*ChE 344 Reaction Engineering and Design* *WINTER 2016*

**Instructor:** Dr. Trent Silbaugh

**Lecture:** TuTh 9:30-11:30 AM 1013 H.H. Dow

**Discussions:** Discussion will take place in the final 30 minutes of the lecture period and will consist of an in-class problem to be solved in assigned groups of 4. GSIs and proctors will be in the room to offer clarification and assistance. At least one member of the group will need to bring a computer to class to complete some ICPs. An announcement will be posted at least one day prior if a computer will be needed.
Sunday review sessions will be held on central campus from 3-5 PM. See room information in the office hours section below (locations may change after the first week of class).

**Personnel Information**

| **Name** | **Role** | **Office** | **Email (@umich.edu)** |
|---|---|---|---|
| Trent Silbaugh | Instructor | 3086 H.H. Dow | tsilbaug |
| Martin De Beer | GSI (Hmwk) | | mapadebe |
| Calvin Boerigter | GSI (ICP) | | cboerigt |
| Robert Polik | IA | | rpolik |
| Lauren Warren | IA | | lmwarr |
| Patrick Lown | Tutor | | plown |

**Course objectives:**

In this course, you will learn how to analyze chemical reactors and reaction systems, develop critical and creative thinking skills, solve open-ended problems in teams, and practice solving reaction engineering problems using computer software.

**Prerequisite:**

ChE 330 and ChE 342

**Course Outcomes:**

- Describe the algorithm that allows students to solve chemical reaction engineering problems through logic rather than memorization
- Size isothermal, adiabatic, and non-adiabatic reactors for homogeneous and heterogeneous reactions
- Analyze multiple reactions carried out both isothermally and non-isothermally in flow, batch, and semi-batch reactors to determine selectivity and yield
- Determine the reaction order and specific reaction rate from experimental data
- Describe the steps in a catalytic mechanism and how one goes about deriving a rate law, mechanism, and rate limiting step that are consistent with experimental data
- Carry out computer simulation of reactors with multiple reactions with heat effects
- Work together to solve both open-ended and closed-ended reaction engineering problems
- Write questions that demonstrate critical thinking on reaction and reactor safety

**Office Hours and Sunday Review**

Monday
- 3-5 PM (3166 HH Dow) Martin and/or Calvin

Tuesday
- After lecture – 12:30 PM (3166 HH Dow) Dr. Silbaugh
- 8-9 PM (Shapiro) Patrick

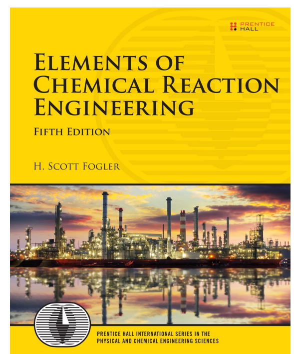
Wednesday
- 3-5 PM (3166 HH Dow) Martin and/or Calvin
- 6-9 PM (CHEM 1640) Robert (6 to 8) and Lauren (7 to 9)

Thursday
- 1-2 PM (3166 HH Dow) Dr. Silbaugh

Friday
- 3-6 PM (Shapiro) Patrick

Sunday Review
- 3-4:30 PM (AH Aud C) Lauren and Robert

**Required Text:**




- Elements of Chemical Reaction Engineering, 5th Edition
  By H. Scott Fogler
- Text ordering information: http://www.informit.com/store/elements-of-chemical-reaction-engineering-9780133887518
- The first 4 chapter will be provided to you free of charge (Thank you Prof. Fogler!), as the new edition will not be available until Jan. 8th.
- Earlier editions have differing text in some places and different problem statements. If you are a risk taker and you go with an older version, you will need to be vigilant of any differences. We will not be responsible for any issues arising from the use of a previous edition.

**Web resources:**

Textbook webpage: http://www.umich.edu/~elements/5e/

CTools - The site will contain:

Homework problem statements
Assignment grades
Announcements and class polls
Homework, In-class problem and exam solutions

Lecture recordings: All lectures will be recorded through the CAEN lecture capture system. Lectures can be accessed through the CTools site.

**In-class problems:**

Students will work in assigned groups of 4 to complete in-class problems. These problems will be graded and all participating members of the group will receive the same score. We will reorganize groups after the first midterm.

**Homework:**

Assignments will be posted one week before the due date. Assignments will be turned in at the start of lecture on Thursday due dates. (See semester schedule below for due dates)

**Guidelines:**

1. On the first page in the upper right hand corner, write:
   Name
   Problem Set and Due Date
   Students you have studied with while working on the assignment
2. Use 8.5 x 11 paper with straight edges (no paper torn from spiral notebook). Solutions can be hand-written or typed
3. All pages should be numbered (e.g. 1/5, 2/5 etc.) and have your name written at the top.
4. Pages should be ***stapled*** together
5. Use a ruler (or computer) when making sketches and drawings.
6. Please be neat and write legibly. If the grader can't read it, they will have to assume it is incorrect.

**Exams:** There will be two midterm exams during the semester and a comprehensive final exam. Midterm 1 will be held during class hours. Midterm 2 will be held 6-8 pm on the indicated date. There will be no lecture on the day of the Midterm 2 exam.

**Request for regrading:** You may request that the grade given on a homework assignment or exam be reevaluated. All such requests must be made in writing and submitted to Martin De Beer. This request should include the assignment or exam in question along with a brief note explaining your concerns. **You will be given one (1) week from the date that an assignment or exam is returned to make such a request.** No requests for regrades will be accepted after this one week has expired. You will also only have one week to notify your instructor that an assignment has not been returned to you.

**Engineering Honor Code:** All exams and homework assignments will be administered under the College of Engineering Honor Code.

**Exams:**

You must write and sign the Honor Pledge "I have neither given nor received aid on this examination, nor have I concealed any violation of the Honor Code." after taking each exam. Failure to do so gives your instructor the right to refuse to grade that exam.

**Individual assignment (Limited collaboration):**

Each assignment is to be completed individually, but not necessarily in isolation. You are allowed to form small study groups (e.g. of less than five students) and to discuss general solution strategies with peers. However, you are expected to attempt every problem on your own before discussing with classmates and you must complete all calculations and write-up, from scratch to final form, on your own.

- It is acceptable to discuss problem-solving strategies with the usage of books and notes, but you may not allow any classmate to copy your solution. Note that creating an unfair advantage for another student is an Honor Code violation.
- Verbatim copying of another student's work is forbidden.
- You are not allowed to possess, look at, use, or in any way derive advantage from the existence of solutions prepared in previous years, whether these solutions were former student's work or copies of solutions made available by instructors or the textbook author.

**Grading:**

Course grades will be calculated according to the following weights:

| | |
|---|---|
| Homework | 15% |
| Midterm Exam 1 | 25% |
| Midterm Exam 2 | 25% |

| | |
|---|---|
| Final Exam | 30% |
| In class problems | 5% |
| Total | 100% |

At the end of the semester, a percentage grading scale will be used to determine the letter grade. The grading will be no tougher than the scale:

A-/B+ cutoff 90%
B-/C+ cutoff 80%
C-/D+ cutoff 70%
E cutoff 65%

Dr. Silbaugh reserves the right to be more generous when assigning letter grades. We expect all students to perform well in the course, provided they actively participate, complete necessary readings and homework assignments, and seek help if needed.

**Students with disabilities:**
Dr. Silbaugh is available to discuss appropriate accommodations that may be required for students with disabilities. Requests for academic accommodations are to be made during the first three weeks of the semester, excluding unusual circumstances, so that necessary arrangements can be made. Students are encouraged to register with the Office of Students with Disabilities, G-664 Haven Hall, (734)763-3000, https://ssd.umich.edu/ to verify their eligibility for appropriate accommodations.

**Course Schedule (*Tentative*)**
Portions of assignments contained problems taken from:
*Elements of Chemical Reaction Engineering 5th Edition, H. Scott Fogler*.
Problem numbers from this text listed below.

| Date | Topic | Chapter | Submit | Other Material |
|---|---|---|---|---|
| Th 1/07/16 | Introduction, Mole Balances, Polymath | Chapter 1 | | ICG 1 |
| Tu 1/12/16 | Design equations | Chapter 2 | | Black Widow Video |
| Th 1/14/16 | Rate Laws | Chapter 3 | HW 1:<br>P1-$1_A$ (a-b),<br>P1-$2_A$ (ICG),<br>P1-$5_B$(omit b),<br>P1-$6_A$ (omit b),<br>P2-$2_A$ (ICG),<br>P2-5 | |
| Tu 1/19/16 | Stoichiometry in Batch | Chapter 4 | | |
| Th 1/21/16 | Stoichiometry in Flow Systems | Chapter 4 | HW 2:<br>P3-$8_A$,<br>P3-$12_A$,<br>P3-13 (a),<br>P4-$6_A$,<br>P4-$8_B$ | |
| Tu 1/26/16 | Isothermal Reactor Design | Chapter 5 | | Chemical Engineering Gone Wrong Video |
| Th 1/28/16 | FE exam question example | Chapter 5 | HW3:<br>P4-2 (ICG),<br>P4-5,<br>P5-$12_B$,<br>P5-$19_B$ | |
| Tu 2/02/16 | Pressure drop in reactors | Chapter 5 | | |
| Th 2/04/16 | Membrane Reactors | Chapter 6 | HW4:<br>P5-2 (ICG),<br>P5-3,<br>P5-$14_B$,<br>P5-$8_B$,<br>P5-$17_B$ | |
| Tu 2/09/16 | Semibatch Reactors | Chapter 6 | | |
| Th 2/11/16 | Analysis of Data and PSSH | Chapter 7 | HW 5:<br>P5-$22_A$,<br>P5-23,<br>P6-$2_D$,<br>P6-$6_C$,<br>P6-$8_C$ | |
| Tu 2/16/16 | **Midterm 1 (9:30-11:30am)** | | | |

