Reactor Design Project - Memo 1
DUE: 30 January 2008

Memo 1: Background & Overall Mass and Energy Balances

The first memo is a written document that includes two sections. Section 1 should contain background information derived from literature about your feedstock (and competing feedstocks) and product as well as published kinetics parameters for the production of acrolein or maleic anhydride in a fixed bed reactor from your group's feedstock. This information will serve as a first draft for the introduction to your final report. Section 2 includes preliminary mass and energy balances for your reaction system. Detailed guidelines for each section follow.

1. Literature Search and Background

1.1. ***Process Background:*** This section will form the basis for the introduction of your final report. Initially, use the general references cited in the Reference List for this work (*e.g.,* Kirk-Othmer, etc.), as well as some information from at least one recent patent on your technology (http://www.uspto.gov; section on Current State of the Art). ***Please cite all references used***.

1.1.1. Include a description of the major uses of your feedstock and product, as well as competing feedstocks[1]. (Understanding the uses provides insight into market prices of both feedstock and product).

1.1.2. Investigate what major companies produce your product, quantity produced each year in the US and the world, and the market price of feedstock and product.

1.1.3. Review the processes and typical process conditions (inlet compositions, operating pressure, and temperature, and typical reactor conversions) for the manufacture of your product – particularly focussing on the process assigned to your group.

1.1.4. Comment on the most typical reactor types employed for this technology.

1.1.5. Give the typical product and byproduct distributions produced by the reactors for your technology.

1.1.6. Consider if a 'greener' route to your product is possible or practiced and discuss.

In later memos more information will be added to the introduction. Reference citations[2] must be contained in this introduction.

1.2. ***Reaction Kinetics:*** Conduct a Chemical Abstracts literature search[3] (SciFinder Scholar) for the kinetics of your reaction technology. Obtain at least ***three*** journal references for possible reaction kinetics for your reactor. (You may not have all these in hand by the due date of the first memo, but put them on request, if necessary, and ***include the citations*** in this memo submission). Your reaction rates should have the ability to predict byproducts of your reaction. You may obtain copies of these journal articles from the library, interlibrary loan or the EJournals from ScienceDirect (Elsevier) or the ACS journals. If you have trouble finding the articles of interest, contact Dr. LaMarca[4] for assistance.

2. Calculations

2.1. Begin by writing a ***balanced*** stoichiometric equation for your chemistry. Calculate an overall mass balance for your group's reactor technology (*i.e.,* Group 1 should use propylene as feedstock for 30K metric ton/yr production rate of acrolein). Base your **inlet composition** and **reaction conversion** on typical literature values determined above in section 1.1.3. **State these assumptions!** (Also, in converting your annual production rate to a reactor feedrate and production rate (in kg/s) you should account for scheduled shutdowns of at least 2 weeks / year).

2.2. Using the methodology for flow systems described in Fogler, Chapter 3, section 3.5, develop a ***general stoichiometric table*** for your reaction system. Give a sample calculation of this mass balance (handwritten).

2.3. Calculate the heat of reaction (ΔH_{rxn}^{298K}) to produce your product from all competing feedstocks and ***comment*** on the differences between feedstocks.

2.4. Calculate an overall energy balance using inlet and outlet enthalpies for a generic reactor assuming ***typical*** reaction conversions determined in section 1.1.3.

2.4.1. **First, calculate an overall isothermal energy balance and determine heat duty required to operate at a typical temperature (as determined in part 1.1.3)[5].**

---

[1] For the acrolein projects you should consider both propane and proplyene as feedstocks. For the maleic anhydride projects you should consider n-butane, n-butene and benzene as feedstocks.

[2] *The ACS Style Guide* provides a standard format for literature citations. While this book is available for purchase and several copies are available in the library, an Internet search reveals several University websites which provide essential information excerpted from this reference. One such reference is found at the University of Wisconsin Chemistry Library: http://chemistry.library.wisc.edu/instruction/acstyle.htm.

[3] A literature search is not a 'Google' search, however, 'Google Scholar' may provide some initial direction to your search.

[4] Daytime phone: (302) 774-2265, e-mail: Concetta.LaMarca@usa.dupont.com.

[5] For both energy balances refer to Felder & Rousseau, Chapter 9 - Balances on Reactive Systems, section 9.5.

2.4.2. **Second, calculate an overall adiabatic energy balance and determine the final temperature.** Use typical inlet temperatures given in either the Kirk-Othmer or McKetta references cited in the overview of the project. Perform calculations using physical property data obtained from either the DIPPR database or the NIST database (NIST WebBook http://webbook.nist.gov/), if possible. Remember to use heat capacities as a function of temperature. (Techniques for integrating these expressions are described in the course handout on "Help with Using DIPPR Properties". Give a sample calculation of heat capacities, enthalpies and the energy balance and show units in this calculation. Remember to cite references for your thermochemical property data.

2.5. UNITS: Please use SI units for all calculations [kg-s-kgmol-m] in this and subsequent memos, as well as in your reactor models.

3. **Group Duties:** Provide a tentative listing of duties for each group member for this project.
4. **Hand Calculations:** Give hand calculations of each representative calculation in an appendix to this short report. You are not required to type these hand calculations.