A. DESCRIPTION

This course focuses on the concepts and applications of chemical thermodynamics and rate processes. The central objective of this course is to extend students' understanding of the elementary concepts of thermodynamics, gas laws and chemical kinetics that they learnt in their previous freshman and sophomore chemistry and physics courses. The first part of the course concentrates on the fundamental principles and applications of thermodynamics, especially its first and second laws. The remainder of the course will focus on rate processes including kinetic theory of gases, reaction kinetics, and transport phenomena. This course uses both a microscopic and macroscopic approach in examining thermodynamics and rate processes. This allows students to experience how both thermodynamics and rate processes are applied to solve a wide range of practical problems from the laboratory scale to the industrial scale.

B. ORGANIZATION

CHEM 4362 is a lecture course in which topics are presented by the instructor. Concurrent enrollment in CHEM 4162, “Thermodynamics and Kinetics Laboratory”, is required only for those students in the Bachelor of Science degree program. Homework assignments are given on a regular basis. There is one mid-term exam, a comprehensive final exam, and an ACS exam.

C. PRE-REQUISITE COURSES

Thermodynamics and kinetics relies heavily on applied mathematics. In order to succeed in this course, students must have a good grounding in applied mathematics and have had prior exposure to freshman physics and chemistry courses. The pre-requisite courses for CHEM 4362 are the following:

1. Calculus I and II (MATH 1431/1432)
2. General Physics I and II (PHYS 1111/1112/1331/1332)
3. General Chemistry I and II (CHEM 1141/1142/1341/1342)
Other courses (not pre-requisite) that will benefit students taking CHEM 4362 are as follows:

1. Differential Equations (MATH 2343)
2. Partial Differential Equations (MATH 4343)
3. Linear Algebra (MATH 3334)
4. University Physics I and II (PHYS 2111/2112/2331/2332)

D. COMPUTATIONAL SOFTWARE

The computer is a standard tool in any modern scientific or engineering discipline. As such, students in CHEM 4362 are required to fully utilize computer technology whenever necessary to solve numerical problems. This course will require the use of MATLAB, a powerful technical computing platform. Students have access to MATLAB on any university computer on campus. Students may also purchase a personal copy of MATLAB at a discounted, student rate. Personal purchases can be made at the following site:

http://www.mathworks.com/academia/student_version/

E. REFERENCES

There is no required textbook for this course. Textbooks and references that supplement or expand on the material covered in class are the following:

Thermodynamics


Kinetics


Applied Mathematics

General Physical Chemistry


F. COURSE TOPICS

<table>
<thead>
<tr>
<th>Topic</th>
<th>Title</th>
<th>Concepts</th>
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</thead>
</table>
| 1 | Material Balances | • General conservation equation  
• Nonreactive and reactive processes  
• Multiple reactions |
| 2 | Energy Balances: First Law of Thermodynamics | • Thermodynamic definitions  
• Energy balance  
• $\Delta U$ and $\Delta H$ for ideal and real gases |
| 3 | Entropy Balances: Second Law of Thermodynamics | • Entropy balance  
• $\Delta S$ for ideal and real gases |
| 4 | Thermodynamic Processes and Cycles | • Rankine cycle  
• Refrigeration cycle |
| 5 | Thermodynamic Properties of Real Substances | • Equations of state of real gases  
• Thermodynamic partial derivatives |
| 6 | Phase Equilibrium and Mixtures | • Phase diagrams and equilibrium  
• Clapeyron and Antoine equations  
• Ideal solutions  
• Properties of mixing |
| 7 | Vapor-Liquid Equilibrium of Mixtures | • Raoult’s Law  
• Modified Raoult’s Law  
• Excess molar Gibbs free energy models |
| 8 | Chemical Reaction Kinetics | • Rate of reaction  
• Complex reaction mechanisms  
• Design of chemical reactors |
G. GRADING PLAN

The coursework is 45% exams and 55% homework assignments:

<table>
<thead>
<tr>
<th>Component</th>
<th>Frequency</th>
<th>Unit Value</th>
<th>Total</th>
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<tr>
<td>Homework Assignments</td>
<td>11</td>
<td>50</td>
<td>550</td>
<td>55</td>
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<tr>
<td>Mid-Term Exam</td>
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<td>140</td>
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<td>ACS Exam</td>
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<td>Final Exam</td>
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<td>250</td>
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Grading Scale

Your final grade for the course will be determined by the following percentage scale:

A  100–93       A–  92–90
B+  89–87       B   86–83       B–  82–80
C+  79–77       C   76–73       C–  72–70
D+  69–67       D   66–60       F   < 60

Homework Assignments

Homework assignments are posted on Blackboard and are due no later than 18:30 on the dates shown in the tentative schedule (see Section M). Late assignments will not be accepted.