| | | | | |
|---|---|---|---|---|
| Th 2/18/16 | Multiple Reactions | Chapter 8 | | |
| Tu 2/23/16 | Multiple Reactions | Chapter 8 | | |
| Th 2/25/16 | Derivation of Energy Balance | Chapter 11 | HW 6:<br>P7-$10_A$,<br>P8-$1_A$ (g+h),<br>P8-$2_A$ (ICG)<br>P8-$6_B$,<br>P8-$10_B$,<br>Study Problem:<br>P8-7 | |
| Tu 3/08/16 | Adiabatic Equilibrium Conversion/ Staging | Chapter 11 | | |
| Th 3/10/16 | Heat Exchange | Chapter 12 | HW 7:<br>P7-7,<br>P7-$8_A$,<br>P8-$13_B$,<br>P8-$16_B$ | |
| Tu 3/15/16 | Multiple Reactions with Heat Effects | Chapter 12 | | |
| Th 3/17/16 | Unsteady State CSTR & Multiple Steady State | Chapter 13 | HW 8:<br>Written problems (attached below),<br>P11-$5_A$,<br>P11-$6_B$,<br>P12-$4_A$ (ICG) | |
| Tu 3/22/16 | **Midterm 2 (9:30-11:30am)** | | | |
| Th 3/24/16 | Safety | Chapter 13 | | |
| Tu 3/29/16 | Catalysis | Chapter 10 | | |
| Th 3/31/16 | Catalysis | Chapter 10 | HW 9:<br>P12-$26_C$,<br>P13-$1_B$ (b) and (f),<br>P12-$17_B$ | |
| Tu 4/05/16 | Catalysis: External mass transfer | Chapter 14 | | |
| Th 4/07/16 | Catalysis: Internal mass transfer | Chapter 15 | HW 10:<br>P10-3,<br>P10-8,<br>P10-11 | |
| Tu 4/12/16 | PSSH Enzyme Kinetics | Chapter 9 | | |
| Th 4/14/16 | Bioreactors | Chapter 9 | HW 11:<br>P14-2,<br>P9-9,<br>P14-8,<br>P15-2,<br>P15-3 | |

| | | | | |
|---|---|---|---|---|
| **Mo 04/25/16*** | **FINAL EXAMINATION** | | | |

**FINAL EXAM: Monday, April 25th, 1:30 pm – 3:30 pm**
* The assigned final exam date and time is based on a 9:00 or 9:30 am class start time.

**ChE344 Homework 8:**

**Problem 1: (10 points)**

The reaction:

$A \leftrightarrow B$

The forward and reverse rate constants are given by:

