



Universidad de Santiago de Chile
Departamento de Ingeniería Química
Programa de Magister en Ciencias de la Ingeniería

Course: Advanced Thermodynamics for Chemical and Process Engineering

Prof. Julio Romero

Units

- 1) A critical review of concepts, fundamentals and definitions
- 2) Thermodynamic properties determination by using equations of state
- 3) Phase Equilibrium
- 4) Thermodynamic aspects of high pressure applications
- 5) Surface processes: advanced topics on adsorption
- 6) Topics of Electrochemistry
- 7) Thermodynamic approach to microscopic processes

Contents

Unit 1: A critical review of concepts, fundamentals and definitions

- Definitions of system, property, state, process, work, heat and energy
- What's the entropy?
- Concepts of Gibbs Energy, Helmholtz Energy, chemical potential and activity
- Thermodynamic equilibrium in common phenomena: when are you using thermodynamics?

Unit 2: Thermodynamic properties determination by using equations of state

- Presentation of different cubic equations
- Applications of modern equations of state (EOS): SRK, Dieterici, PR, etc.
- Special equations for specific types of compounds or calculations

Unit 3: Phase Equilibrium

- UNIFAQ, UNIQUAC and Modified ASOG method to estimate vapour-liquid equilibrium (VLE)
- Applications in solid-gas equilibrium
- Liquid-liquid equilibrium

Unit 4: Thermodynamic aspects of high pressure applications

- What's a supercritical fluid?
- Main applications of near-critical and supercritical fluids (carbon dioxide, water and propane)
- Determination of properties in near-critical and supercritical conditions
- Dense gas extraction
- Chemical reaction under high pressure conditions
- Other applications (particle and thin film formation, pasteurization, bioprocesses)

Unit 5: Surface processes: advanced topics on adsorption

- Deduction of sorption isotherms (Langmuir, Freundlich, Temkin, BET and GAB model)
- New classification of sorption isotherms
- Adsorption in microporous materials
- Adsorption effects in mass transfer
- New applications considering thermal aspects

Unit 6: Topics in Electrochemistry

- Debye-Hückel Theory
- Concepts of ionic atmosphere, charge density, ionic strength and mean activity coefficient
- Electrodes and its applications

Unit 7: Thermodynamic approach to microscopic processes

- Interest in microscopic processes: nanotechnology
- Microscopic interactions: some cases

References

J.M. Smith, H.C. Van Ness, and M.M. Abbott, Introducción a la Termodinámica en Ingeniería Química, 6º Ed. McGraw-Hill (2003)

L. Pauling "General Chemistry" Dover (1970)

P. W. Atkins "The Elements of Physical Chemistry" Oxford University Press (1993)

I. N. Levine "Physical Chemistry" McGraw-Hill (1995)

D. L. Goodstein "States of Matter" Dover (1985)