# ENCH 640 Advanced Chemical Reaction Kinetics

**Instructor**:
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**Class Schedule**:
Class will meet on TU/TH 11:30 AM - 12:45PM (Physics 107).

**Office Hours**:
9:00 a.m. - 9:50 a.m. on Fridays or by appointment.
Outside of these hours, students will usually be welcomed, but may sometimes be advised to come back later.

**Description**:
This course will provide an overview of advanced chemical kinetics and reaction engineering at an intermediate to advanced level. Coverage will be relatively broad and shallow. The goal is to provide students with the vocabulary, modeling tools (Matlab programing code), and theoretical background to understand current chemical kinetics and reaction engineering literature and to tackle the sort of complex problems that they may encounter in their research and beyond.

This course will cover Matrix Methods and Notation; Solution of linear ODEs using Laplace transform methods; Stochastic methods for analyzing chemical reaction processes; Sensitivity analysis and determination of rate parameters; Collision theory of reaction rates; Potential Energy Surfaces; Transition State Theory; Reactions in Liquids; Reactions at solid surfaces; Transport effects on reactions at solid surfaces (and in catalyst pellets); Fundamental Balance Equations for Reactor Engineering; Batch and Semibatch Reactors; The ideal plug flow reactor (PFTR); Multi-stability and optimal operating conditions in CSTR; Linear stability analysis of the systems ODEs; Residence time distributions (RTD's) and non-ideal flow patterns; Numerical Solution of Boundary Value Problems; The fixed bed catalytic reactor and fluid bed reactor et al.

**Prerequisites**:
Students are expected to be familiar with the material commonly presented in undergraduate kinetics and reaction engineering courses (see for example the texts by Fogler, Schmidt, or Hill listed on the Bibliography page). ***Only a brief review of undergraduate material will be presented***. However, knowledge of it will be necessary to succeed on the course exams and homework. **Background in calculus, ordinary differential equations, linear algebra, numerical methods, statistical mechanics, quantum mechanics, and general physical chemistry** will also be helpful at various points in the course.

**Textbook**:
***There is no required textbook for this course. Lecture notes in pdf format will be posted on the course web page prior to class***. ***Documents provided courtesy of Dr. Mark Swihart from SUNY-Buffalo***. Much of the material in the chemical kinetics portion of the course is based on 'Chemical

Kinetics and Dynamics' by Steinfeld, Francisco, and Hase. Much of the reaction engineering portion of the course is based on 'Chemical Reactor Analysis and Design' by Froment and Bischoff. Other books that you may find useful are listed on the bibliography part of this document.

**Grade Basis**:

<u>*Exams*</u>:

There will be two exams, each determining 30% of the final grade. Exam problems will be closely related to the homework assignments. The first exam (mid-term exam) will cover the chemical kinetics portion of course. The second exam (during finals week) will cover the reaction engineering portion of course. **The exams will be closed-book format. You may use a scientific calculator and two letter-size sheets (2-sided) of notes to aid you on the two exams**.

<u>*Homework*</u>:

Problem sets will be assigned each Thursday, due the following Thursday. ***There will be 12 homework sets. These 12 homework sets will count for 40% of the final grade***. Every student has three quotes to turn in their homework with a ***2-day*** (***48 hour) extended due date***. You still receive full grades as long as you haven't run out of your three quotes. **However, you can only receive maximally 80% of the total points if you submitted your homework late AND you have run out of your three late quotes**. Decide wisely when you are going to use this quote. <u>My suggestion is to: always submit your homework on time and never use this quote</u>. Most of the homework will be an independent project with application-based problem sets, all the homework data is retrieved from original research paper. A computational software package (Matlab or Polymath or Fortran or Maple or Mathematica or whatever you prefer) with plotting function will be necessary to solve most of the homework. However, detailed examples of lecture notes and homework solutions will be provided with Matlab or Maple format. Working together on homework problems is encouraged. Copying from homework solutions is not allowed. If you simply copy or adapt these previous solutions without fully understanding how to solve the problems, you are unlikely to be very successful on the course exams, and as a result are likely to do poorly in the course. Moreover, copying from these solutions constitutes academic dishonesty, which has severe consequences. *Homework regrading must be formally submitted to the instructor within 48 hours of return of your homework. You must present evidence why you think I should raise your points based on your submitted homework. You cannot simply say "I forgot adding ...."; or "I misunderstood..."; or "my computer is crashed, or I lost my data".*

**Grading policy**:

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|---|---|
| A (4.0): | >=91% |
| A- (3.7 ): | 87%~91% |
| B+ (3.3 ): | 83%~87% |
| B Good (3.0 ): | 79%~83% |
| B- (2.7 ): | 75%~79% |
| C+ (2.3 ): | 71%~75% |
| C Not Satisfactory (2.0 ): | 67%~71% |
| C- (1.7 ): | 63%~67% |
| D Unacceptable (1.0 ): | 60%~63% |
| F Failure (0 ): | <60% |

AU Audit (No Credits Attempted or Earned)

**Bibliography of Useful Texts and References**:


*Review of undergraduate kinetics and reaction engineering*:

Fogler, H.S., “Elements of Chemical Reaction Engineering”, 4th Ed., Prentice Hall, Englewood Cliffs, New Jersey, 2005.

Schmidt, L.D., “The Engineering of Chemical Reactions, 2nd. Ed.”, Oxford University Press, New York, 2004.

Hill, C.G., Jr., “An Introduction to Chemical Engineering Kinetics and Reactor Design”, John Wiley and Sons, New York, 1977.

*Chemical Kinetics*:

Masel, R.I., “Chemical Kinetics & Catalysis”, Wiley, 2001.

