CM3230
Thermodynamics for Chemical Engineers

Curricular Designation: Required

Catalog Description:

First and second law applied to closed and open systems. Topics include energy conversion, power cycles, entropy and enthalpy calculations on engineering systems; property estimation for non-ideal vapors, liquids, and other substances, non-ideal multicomponent equilibria, chemical reaction equilibria.

Credits: 4.0, Lec-Rec-Lab: (4-0-0), Semesters Offered: Fall, Spring

Prerequisites:

- CH 3510 - Physical Chemistry I - Thermodynamics, Equilibrium and Kinetics
- MA 3160 - Multivariable Calculus with Technology and
  (MA 3520(C) - Elementary Differential Equations or
  MA 3521(C) - Elementary Differential Equations or
  MA 3530(C) - Introduction to Differential Equations or
  MA 3560(C) - Mathematical Modeling with Differential Equations)

Textbooks(s) and/or Other Required Materials:


Course Objectives

1. Master the principles of thermodynamics of ideal and non-ideal mixtures of gases and liquids;
2. Master the principles of the fundamental equations governing thermodynamics: e.g., the Maxwell equations, equations of state;
3. Master the application of energy balances on process systems recognizing the constraints implied by the second law;
4. Familiarity with heat engines and common gas-cycle engines.
5. Familiarity with the analysis of Rankine and refrigeration cycles;
6. Mastery of the principles and application of fugacity and activity coefficients to non-ideal multiphase equilibrium;
7. Mastery of the application of thermodynamics principles to common chemical engineering process problems;
Topics Covered:

1. Introduction and Basic Concepts
   - Systems, boundaries and surroundings
   - Intensive and extensive properties
   - PVT surface for pure substances
   - Steam tables
   - Ideal Gas Law

2. First Law of Thermodynamics
   - Forms of energy: kinetic, potential and internal
   - Modes of energy transfer: work and heat
   - Reversible and irreversible processes
   - First law for closed systems
   - Enthalpy and first law for open systems
   - Thermochemical data: heat capacity, latent heats and heats of reaction
   - Application to process equipment
   - Thermodynamic Cycles: Carnot and Rankine Cycles

3. Entropy and Second Law of Thermodynamics
   - Entropy
   - Second law of thermodynamics
   - Application to closed systems
   - Application to open systems
   - Entropy change for ideal gas systems
   - Mechanical energy balances
   - Power cycles and refrigeration cycles: efficiencies and COP

4. Equations of State (EOS)
   - Principle of corresponding states
   - Van der Waals EOS
   - Cubic EOS: Redlich-Kwong, Peng-Robinson, Soave-Redlich-Kwong
   - Virial EOS: Beattie-Bridgeman, Benedict-Webb-Rubin
   - EOS for liquids and solids
   - Generalized compressibility charts: Lee-Kesler

5. Thermodynamic Properties and Relationships
   - Fundamental properties
   - Maxwell relations and cyclic rules
   - The thermodynamic web
   - Change in thermodynamic properties based on EOS
   - Departure functions
   - Joule-Thomson expansion and liquefaction

6. Phase Equilibria 1
   - Phase equilibrium criteria for pure substances
   - Application: Clapeyron equations
   - Partial molar properties
   - Gibbs-Duhem equations
   - Property changes of mixing
   - Determination of partial molar properties
7. Phase Equilibria 2
   - Fugacity: definition
   - Fugacity in vapor phase
     - Fugacity coefficients
     - Mixing of ideal gases
   - Fugacity in liquid phase
     - Ideal Solutions (Lewis/Randall) and Henry’s Law
     - Activity coefficients
     - Excess Gibbs energy
     - Models for binary activity coefficients: Margules, Van Laar, Wilson, NTRL
   - Fugacity in solid phase

8. Phase Equilibria 3
   - Vapor-liquid equilibrium
     - Raoult’s Law
     - Bubble-point and dew-point calculations
     - Non-ideal liquids and azeotropes
     - Applications for flash and distillation process
     - Activity coefficients from VLE data
     - Solubility of gases in liquids
     (As time allows)
       - Liquid-liquid equilibrium
       - Vapor-liquid-liquid equilibrium
       - Solid-liquid and solid-solid equilibrium
       - Colligative properties

9. Chemical Reaction Equilibria (brief discussions only and as time allows)
   - Equilibrium for single reaction
   - Equilibrium constants and their temperature dependence
   - Heterogenous reaction
   - Multiple reactions
   - Gibbs phase rule
   - Reaction equilibria via minimization of Gibbs energy

Class/Laboratory Schedule: Class: 3 hours/week for 14 weeks

Contribution of Course to Curriculum: Engineering and Science
<table>
<thead>
<tr>
<th>Outcome</th>
<th>Contribution</th>
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<tbody>
<tr>
<td>a) An ability to apply knowledge of mathematics, basic science and engineering science</td>
<td>Substantial</td>
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<td>b) An ability to design and conduct experiments as well as to analyze and interpret data</td>
<td>Minimal</td>
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<td>c) An ability to design a system, component or process to meet needs within realistic constraints</td>
<td>Minimal</td>
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<td>d) An ability to function on multidisciplinary teams</td>
<td>Minimal</td>
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<td>e) An ability to identify, formulate, and solve engineering problems</td>
<td>Substantial</td>
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<td>f) An understanding of professional and ethical responsibility</td>
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<td>g) An ability to communicate effectively</td>
<td>Minimal</td>
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<tr>
<td>h) The broad education necessary to understand the impact of engineering solutions in a global, economic, environmental, and social context.</td>
<td>Moderate</td>
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<tr>
<td>i) A recognition of the need for, and the ability to engage in lifelong learning</td>
<td>Moderate</td>
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<td>j) A knowledge of contemporary issues</td>
<td>Minimal</td>
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<tr>
<td>k) An ability to use the techniques, skills, and modern engineering tools necessary for engineering practice</td>
<td>Substantial</td>
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**Prepared by:**

Assoc. Prof. Tomas Co  
February 8, 2017