$f_{CO} = \frac{\xi_1 + \xi_3}{n^0_{CO}}\left(100\%\right)$$

You should submit a single MATLAB file with the filename being (your last name)_M1.m. To assign a grade, the TA will quickly examine your file and then execute it. To receive full credit, the last things it displays should be ***the correct values*** of the partial pressure of methanol and the fractional conversion. In other words, if your code does not run or it does not display the correct answer upon running, you will not receive full credit.

Warning: Non-linear equations can have more than one solution; your code must display results calculated using the solution that is physically meaningful, not any other solution to the equations above.