Aalto University

CHEM-E6115
Thermodynamics of modeling and simulation

Introduction

Spring 2021

CHEM-E6115 Thermodynamics of Modeling and simulation (5 cr)

Responsible teacher:
Professor Daniel Lindberg

Learning outcomes

- After the course the student can
  - Describe industrial problems as a system, in terms of its thermodynamic variables
  - Use thermochemical properties of systems and their analytical expressions in the simulation of properties and processes
  - Analyse and model experimental data in chemical equilibrium calculations
- The course deepens the contents of the courses “Fundamentals of Chemical Thermodynamics” (E6100) and “Thermodynamics of solutions” (E6105) in thermodynamic analysis of experimental data

Teaching methods

- Lectures
- Tutorials and guided assessments
- Project work in groups of two from a selected individual topic, including reporting
- Independent study and exam
- Prerequisite knowledge: “Fundamentals of Chemical Thermodynamics” and “Thermodynamics of solutions” or similar courses
- Course materials
  - A. Pelton, Phase Diagrams and Thermodynamic Modeling of Solutions
  - https://www.sciencedirect.com/book/9780128014943/phase-diagrams-and-thermodynamic-modeling-of-solutions
  - Handouts from lectures
  - Selected papers and presentations from http://www.crct.polymtl.ca/courses.html

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

Course information

- Mainly through myCourse portal and in lectures as well as tutorials
- Group e-mails from WebOodi will be used if necessary

- Exam and workshop marks will also be posted in MyCourses

Course personnel

- Prof. Daniel Lindberg (Daniel.k.Lindberg@aalto.fi)
- Mr David Sibarani (David.sibarani@aalto.fi)

Work load

- Lectures 8 h
- Tutorials 8 h
- Project (home) work 57 h
- Independent (group) studies 58 h
- Project seminar

Project work

- Thermodynamic assessment of a binary metallic, oxide or halide system (or other suitable systems) – Calphad modeling
  - Develop a database to calculate thermodynamic properties and phase equilibria based on literature experimental data
  - Model the thermodynamic properties of a binary system, including non-ideal solution properties of the liquid phase and optimize the solution parameters
  - Utilize database for process simulation
  - Write a report on the study
  - Present the work at a seminar in May

Course evaluation

- Examination (25%)
- Project work (75%)
- All must be ’passed’.

Schedule

- 9.3.2021: Introduction
- 16.3.2021: lecture
- 23.3.2021: lecture – move to 24.3.2021
- 30.3.2021: lecture/introduction of project work
- Exam 14.4.2021 at 9 o’clock
- Presentation of project work – mid/end of May
- Deadline for project work – end of May