Stevens Institute of Technology
Syllabus

Course Number: CHE 620-MT 603

Chemical and Materials Engineering Thermodynamics
Fall 2016

Monday, 6:15-8:45 PM in Pierce-116

No class on Monday, September 05 (Labor Day)
No class on Monday, October 10 (Columbus Day).
Class on Tuesday, October 11 (Monday schedule).
Last day of classes will be on December 09.

http://goo.gl/yeQzr

Professor: Simon Podkolzin **Office:** Burchard 426 **E-mail:** Simon.Podkolzin@Stevens.edu	**Office Hours:** Tuesday 4-7 pm

Overview

The course will employ lectures, class discussions, class presentations and homework. Participation in class discussions is expected from every student.

Students are expected to complete a midterm test, an individual term project with a class presentation, and a final exam.

Homework will be assigned each week.

Textbooks

Required: H.W. Tester and M. Modell, "Thermodynamics and Its Applications", 3rd Edition, Prentice Hall, ISBN: 978-80139153563

Recommended: Terrell L. Hill, "An Introduction to Statistical Thermodynamics", Dover Publications, ISBN: 978-0486652429

Optional. Only l*ectures on Thermodynamics of Surfaces will be based on this book, and lecture notes will be provided:* Richard I. Masel, "Principles of Adsorption and Reaction on Solid Surfaces", Wiley-Interscience, ISBN: 978-0471303923.

Grading

1. Class participation	5
2. Class presentation	15
3. Homework	24
4. Midterm test	23
5. Final exam	33

Letter grades will be assigned based on the absolute scale:

A	91-100
A-	86-90
B+	81-85
B	75-80
B-	70-74
C+	65-69
C	60-64
C-	55-59
D+	50-54
F	below 50

Testing

Class tests and the final exam will be open book, open notes. You do not have to memorize lengthy formulas or definitions. You do, however, need to understand the material and know how to apply it for solving problems. If you do not know the material, you will run out of time on the tests.

Grading

Homework is due at the beginning of the class. No late homework will be accepted for any reason. If you unable to attended the class and still want to submit your homework, please scan and send it by email as an Adobe pdf file. You can miss one homework assignment and still receive full credit for it. If you submit all homework assignments, your lowest homework score will be adjusted to 100%.

CHE 620 - MT 603

Chemical and Materials Engineering Thermodynamics

1. The Scope of Classical Thermodynamics

2. Basic Concepts and Definitions

- 2.1. System and Boundaries
- 2.2. Primitive Properties
- 2.3. Classification of Boundaries
  - 2.3.1. The Adiabatic Wall
  - 2.3.2. Simple and Composite Systems
- 2.4. State of a System
- 2.5. Stable Equilibrium States
  - Postulate I
  - Postulate II
- 2.6. Thermodynamic Processes
- 2.7. Derived Properties
- 2.8. Nomenclature and Units

3. First Law

- 3.1. Work Interactions
- 3.2. Adiabatic Work Interactions
- 3.3. Energy
- 3.4. Heat Interactions
- 3.5. The First Law for Closed Systems
  - 3.5.1. Specific Heats
  - 3.5.2. Standard States
  - 3.5.3. Heats of Reactions
  - 3.5.4. Heats of Formation
  - 3.5.5. Process Calculations for the Ideal gas
- 3.6. The First Law for Open Systems
  - 3.6.1. Applications of the First Law for Open Systems

4. Second Law

- 4.1. Heat Engines
- 4.2. Reversible Processes
- 4.3. Thermodynamic Temperature
- 4.4. The Theorem of Clausius
- 4.5. Entropy
- 4.6. Internal Reversibility
- 4.7. Combined Statement of First and Second Law for Closed Systems
- 4.8. Reversible Work of Expansion or Compression in Flow Systems
- 4.9. The Chemical Potential
  - 4.9.1. Introduction of the Chemical Potential
  - 4.9.2. Extensive Properties
  - 4.9.3. Partial Molar Properties

- 4.9.3.1. Definition and Relationships
- 4.9.3.2. Graphical Representation: The Method of Intercepts
- 4.9.3.3. Independent Variables

5. The Calculus of Thermodynamics

- 5.1. Fundamental Equations
- 5.2. Intensive and Extensive Properties
- 5.3. Methods for Transforming Derivatives
- 5.4. Legendre Transformations
- 5.5. Non-Simple Systems

6. Equilibrium Criteria

- 6.1. Classification of Equilibrium States
- 6.2. Derivations of the Conditions of Equilibrium in a Heterogeneous System
    - 6.2.1. Membrane Equilibrium
    - 6.2.2. Phase Equilibria
    - 6.2.3. Chemical Reaction Equilibria
- 6.3. Applications of the Conditions of Equilibrium in a Heterogeneous System
    - 6.3.1. Examples
    - 6.3.2. Common Tangent Construction
    - 6.3.3. Phase Rule

7. Stability

- 7.1. Stable and Unstable Equilibria
- 7.2. One-Component System
    - 7.2.1. Gibbs Free Energy Function
    - 7.2.2. Clausius-Clapeyron Equation
    - 7.2.3. Triple Points
    - 7.2.4. Critical Points
- 7.3. General Discussion of Stability Conditions with Respect to Infinitesimal Fluctuations
- 7.4. Stability Criteria for Infinitesimal Fluctuations
- 7.5. Spinodal Line and Critical Point
- 7.6. Thermodynamic Calculations Associated with the Nucleation and Growth of Precipitates
    - 7.6.1. Free energy Changes
    - 7.6.2. Selection of the Displacement Variable
    - 7.6.3. Driving Forces

8. Properties of Pure Materials

- 8.1. Fundamental Equations
- 8.2. PVT Behavior of Pure Fluids and the Theorem of Corresponding States
- 8.3. PVTN Equations of State
    - 8.3.1. Cubic Equation of State
    - 8.3.2. Volume Translated Cubic Equation of State
    - 8.3.3. Hard-Sphere Equation of State
    - 8.3.4. Virial Expansions

11. Chemical Equilibria

11.1. Problem Formulation and General Approach
11.2. Conservation of Atoms
11.3. Non-Stoichiometric Formulation
11.4. Stoichiometric Formulation
11.5. Equilibrium Constants
11.6. The Phase Rule for Reacting Systems
11.7. Effect of Chemical Equilibrium on Thermodynamic Properties
11.8. Le Chatelier Principle

12. Introduction to Statistical Thermodynamics

12.1. Statistical-Mechanical Ensembles and Postulates
12.2. Ideal Monoatomic Gas
12.3. Ideal Monoatomic Crystals
12.4. Lattice Statistics
12.5. Chemical Equilibrium
12.6. Chemical Reaction Rates

13. Thermodynamics of Solid Surfaces

13.1. Crystal Planes, Surface Reconstruction and Relaxation
13.2. Energetics of Adsorption, Gas Adsorption Isotherms
13.3. Reactions on Solid Surfaces
13.4. Rate Laws for Surface Reactions And Chemical Kinetics
13.5. Rates And Mechanisms of Surface Reactions