Reactor Design Project Overview

The design project is structured to comprise five memos and a final report, each to be completed at approximately two-week intervals throughout the semester. The project will conclude with an oral presentation. You will work together in your homework teams, each team on a slightly different problem. The design project will count as 20% of your final grade.

Project Description:

The project objective is to design a reactor for the production of either 1) maleic anhydride by the catalytic partial oxidation of n-butane, benzene or n-butene, or 2) for the production of acrolein by the catalytic oxidation of propylene or propane. While various reactor technologies have been practiced for these reactions, fixed bed reactor technology will be the focus of your design for this project.

The project work will involve a review of the literature for background on the product and production technologies, and for reaction kinetics for your system. Most of your work will focus on the reactor design and simulation based on these kinetics relationships from the literature. Your initial design will be for an ideal isothermal reactor using a simple rate equation. As we proceed through the semester, you will add in pressure drop calculations, energy balances and more complex chemistry to describe competing reactions.

You will perform reactor analysis and sizing using hand calculations and POLYMATH®, and reactor simulation using the Aspen Plus® process simulator. Detailed expectations will be outlined in individual instructions for each memo.

Group Assignments:

Group #	Team Members	Product	Reactant	Reactor Type	Production Rate
1	Nicole Cosgrove Michael Glasspool Sarah Wilson	Acrolein	Propylene	Fixed Bed Reactor	30000 M tons/yr
2	Kyle Lynch David Teicher Shu Xu	Acrolein	Propylene	Fixed Bed Reactor	75000 M tons/yr
3	Kerri May Megerle Scherholz Christopher Watts	Acrolein	Propylene	Fixed Bed Reactor	135000 M tons/yr
4	Yousef Ghotok Joseph Havelin Karen Osborn	Maleic Anhydride	n-Butane	Fixed Bed Reactor	25000 M tons/yr
5	Derek Becht Matthew Hunnemeder Eric Nette Michael Raymond	Maleic Anhydride	Benzene	Fixed Bed Reactor	50000 M tons/yr
6	Caitlin Boyd Katherine Ross David Schiavi	Maleic Anhydride	n-Butene	Fixed Bed Reactor	40000 M tons/yr
7	Joseph Haupt Pamela Kubinski Bethany Schmid Keith Weigand	Maleic Anhydride	n-Butane	Fixed Bed Reactor	40000 M tons/yr

Schedule: Due Date

Memo 1: Background & Overall Mass and Energy Balances	Wednesday, 30 Jan 2008
Memo 2: Isothermal Reactor Sizing with Simple Kinetics	Wednesday, 13 Feb 2008
Memo 3: Pressure Drop and Reactor Size Optimization	Wednesday, 27 Feb 2008

Reactor Design Project Overview

Memo 4: Multiple Reactions	Wednesday, 12 Mar 2008
Memo 5: Energy Balances with Multiple Reactions	Wednesday, 9 Apr 2008
Final Report and Oral Presentations	Wednesday, 23 Apr 2008

Contact Information:

Dr. LaMarca can be reached by phone during daytime hours at (302) 774-2265, or by email: Concetta.LaMarca@usa.dupont.com.

Project Memo Submissions:

Memos must be submitted at 8 am on the due date in class. Late submissions will be awarded partial credit in accordance with the policy outlined in the course syllabus. Your memos will be graded, and you will be eligible for 50% of the points missed on a resubmission due with the subsequent memo.

Memo submissions will include hand calculations, typewritten report material, POLYMATH® models and AspenPlus® models. Hand calculations and typewritten material as well as printed copies of POLYMATH® models and Aspen report files should be handed in as a hard copy at the beginning of class. Electronic copies of your POLYMATH® models and AspenPlus® backup files (*.bkp) should be submitted to Dr. La Marca by email before the start of the class on the due date. (Concetta.LaMarca@usa.dupont.com).

Clearly state all assumptions AND your solutions in the discussion section of each memo. A simple printout of a spreadsheet or model alone, is not complete, so be sure to state clearly your results and show your work.

Project Grading Components:

1. Background on product and raw materials.
2. Literature review / kinetics research.
3. Mass & energy balances.
4. Reactor Design
   - POLYMATH® Model
   - Aspen Plus® Model
5. Final report / writing comprehensiveness
6. Graded memos.

Reactor Design Project Overview

RESOURCES FOR YOUR PROJECT:

BOOKS ON RESERVE:

- Rate equations of solid-catalyzed reactions, edited by Reiji Mezaki and Hakuai Inoue. Tokyo, University of Tokyo Press, c1991. Call#: QD502.R38 1991. *(This is a good source of kinetics expressions; however, you still need to request the original reference article).*
- The properties of gases and liquids. Robert C. Reid, John M. Prausnitz, Bruce E. Poling. 4th Ed. New York, McGraw-Hill, c1987. Call#: TP242.R4 1987.
- Plant design and economics for chemical engineers, Max S. Peters, Klaus, D. Timmerhaus, 4th Ed. New York, McGraw-Hill, c1991. Call#: TP155.5.P4 1991.
- Heterogeneous catalysis in industrial practice, Satterfield, Charles N. 2nd Ed. New York, McGraw-Hill, c1991. Call#: TP156.C35S27 1991.
- An introduction to chemical engineering kinetics & reactor design, Hill, Charles G., New York: Wiley, 1977. Call#: QD502 .H54
- Handbook of commercial catalysts: heterogeneous catalysts, Howard F. Rase, Boca Raton, Fla.: CRC Press, c2000, TP159.C3 R37 2000.
- Green Engineering: environmentally conscious design of chemical processes, Allen, David T. and David R. Shonnard.: Prentice Hall, c2002. Call Number: TP155.2.E58 A54 2002.