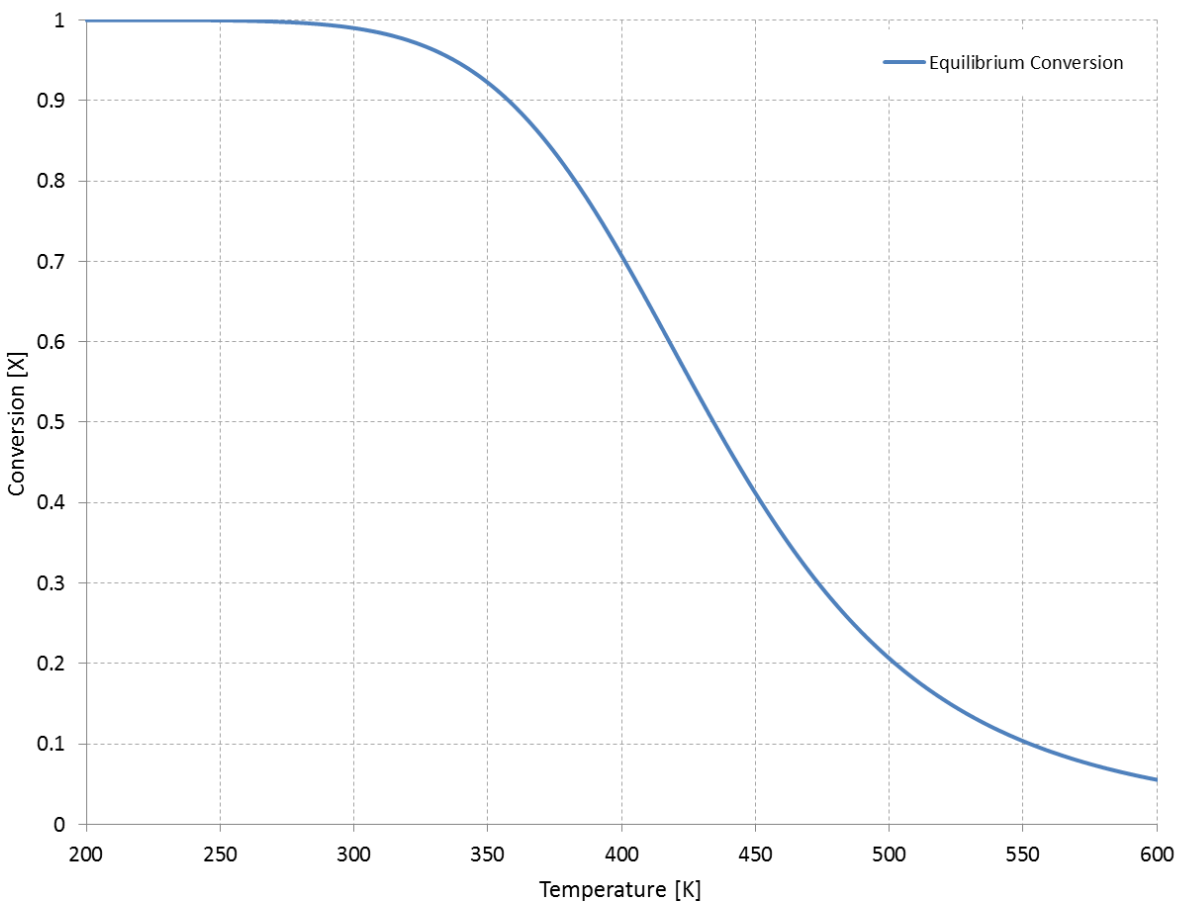
$$k_f = 0.1 \exp\left(-\frac{30000}{RT}\right)$$

$$k_r = 2848 \exp\left(-\frac{67044}{RT}\right)$$

The heat capacities are as follows: $C_{p,A} = 100$, $C_{p,B} = 400\ J.mol^{-1}.K^{-1}$

Consider a series of three reactors with interstage cooling. The inlet to the first reactor is pure A at a temperature of 300K and the interstage coolers bring the fluid back to this temperature. The three reactors are maintained at temperatures of 440, 400, 370K, in that order.

What is the exit conversion from the cascade? (You can redraw the plot below or submit your answer directly on this page)



**Problem 4: (10 points)**

The elementary liquid-phase reaction:

$$A + B \leftrightarrow C$$

Is to be carried out in a set of tubular reactors packed with a resin catalyst and arranged in series. The feed consists of 25 mol % A, 25 mol % B, and 50 mol % inerts at 300K. There are many heat exchangers available to you which are able to cool the reaction stream to temperatures as low as 300K. The reactors have sufficient catalyst to reach 95% of the corresponding equilibrium conversion. What is the smallest number of reactors in series necessary to obtain an exiting conversion above 50%? What would you need to do in order to increase the conversion to 95%? What concerns would you have about reaching 95% conversion?

Additional information:

$$C_{P_A} = 2.0 \frac{cal}{g\ mol\ °C} \qquad C_{P_C} = 7.0 \frac{cal}{g\ mol\ °C}$$

$$C_{P_B} = 5.0 \frac{cal}{g\ mol\ °C} \qquad C_{P_I} = 1.5\ cal/(g\ mol\ °C)$$

$$\Delta H^o_{Rx}(273K) = -10000 \frac{cal}{g\ mol\ A} \qquad F_{A0} = 10\ mol/min$$

| $T(K)$ | 350 | 400 | 450 | 500 | 550 | 600 | 650 | 700 |
|---|---|---|---|---|---|---|---|---|
| $X_e$ | 1.00 | 0.97 | 0.74 | 0.4 | 0.2 | 0.1 | 0.06 | 0.04 |

**BONUS PROBLEM (10 points)**

Operating a reactor along the adiabatic trajectory (i.e. the conversion-temperature path a reaction with no heating/cooling will follow) is, obviously, not the best way to operate a reactor. Instead there is a “maximum rate path” which is the trajectory a reaction mixture will follow when the temperature is controlled to maximise the reaction rate at any conversion level.

Sketch the maximum rate path for Problem 1.

**Study Problem:** P11-$9_A$ ECRE $5^{th}$ Edition