Memo 5: Energy Balances **Due Wednesday, 9 April 2008**

In this memo you will add the energy balance to your Polymath and Aspen models. Instead of assuming isothermal conditions in your reactor, you will now model the heat transfer in the multi-tubular reactor.

For exothermic reactions we typically configure the multi-tubular reactor with co-current cooling, offering the best conditions for reactor dynamic stability by maintaining a relatively constant driving force for heat transfer. For simplicity in this memo, however, we will assume a constant coolant temperature so that you won't need to consider the energy balance on the coolant. You will need to include the energy balance for the process fluid.

Monitoring the reactor 'hotspot' – the hottest axial temperature in the reactor – provides an indication of the viability of your reactor design from the perspective of reaction selectivity and reactor dynamic stability. While dynamic modeling of reactor behavior is outside the scope of this course, we can use a well-established steady-state measure as an indicator of reactor stability. One "rule-of-thumb" test for dynamic stability is to consider the reactor "gain". This metric asks the question – when you increase the reactor coolant temperature by 1ºC, how much does the hotspot temperature increase?

$$Gain = \frac{\Delta T_{HS}}{\Delta T_{coolant}}$$

For a cooled reactor, we generally want this quantity to be less than 2 to assure dynamic stability. (A similar measure is evaluated for an adiabatic reactor where we look at how the exit temperature varies with a variation in inlet temperature).

Polymath Model

1. Add the energy balance to your Polymath model developed in Memo 4. Equation 8-35 (in the 4th edition of Fogler) provides the energy balance on the process fluid for a tubular reactor in terms of (dT/dV) and molar flow rates. Derive the expression in terms of catalyst weight (dT/dW) using your catalyst bulk density, and ***include these calculations in your memo***. As a simplification for your Polymath model, you may wish to use component C_p values at your reactor feed temperature so that you can calculate these values *a priori* in a spreadsheet. You will also need to research a value for an overall heat transfer coefficient for a packed bed reactor, and select a coolant temperature. ***Be clear about what you are assuming and state your assumptions in your memo.***
    a. Examine your reactor temperature profiles and selectivity to your desired product as a function of gas inlet temperature and coolant temperature. Where is your hotspot? How can you moderate this hotspot temperature with process variables? ***Explore these ideas and submit your results with your model in this memo.***
    b. What is the "gain" for your selected reactor operating conditions? Do you expect your reactor to be stable dynamically, and if not, how can you modify your process conditions to specify a stable reactor?

c. How does isothermal operation compare with operating a real reactor with heat transfer?

Aspen Model

2. In your Aspen model, you will change the RPLUG reactor type to Reactor with constant coolant temperature. This option will require a value for an overall heat transfer coefficient (as in part 1 above) and a coolant temperature. To examine the temperature profiles and correctly identify the position of the hotspot, you will want to modify the number of intervals displayed in your reactor block results. To do so, select the Report item under your reactor block description and increase the number of intervals beyond the default value of 10.
    a. Where is the reactor hotspot and how can it be modified with process variables?
    b. How does the reactor performance – in terms of reaction selectivity – compare with the results in an isothermal reactor?
    c. What is your predicted "gain"? Do you expect your reactor to perform viably in operation, and if not, what can you do to find conditions where it can?
    d. How does the coolant temperature impact the results?

Special Note:

Some groups may still be working to successfully get good expressions for multiple reaction steps into their models. Please make this a priority. If we don't get the kinetics right, the rest is meaningless. Please ask for help if you need it.