REFERENCE SECTION:

- Kirk-Othmer Encyclopedia of Chemical Technology. Editorial board, Herman F. Mark *et al.*; executive editor, Martin Grayson, associate editor, David Eckroth. 4th Ed. New York, Wiley, c1991-. Call#: TP9.E685 1991 Reference Section.
- Kirk-Othmer encyclopedia of chemical technology [electronic resource] Rm. 219 Computer 16, 17, 18 in the library. To print, select the text desired and print. (Otherwise the figures will not be legible).
- Encyclopedia of Chemical Processing and Design. Executive editor, John J. McKetta, associate editor, William A. Cunningham. New York, M. Dekker, c1976-. v. <1-64 >. Call#: TP9.E66 Reference Section. See section on your process as well as physical properties, and cost estimation.
- Perry's Chemical Engineers' Handbook. 6th ed., late ed. Robert H. Perry; ed., Don W. Green; asst. ed., James O. Maloney. New York, McGraw-Hill, c1984. Call#: TP151.P45 1984. (This is also available from the all computer rooms in Rowan Hall under the 'Start -> All Programs -> Chemical Eng Apps -> Perry's' menus).

Costing information

- Turton, R, R. C. Bailie, W. B. Whiting, J. A. Shaeiwitz, *Analysis, Synthesis, and Design of Chemical Processes*, Prentice Hall PTR, New Jersey 1998
- Holland, F. A., J. K. Wilkinson, "Section 9 Process Economics," in *Perry's Chemical Engineers' Handbook 7th Edition*, Editors Perry, R. H., D. W. Green, J. O. Maloney McGraw Hill, New York 1999. See Table 9-50.
- Siebert, Oliver W. and John G. Stoecker, "Section 28 Materials of Construction," in *Perry's Chemical Engineers' Handbook 7th Edition*, Editors Perry, R. H., D. W. Green, J. O. Maloney McGraw Hill, New York 1999.

PHYSICAL PROPERTIES:

- The DIPPR database contains 29 fixed-value properties and 15 temperature-dependent properties of approximately 1811 industrially important compounds. (This database is accessible from the presentation computer in the 3rd floor computer room, http://dippr.byu.edu/public/ , username: rowanthermo, password: che&dippr). More info is available from the course website.
- Physical and thermodynamic properties: NIST WebBook http://webbook.nist.gov/
- Perry's, *Chemical Engineer's Handbook*
- *CRC Handbook of Chemistry and Physics*

Reactor Design Project Overview

JOURNAL ARTICLES

Comprehensive literature searches can be performed using Scifinder Scholar. You can access this program in the Rowan Hall computer rooms as follows. Start -> All Programs -> Chemical Eng. Apps -> Scifinder Scholar.

Many of the journal articles that you will need for this project can be obtained online, from the Library, Interlibrary Loan or from Dr. LaMarca. You need to locate references for your reaction immediately so that you can meet the first deadline. **You will be required to have three reaction rate expressions for your reactor taken from original references.** These expressions should include a simple power-law rate expression as well as a complex, Langmuir-Hinshelwood type expression that includes byproduct formation rates. Prices of chemicals can be found in the *Chemical Market Reporter* (ISSN: 1092-0110) which is located in the current periodicals room.

On-line journals can be found:

- From the library site http://www.rowan.edu/open/library/ under E-Journal Finder (at the right).
- Or directly for the most journals:
  Science Direct (Elsevier Journals) http://www.rowan.edu/library/databases/science_direct.htm such as *Chemical Engineering Science, Applied Catalysis A: General and Applied CatalyisB: Environmental, Applied Catalysis*
  ACS publications http://pubs.acs.org/journals/aoc/subselect.html of interest are: *Industrial and Engineering Chemistry Research, Chemical & Engineering News*.

PATENTS: Patents will not provide specific process information (or kinetics) for design; however, they contain a very useful section on the "Review of Current Art" which will help provide additional perspective for your process background. To search and access issued patents in the U. S. online, visit the following site: http://www.uspto.gov

ACADEMIC CONDUCT:

As stated in the syllabus, the policy in this class in matters of academic misconduct will follow that stated in "Rowan University Student Handbook." Plagiarizing from literature sources or from another team is a violation of University Academic Conduct policy.

In accordance with your guidelines for cooperative learning, you are expected to work together with your team members. Each team's project submissions should represent unique work done by the members of the team.