



Aalto University

CHEM-E6115

Thermodynamics of modeling and simulation

Introduction

Spring 2022

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

Course personnel

- Prof. Daniel Lindberg (Daniel.k.Lindberg@aalto.fi)
- Dr Willem Malan (willem.malan@aalto.fi)

Work load

- Lectures 10 h
- Tutorials 8 h
- Project (home) work 57 h
- Independent (group) studies 56 h
- Project seminar

Project work

- Thermodynamic assessment of a binary 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

- 8.3.2022: Introduction
- 15.3.2022: lecture
- 22.3.2022: lecture
- 29.3.2022: lecture/introduction of project work
- 5.4.2022
- Exam 13.4.2022 at 9-13 (Wednesday)
- Presentation of project work – mid/end of May
- Deadline for project work – end of May