Spring 2020

CHE 349-002: Kinetics and Reactor Design

Robert Barat

MEMORANDUM

To: ChE 349 Class
Date: January 23, 2020
From: Prof. Robert Barat
Re: Course Introduction (v.1)

Course Description: *ChE 349 Kinetics and Reactor Design (3-0-3).*

Derive and solve species and energy balances for single chemical reactors processing liquid and gaseous systems; chemical reactor process safety; multiple reaction applications; catalysis, including mechanisms, rates, reactor design.

Prerequisites: Chem 236 (Physical Chemistry), ChE 342 (Thermodynamics), ChE 370 (Heat & Mass Transfer), Math 222 (Differential Equations)

Class Meetings: Mondays, Thursdays 10-11:20 AM, KUPF 106

Attendance: Class attendance will not be monitored. But you are strongly encouraged to not miss classes. Remember that you're responsible for in-class topics.

Instructor Information: Location: 374 Tiernan Hall
Office Hour: Mondays 1-2:30 PM. If I'm in my office, the door is open – stop in; or email me for an appointment; individual or group visits are OK.
Office phone: (973) 596-5605 Email (preferred contact): barat@njit.edu

Text: *Essentials* of Chemical Reaction Engineering, H. S. Fogler, 2nd ed. -- Prentice Hall (2018). The book also contains many links to useful resources. NOTE: Such texts are heavy and often expensive. Feel free to share a copy between a few of you.

Web-Based Textbook Resource: http://www.umich.edu/~essen/

Course Requirements:
Term tests* (3) .... 50% (2 before the drop date)
Group project ………15%
Homework ……….... 15%
Final test*………….... 20%
* All tests are "Open-Book" and "Open-Notes"

Grading Scale *(historical – subject to change):* Total points normalized to 100

A	B+	B	C+	C	D	F
90-100	84-89	78-83	72-77	66-71	60-65	< 60

Homework: Problem sets will be assigned, collected, T/A graded, and then returned. Solutions will be reviewed in class as time allows. All solutions will be posted on the course *Canvas* site. If you have questions about HW grading, contact the T/A directly. All HW problems are original – none from the text.

Homework Grader: TBA If you have questions about HW grading, contact TBA. For questions about the course material, please see the instructor. The tests and the Term Project are all graded by the instructor.

Term Project: Work in groups (you form). A Peer & Self Evaluation will be done at the conclusion of the project that will impact your grade; more details later.

***Canvas* Site:** http://canvas.njit.edu --- Please check this site and your email often (at least once a day). Practice problems will be posted, as well as HW and test solutions, group projects, some in-class work, and useful memos.

Math Solver: You must have access to and know how to use one math solver software package. Examples include *Polymath, Maple, Matlab, Mathcad,* and *Mathematica.* It will be needed for the term project and some homeworks. A solver is NOT needed on tests.

Polymath is available on dep't PCs in 411 Tiernan. The **license** info for download of *Polymath* onto your laptop is posted on the Canvas site. Three podcasts (Algebraic Equations, ODE's, Regressions) are available in the Media Gallery of the course *Canvas* site to help you learn *Polymath*, if you choose to use it.

Course Topics: Constant density (liquid) reactors – species balance
Variable density (gas) reactors – species balance
Simultaneous species and energy balances
Chemical reactor process safety
Multiple reaction systems
Catalysis – homogeneous and heterogeneous

Assigned Readings: The semester schedule (separate posting) lists recommended readings in the Fogler text. Ultimately, for quizzes and exams, you are responsible for the material *covered in class.*

Recommended Link: You should check out this link: www.essentialchemicalindustry.org
This is a treasure of information about our profession.

Policy on Integrity: Professional behavior is expected at all times in this course.

- On-time arrival for the start of class is expected.
- Cheating on exams will not be tolerated. If calculations are required, only calculators are permitted. All cell phones must be away during exams.
- Collaboration on homework assignments is not discouraged. In fact, homework and study groups might be helpful. All homework assignments, however, must be individually *submitted before the solutions are reviewed in class*.
- Everyone within a Term Project group must contribute effort equally. A Peer & Self Evaluation will be done after the group projects are submitted.
- If you use *Polymath*, you must obey the license terms – no commercial use; for education use only.

Specific goals (Learning Attributes) for this course:

a. Students will be able to:

1. Write reaction rate laws for single elementary reactions and/or stated complex liquid phase reactions
2. Express concentrations in terms of conversion for liquid (constant density) systems using the given reaction stoichiometry and reactor feed
3. Calculate the requested unknown (e.g. volume, space time) using the appropriate species balance for the assigned liquid phase steady-state flow reactor (CSTR, PFR)
4. Write reaction rate laws for single elementary reactions and/or stated complex gas phase reactions
5. Express concentrations in terms of conversion for gas (variable density) systems using the given reaction stoichiometry and reactor feed
6. Simplify concentration expressions for dilute gas systems using problem-specific appropriate assumptions
7. Calculate the requested unknown (e.g. volume, space time) using the appropriate species balance for the assigned gas phase steady-state flow reactor (CSTR, PFR)
8. Derive the appropriate energy balance for the assigned steady-state flow reactor
9. Combine species, energy balances to determine unknown quantity (time, conversion, energy transfer rate, temperature) for steady-state flow reactors
10. Model (species, energy balances) the pre-upset (steady-state) condition for a CSTR with emphasis on process safety (e.g. runaway)
11. Model (species, energy balances) the upset (transient) condition for a CSTR and for a batch reactor with emphasis on process safety (e.g. runaway)
12. Derive a rate expression based on an elementary mechanism using the Pseudo Steady State Hypothesis or Langmuir–Hinshelwood algorithm for homogeneous and heterogeneous catalytic systems
13. Express concentrations in terms of conversion for both liquid and gas catalytic systems using stoichiometry and feed/charge conditions
14. Calculate the required unknowns (e.g. volume, time) using the appropriate species balance for assigned catalytic reactor
15. Derive species net reaction rates from multiple reaction networks
16. Design the required reactor using the energy and species balances in a multiple reaction problem
17. Complete a team-based term project by preparing the basic reactor design using energy and species balances
18. Produce a professional, team-based memo with sound presentation of results and quality graphs
19. Solve algebraic (linear, quadratic) equations and ODEs (separation of variables) analytically (by hand)
20. Solve term project multiple-equation (algebraic, ODEs) problems using computer-based numerical software

b. This course explicitly addresses ABET student outcomes 1, 2, 3, 4:

1. An ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics
2. An ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors
3. An ability to communicate effectively with a range of audiences
4. An ability to recognize ethical and professional responsibilities in engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts