Homework Set 10

Due: Thursday, December 1 (sections 001, 003, and 004)/Friday, December 2 (section 002)

This assignment is to be completed in assigned homework groups. Be sure to include the group number as well as first and last names of all contributing group members in addition to the assignment number and instructor name on the submitted homework. The assignment must be in one person's handwriting. 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 in equation solving. All problems are from the end of the chapters in the 4th edition of the Felder, Rousseau, and Bullard (FR&B) text unless otherwise stated.

1. (**20 pts**) Synthetically produced ethanol is an important industrial commodity used for various purposes, including as a solvent (especially for substances intended for human contact or consumption); in coatings, inks, and personal care products; for sterilization; and as a fuel. Industrial ethanol is a petrochemical synthesized by the hydrolysis of ethylene:

$$C_2H_4(g) + H_2O\ (v) \rightleftharpoons C_2H_5OH\ (v)$$

Some of the product is converted to diethyl ether in the undesired side reaction:

$$2\ C_2H_5OH\ (v) \rightleftharpoons (C_2H_5)_2O\ (v) + H_2O\ (v)$$

The combined feed to the reactor contains 53.7 mole% C_2H_4, 36.7% H_2O, and the balance nitrogen, and enters the reactor at 310°C. The reactor operates isothermally at 310°C. An ethylene conversion of 5% is achieved, and the yield of ethanol (moles ethanol produced/moles ethylene consumed) is 0.900. *Hint*: treat the reactor as an open system.

Data for Diethyl Ether:

$$\Delta\hat{H}_f^o = -271.2 \text{ kJ/mol } \textit{for the liquid}$$
$$\Delta\hat{H}_v = 26.05 \text{ kJ/mol } (\textit{assume independent of } T)$$
$$C_p[\text{kJ/(mol}\cdot\text{C)}] = 0.08945 + 40.33\times10^{-5}T(^\circ\text{C}) - 2.244\times10^{-7}T^2$$

(a) Calculate the reactor heating or cooling requirement in kJ/mol feed.

(b) Why would the reactor be designed to yield such a low conversion of ethylene? What processing step (or steps) would probably follow the reactor in a commercial implementation of this process?

2. **(20 pts)** Lime (calcium oxide) is widely used in the production of cement, steel, medicines, insecticides, plant and animal food, soap, rubber, and many other familiar materials. It is usually produced by heating and decomposing limestone (CaCO3), a cheap and abundant mineral, in a *calcination* process:

$$CaCO_3\ (s) \xrightarrow{heat} CaO\ (s) + CO_2\ (g)$$

(a) Limestone at 25°C is fed to a continuous calcination reactor. The calcination is complete, and the products leave at 900°C. Taking 1 metric ton (1000 kg) of limestone as a basis and elemental species [Ca(s), C(s), O2(g)] at 25°C as references for enthalpy calculations, prepare and fill in an inlet–outlet enthalpy table and prove that the required heat transfer to the reactor is 2.7 x 10^6 kJ.

(b) In a common variation of this process, hot combustion gases containing oxygen and carbon monoxide (among other components) are fed into the calcination reactor along with the limestone. The carbon monoxide is oxidized in the reaction

$$CO\,(g) + 1/2\; O_2\,(g) \longrightarrow CO_2\,(g)$$

Suppose

- the combustion gas fed to a calcination reactor contains 75 mole% N_2, 2.0% O_2, 9.0% CO, and 14% CO_2;
- the gas enters the reactor at 900°C in a feed ratio of 20 kmol gas/kmol limestone;
- the calcination is complete;
- all of the oxygen in the gas feed is consumed in the CO oxidation reaction;
- the reactor effluents are at 900°C.

Again taking a basis of 1 metric ton of limestone calcined, prepare and fill in an inlet–outlet enthalpy table for this process [don't recalculate enthalpies already calculated in Part (a)] and calculate the required heat transfer to the reactor.

(c) You should have found that the heat that must be transferred to the reactor is significantly lower with the combustion gas in the feed than it is without the gas. By what percentage is the heat requirement reduced? Give two reasons for the reduction. State another benefit of feeding the combustion gas, besides the reduction of the heating requirement.

3. (20 pts) A gas mixture containing 85 mole% methane and the balance oxygen is to be charged into an Evacuated well-insulated 20-liter reaction vessel at 25°C and 200 kPa. An electrical coil in the reactor, which delivers heat at a rate of 100 watts, will be turned on for 85 seconds and then turned off. Formaldehyde will be produced in the reaction:

$$CH_4 + O_2 \longrightarrow HCHO + H_2O$$

The reaction products will be cooled and discharged from the reactor.

