Homework Set 5 Solutions

<u>Due</u>: Thursday, September 29 (sections 001, 003, and 004)/Friday, September 30 (section 002)

This assignment is to be completed <u>individually</u>. The number in parentheses next to each problem shows how many points the problem is worth in the overall assignment. Please show all work and use correct significant figures to receive full credit. Be sure to follow the problem formatting instructions to avoid unnecessary deductions. If you use an equation-solving tool (calculator, APEx, Solver, MATLAB), write out the equation(s) and note the tool that you used; otherwise, show all hand calculations used to solve any equations.

1. (**20 pts**) At low to moderate pressures, the equilibrium state of the water–gas shift reaction $\mathrm{CO} + \mathrm{H_2O} \rightleftharpoons \mathrm{CO_2} + \mathrm{H_2}$ is approximately described by the relation

   $\frac{y_{CO_2} y_{H_2}}{y_{CO} y_{H_2O}} = K_e(T) = 0.0247\exp[4020 / T(\mathrm{K})]$ where T is the reactor temperature, K_e is the reaction equilibrium constant, and y_i is the mole fraction of species i in the reactor contents at equilibrium. The feed to a batch shift reactor contains 20.0 mole% CO, 10.0% CO2, 40.0% water, and the balance an inert gas. The reactor is maintained at T =1123K.

   (a) Assume a basis of 1 mol feed and draw and label a flowchart. Carry out a degree-of-freedom analysis of the reactor based on extents of reaction and use it to prove that you have enough information to calculate the composition of the reaction mixture at equilibrium. Do no calculations.

   (b) Calculate the total moles of gas in the reactor at equilibrium (if it takes you more than 5 seconds you're missing the point) and then the equilibrium mole fraction of hydrogen in the product. (*Suggestion:* Begin by writing expressions for the moles of each species in the product gas in terms of the extent of reaction, and then write expressions for the species mole fractions.)

   (c) Suppose a gas sample is drawn from the reactor and analyzed shortly after startup and the mole fraction of hydrogen is significantly different from the calculated value. Assuming that no calculation mistakes or measurement errors have been made, what is a likely explanation for the discrepancy between the calculated and measured hydrogen yields?

   (d) Write a spreadsheet to take as input the reactor temperature and the feed component mole fractions x_{CO} , x_{H2O}, and x_{CO2} (assume no hydrogen is fed) and to calculate the mole fraction y_{H2} in the product gas when equilibrium is reached. The spreadsheet column headings should be

   T x(CO) x(H2O) x(CO2) Ke … y(H2)

   Columns between Ke and y(H2) may contain intermediate quantities in the calculation of y_{H2}. First test your program for the conditions of Part (a) and verify that it is correct. Then try a variety of values of the input variables and draw conclusions about the conditions (reactor temperature and feed composition) that maximize the equilibrium yield of hydrogen.

   Please print and submit the Excel spreadsheet for part (d) of this problem with the homework set. <u>You will also need to submit the Excel file via Moodle.</u> Please name your file LastName_Section_HW 5.xlsx (e.g. Bullard_002_HW5.xlsx). *Review the syllabus instructions about academic integrity related to spreadsheets.*

2. (**20 pts**) Methanol is synthesized from carbon monoxide and hydrogen in a catalytic reactor. The fresh feed to the process contains 32.0 mole% CO, 64.0% H_2, and 4.0% N_2. This stream is mixed with a recycle stream in a ratio 5 mol recycle/1 mol fresh feed to produce the feed to the reactor, which contains 13.0 mole% N_2. A low single-pass conversion is attained in the reactor. The reactor effluent

goes to a condenser from which two streams emerge: a liquid product stream containing essentially all the methanol formed in the reactor, and a gas stream containing all the CO, H2, and N2 leaving the reactor. The gas stream is split into two fractions: one is removed from the process as a purge stream, and the other is the recycle stream that combines with the fresh feed to the reactor.

(a) Assume a methanol production rate of 100 kmol/h. Draw and fully label the flowsheet. Perform the DOF for the overall system and all subsystems to prove that there is **insufficient** information to solve for all unknowns.

(b) Briefly explain in your own words the reasons for including (i) the recycle stream and (ii) the purge stream in the process design.

3. (**10 pts**) Liquid methanol is fed to a space heater at a rate of 12.0 L/h and burned with excess air. The product gas is analyzed and the following dry-basis mole percentages are determined: CH_3OH = 0.45%, CO_2 = 9.03%, and CO = 1.81%.

    (a) Draw and label a flowchart and verify that the system has zero degrees of freedom.

    (b) Calculate the fractional conversion of methanol, the percentage excess air fed, and the mole fraction of water in the product gas.

    (c) Suppose the combustion products are released directly into a room. What potential problems do you see and what remedies can you suggest?

(**50 pts**) The remainder of the assignment (4 problems) will be completed online using WileyPLUS. *You do not have to turn in any paperwork with this portion of the assignment.* Use the link for your class on the Moodle site, and then you can access the Assignment within WileyPLUS. The due date for the WileyPLUS completion is the same as for the homework assignment – the beginning of your class period. Note that the WileyPLUS assignment cannot be submitted late.

Challenge Problem: FR&B 4.82