Memo 4: Multiple Reactions **Due Wednesday, 12 March 2008**

In this memo, you will modify your reactor models to include multiple reactions. In part 3 of memo 3 you were asked to present kinetics expressions you found in the literature for reaction networks that allow prediction of your primary product, as well as byproducts. You will use these kinetics in this memo. ***Recall that your selected model(s) must be approved for use by Dr. LaMarca.***[i] Based on your journal articles, you should try several of the reaction mechanisms. Then choose a reaction rate mechanism that you believe is appropriate for your reactor. Give a statement justifying why you believe your chosen mechanism is the best reaction mechanism for your reactor.

Remember to state all your assumptions for your design in the text describing your model. (Include target conversion of your feedstock, assumed T and pressure, reactor configuration – number of tubes and length and provide references for your choices).

This reactor does not have to be optimized and may be different from the final design submitted in your final report.

1. Present the calculations and results for the design of your reactor. Your POLYMATH model must include mole balances with **multiple reactions,** as well as a momentum balance using the Ergun equation, developed for Memo 3. Use catalyst particle size of 5 mm in diameter, unless you have a good reference for catalyst particle size in a fixed bed reactor. Assume an isothermal reactor.
   Hand in the following:
   a. Hand derivation of equations for your POLYMATH model.
   b. Plots of molar flows of each species as a function of catalyst weight.
   c. Reaction pathway diagram for your multiple reactions.
   d. Choose 3-5 reaction temperatures and compare reaction selectivity to your group's primary product (as well as valuable byproducts, if appropriate), for a constant feedstock conversion as a function of temperature. Discuss these results.
   e. References for all data.
   f. **Give hand calculations of each representative calculation**.

2. Present a preliminary design of your reactor based on the kinetics used in part 1 using Aspen Plus. Assume that you have an isothermal reactor with initial conditions and reactor configuration identical to that in part 1 above.
   Hand in the following:
   a. Your full Aspen Plus report file.
   b. Plots of molar flows of each species as a function of reactor length from your Aspen model.
   c. Sample calculations in which you compare your hand calculation of the reaction rate to the first volume step output by the Aspen program.
   d. References for all data (target conversion used, temperature, inlet T and P, approximate reactor volume etc.).
   e. Compare the results obtained from POLYMATH with those obtained from Aspen.

[i] From memo 3 instructions part 3: Present a preliminary evaluation of the reaction rates expressions that you have obtained from the literature for use in your reactor for **approval by Dr. LaMarca**. This will consist of hand calculations of the reaction rates at your reactors initial conditions. You must compare your hand calculations with results given in the paper. Your reaction rates should have the ability to predict byproducts of your reaction. These reaction rates must be obtained from a journal source and be appropriately referenced.