Mid-Term Exam

Mid-term exam will take place on the date shown in the tentative schedule (see Section M) in Robertson B113. The exam will commence at 13:30 and end at 16:00. This is an open-book exam. You are allowed to use your notes and homework assignments. The only allowed electronic resources are the Blackboard course website, scientific calculator, and the MATLAB software. Other software and websites are strictly prohibited.

ACS Exam

The ACS exam will take place on the date shown in the tentative schedule (see Section M) in Malloy 019. The exam will commence at 13:30 and end at 15:30. This is a closed-book exam. Calculators and computers are not allowed.

Final Exam

The final exam is comprehensive and will take place on the date shown in the tentative schedule (see Section M) in Robertson B113. The exam will commence at 08:30 and end at 11:00. This is an open-book exam. You are allowed to use your notes and homework assignments. The only allowed electronic resources are the Blackboard course website, scientific calculator, and the MATLAB software. Other software and websites are strictly prohibited.
Important Notice

Please note that all exams must be taken at the scheduled time. No substitute exams will be given. Academic honesty is expected. Any questionable conduct will be treated as dishonest behavior. Please see the current undergraduate catalogue for details concerning the University’s policy on academic dishonesty.

H. CLASSROOM RULES OF CONDUCT

1. Silence or disable cell phones in class.
2. Use of cell phones for texting or browsing the web in class is prohibited.
3. Use of the desk computer for social activities in class is prohibited.
4. Class attendance is highly recommended.

I. HOW TO TAKE THIS COURSE

This is a very mathematically challenging and demanding course. You will be applying the material you have covered in your previous mathematics, physics, and chemistry courses to solve problems in thermodynamics and kinetics. The key to success is organization:

- Review the material you have covered in your previous courses. Once you know the basics, then it is just a matter of applying the basics to new concepts, definitions, etc.
- Attend classes.
- Follow the slide presentation on your computer or in print, annotating it with the important notes that are mentioned in class. The slide presentations will be posted on Blackboard a day before presentation.
- Work through the example problems as they are presented in class. After class, work through them again.
- Do, understand and know how to solve all problems in the homework assignments.
- Some students find it effective to work in study groups. This is highly encouraged and recommended. But remember: do not copy other people’s work; you will not learn anything.
- See me if you are unsure about anything. I keep an open-door policy.

J. ACCOMODATIONS AND DISABILITY

Any student with a documented disability requiring accommodations in this course is encouraged to contact me after class or during office hours. Additionally, students will need to contact Counseling and Disability Services in Crooker Center. This office can be reached at (713) 525–6953/3162

K. ABOUT YOUR PROFESSOR

I am an associate professor in the Department of Chemistry and Physics. I teach general chemistry, quantum chemistry, and thermodynamics and kinetics. My research interest is on fuel science and technology, with a particular focus on pyrolysis, gasification, and combustion of fossil fuels and biomass. My interests outside of academia are landscape and nature photography, camping and hiking, classical Latin and Greek, Baroque music, and the performing arts.
## L. TENTATIVE SCHEDULE

<table>
<thead>
<tr>
<th>Date</th>
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<th>Topic</th>
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<tr>
<td>JAN 20</td>
<td>FRI</td>
<td>1 Material Balances</td>
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<td>2 Energy Balances: First Law of Thermodynamics</td>
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<td>3 Entropy Balances: Second Law of Thermodynamics</td>
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<td>27</td>
<td>MON</td>
<td>4 Thermodynamic Processes and Cycles</td>
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<td>20</td>
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<td>6 Phase Equilibrium and Mixtures</td>
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