Steinfeld, J.I., J.S. Francisco, and W.L. Hase, “Chemical Kinetics and Dynamics”, 2nd edition, Prentice Hall, Upper Saddle River, New Jersey, 1998.

Masel, R.I., “Principles of Adsorption and Reaction on Solid Surfaces”, John Wiley and Sons, New York, 1996.

Pilling, M.J., and P.W. Seakins, “Reaction Kinetics”, Oxford, 1995.

Laidler, K.J., “Chemical Kinetics”, 3rd Ed., Harper and Row, New York, 1987.

Benson, S.W., “Thermochemical Kinetics”, 2nd Ed., John Wiley and Sons, New York, 1976.

Robinson, P.J., and Holbrook, K.A., “Unimolecular Reactions”, Wiley-Interscience, New York, 1972.

Boudart, M., “Kinetics of Chemical Processes”, Prentice Hall, Englewood Cliffs, New Jersey, 1968.

Benson, S.W., “The Foundations of Chemical Kinetics”, McGraw-Hill, New York, 1960.

Gates, B.C., “Catalytic Chemistry”, John Wiley and Sons, New York, 1992.

*Reaction Engineering/Reactor Design*:

Butt, J.B., “Reaction Kinetics and Reactor Design”, 2nd Ed., Marcel Dekker, Inc., New York, 2000.

Coker, A. Kaycode, “Modeling of Chemical Kinetics and Reactor Design”, Gulf Professional Publishing, 2002.

Froment, G.F. and K.B. Bischoff, “Chemical Reactor Analysis and Design”, 2nd ed., John Wiley and Sons, New York, 1990.

Levenspiel, “Chemical Reaction Engineering”, 3rd Ed., John Wiley and Sons, New York, 1999.

Carrberry, J.J., “Chemical and Catalytic Reaction Engineering”, McGraw-Hill, New York, 1976.

Denbigh, K.G., and J.C.R. Turner, “Chemical Reactor Theory”, 2nd Ed., Cambridge University Press, London, 1971.

Aris, R., “Elementary Chemical Reactor Analysis”, Prentice Hall, Englewood Cliffs, New Jersey, 1969. (Reprinted by Butterworths, 1989).

*Microbial growth kinetics and bioreactor*:

Clark, D.S & Blanch, H.W, “Biochemical engineering”, 2nd Ed., CRC Press, 1997.

## Tentative Course Schedule

| Week | Tuesday | Thursday |
|---|---|---|
| **1/29-2/2** | *Undergraduate Kinetics Review*<br><br>Introduction and Review – Matrix representation of reaction networks | *Undergraduate kinetics Review*<br><br>More review – definitions, classical approximation methods |
| **2/5-2/9** | *Kinetic Simulations*<br><br>Classical matrix methods for systems of 1$^{st}$ order reactions; | *Kinetic Simulations*<br><br>Stochastic methods and Kinetic Monte Carlo |
| **2/12-2/16** | *Kinetic Simulations*<br><br>Numerical methods and codes for stiff ODE's | *Kinetic Simulations*<br><br>Sensitivity analysis and rate parameter fitting |
| **2/19-2/23** | *Kinetic Simulations*<br><br>Sensitivity analysis and rate parameter fitting | *Reaction Rate Theory*<br><br>Simple collision theory; Potential energy surfaces |
| **2/26-3/2** | *Reaction Rate Theory*<br><br>Potential energy surfaces | *Reaction Rate Theory*<br><br>Transition state theory; Unimolecular Reactions and Pressure Dependent Rate Parameters |
| **3/5-3/9** | *Reaction Rate Theory*<br><br>Thermochemical and kinetic estimation methods; Reactions in liquids | *Condensed Phase and Surface Reactions*<br><br>Reactions at Surfaces; Heterogeneous catalysis |
| **3/12-3/16** | *Condensed Phase and Surface Reactions*<br><br>Heterogeneous catalysis | *Coupled Reaction and Transport*<br><br>Interfacial gradient effects |
| **3/19-3/23** | ***Spring break, No class*** | ***Spring break, No Class*** |
| **3/26-3/30** | **First Exam: Chemical Kinetics**<br><br>**2.0 hour** | *Fundamental Equations for Reactor Engineering*<br><br>Mass balance equations |

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|---|---|---|
| **4/2-4/6** | *Fundamental Equations for Reactor Engineering*<br><br>Simplifications for CSTR, PFTR | *Batch and Semi-Batch Reactors*<br><br>Basic models, Optimization |
| **4/9-4/13** | *The Ideal Plug Flow Reactor*<br><br>Basic models, Optimization | *The Ideal Plug Flow Reactor*<br><br>Optimal Temperature |
| **4/16-4/20** | *The Continuous Stirred-Tank Reactor (CSTR)*<br><br>Basic Cases, Optimal Operation | *The CSTR (cont.)*<br><br>Transient solutions, multiplicity, stability of steady states, phase plane |
| **4/23-4/27** | *Fermentation and Biochemical reactions*<br><br>Microbial growth kinetics, non-structural kinetic modeling of substrate consumption, product formation | *Fermentation and Biochemical reactions*<br><br>Chemostats, recycled reactor (perfusion reactor), multistage CSTR |
| **4/30-5/4** | *Non-Ideal Reactors*<br><br>Residence time distributions | *Numerical Solution of Boundary Value Problems* |
| **5/7-5/11** | *The Fixed-Bed Catalytic Reactor* | *Detailed Example of Fixed-bed Catalytic Reactor Design* |
| **5/14-5/18** | *Complex Reactors*<br><br>Fluidized bed reactor | *No class* |
| Final week | **Final Exam: Reactor Engineering TBD, during final exam week, 2.0 hour** | |