Aalto University

CHEM-E6105 Thermodynamics of solutions

Introduction

January 2024

Teaching of Chemical Thermodynamics for Metallurgists at Aalto University

Fundamentals of Chemical Thermodynamics – CHEM-E6100:

- General concepts of laws of thermodynamics
- Thermodynamic properties of materials and how different properties are connected
- Simple energy balances and chemical equilibrium between pure phases and gas

Thermodynamics of solutions – CHEM-E6105:

- Thermodynamics of mixtures and solutions (e.g. alloys, slags, gases)
- Important concepts: Partial thermodynamic properties, chemical potential, Gibbs-Duhem law, regular solution, activity coefficients, non-ideal solutions
- Chemical equilibrium between multicomponent phases (slag-matte-gas), trace element behavior

Thermodynamics of Modeling and Simulation – CHEM-E6115:

- Project work related to determining thermodynamic properties from experimental data
- Important concepts: Phase diagrams, Experimental techniques for thermodynamic and equilibrium measurements, solution models
- Calculation of phase diagrams based on own databases

General

- **Course personnel**
  - Prof. Daniel Lindberg
  - Senior lecturer Jari Aromaa (tutorials and workshops)

Contents

Thermodynamics of solution phases and their analytical forms in condensed systems,

Use and development of analytical (Gibbs energy) descriptions for solution phases

Applications of Gibbs energy minimisation techniques for chemical process simulations.

Course material:

A. Pelton, Phase Diagrams and Thermodynamic Modeling of Solutions

https://www.sciencedirect.com/book/9780128014943/phase-diagrams-and-thermodynamic-modeling-of-solutions

D. Gaskell, Introduction to the thermodynamics of materials, 4. Ed., Taylor & Francis, 2003, UK.

Learning outcomes

After the course the student can

- Understand and calculate thermodynamic mixing properties and partial properties
- Understand the thermodynamic properties of solutions, and calculate chemical equilibria involving non-ideal phases
- Understand the structure of a thermochemical solver (i.e. a Gibbs energy minimiser).
- Handle equilibria in heterogeneous multi-component (non-ideal) systems.
- Do equilibrium simulations in multi-component heterogeneous systems.

General - workload

- **Course is composed of lectures, tutorials and project work**

- **Lectures 12 h,**
  - Tuesdays 12-14, 9.1, 16.1, 23.1, **30.1**, 7.2, 14.2

- **Tutorials 24 h**
  - Wednesdays 10-12 & Thursdays 12-14

- **Project (home) work 37 h**
  - Three separate tasks to be completed in 2 or 3-person teams; deadline in IV period (to be announced later)

- **Independent (group) studies 62 h**

Course evaluation

Examination (50%) – max 30 points

Project work (40%) – max 3 x 8 points = 24 points

Weekly quizzes (10%) – max 6 x 1 points = 6 points

Course exam 20.2.2021 at 9-13

Additional 1 point if over half of the participants hands in official course feedback

To pass the course, minimum 30 points are needed

Skills needed

- **General chemical thermodynamics, inorganic and physical chemistry form the key disciplines and they are the necessary background of the course.**

Course information

- **Mainly through myCourse portal and in lectures as well as tutorials**

- **Exam and workshop marks will also be posted in MyCourses**

Study materials

- **The lecture hand-outs will be available as pdf files in myCourses**

- **Textbook:**
- **A. Pelton, Phase Diagrams and Thermodynamic Modeling of Solutions**

https://www.sciencedirect.com/book/9780128014943/phase-diagrams-and-thermodynamic-modeling-of-solutions

- **D.R. Gaskell, Introduction to the Thermodynamics of Materials (4th or 5th edition); available to you as e-book in the Aalto library**

- **Written docs in tutorials**