(a) Calculate the maximum pressure that the reactor is likely to have to withstand, assuming that there are no side reactions. If you were ordering the reactor, why would you specify an even greater pressure in your order? (Give several reasons.)

(b) Why would heat be added to the feed mixture rather than running the reactor adiabatically?

(c) Suppose the reaction is run as planned, the reaction products are analyzed chromatographically, and some CO2 is found. Where did it come from? If you had taken it into account, would your calculated pressure in Part (a) have been larger, smaller, or can't you tell without doing the detailed calculations?

4. **(20 pts)** Ammonia is oxidized in a well-insulated continuous reactor:

$$4NH_3\;(g) + 5O_2\,(g) \longrightarrow 4NO\;(g) + 6H_2O\;(v) \qquad \Delta H_r^o = -904.7\text{kJ}$$

The feed stream enters at 200°C and the products leave at temperature *T*out(°C). The inlet–outlet enthalpy table for the reactor appears as follows:

References: $NH_3(g)$, $O_2(g)$, $NO(g)$, $H_2O(v)$ at 25°C, 1 atm

Substance	$\dot{n}_{in}$ (mol/s)	$\hat{H}_{in}$ (kJ/mol)	$\dot{n}_{out}$ (mol/s)	$\hat{H}_{out}$ (kJ/mol)
$NH_3(g)$	4.00	$\hat{H}_1$	—	—
$O_2(g)$	6.00	$\hat{H}_2$	$\dot{n}_3$	$\hat{H}_3$
$NO(g)$	—	—	$\dot{n}_4$	$\hat{H}_4$
$H_2O(v)$	—	—	$\dot{n}_5$	$\hat{H}_5$

(a) Draw and label a process flowchart and calculate the molar amounts of the product stream components and the extent of reaction, ξ. Fill in the values of $\dot{n}_3$, $\dot{n}_4$, and $\dot{n}_5$ in the enthalpy table.

(b) The energy balance for this reactor reduces to $\Delta \hat{H} \approx 0$. Summarize the assumptions that must be made to obtain this result.

(c) Calculate the values of $\hat{H}_1$ and $\hat{H}_2$ and write expressions for $\hat{H}_3$, $\hat{H}_4$ and $\hat{H}_5$ in terms of the outlet temperature, T_{out}, and the heat capacity formulas in Table B.2. Then calculate T_{out} from the energy balance, using a spreadsheet. (See Example 9.5-3.)

(d) A design engineer obtained a preliminary estimate of the reactor outlet temperature using only the first terms of the heat capacity formulas in Table B.2. [For example, $\left(C_p\right)_{NH3} \approx 0.03515$ kJ/(mol·C)]. What value did she calculate? Taking the result of Part (c) to be correct, determine the percentage error in T_{out} that results from using the one-term heat capacity formulas.

(e) The preliminary estimate of Part (d) of T_{out} was mistakenly used as the basis of the design and construction of the reactor. Was this a potentially dangerous error from the standpoint of reactor safety or did it in fact lower the hazard potential? Explain.

(20 pts) The remainder of the assignment (4 problems) will be completed online using WileyPLUS. You can work with your team members to solve these problems, although note that each person may have unique values for some variables. **Each person should submit their own solutions through their own WileyPLUS link.** *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. (There are no Excel problems to be submitted in this assignment).

Challenge Problem: F&RB 9.70

Extra Credit: If you are not in a problem session that had extra credit opportunity through quizzes (i.e. Monday section), you may earn up to **10 points** of extra credit on your lowest HW grade by submitting a creative expression of your experience in CHE 205. This might include a poem, song, puzzle, craft, artwork—the sky's the limit! The only constraints are that your work must be original and your submission must be in good taste (something that could be shared with the rest of the class). You may work in groups if your idea requires multiple people to execute or is too big for one person to complete individually (but group projects will have a higher bar for assigning credit). Grading will be based on originality, effort expended, and quality of the final product. **The creative extra credit is due the last week of class (your instructor will tell you which day) and should be brought to class that day.** If you are in the T and W problem sessions and have already participated in the extra credit quizzes, we also **welcome** your creative contributions to be shared in class (even though you can't get extra, extra credit). The more participation we have, the more fun it is to celebrate crossing the finish line! (And food-related creative items are always appreciated!)