



COURSE SYLLABUS

Chemical Thermodynamics, 7.5 credits

Chemical Thermodynamics, 7,5 högskolepoäng

Course Code: TCHR21	Education Cycle: Second-cycle level
Confirmed by: Dean Mar 1, 2021	Disciplinary domain: Technology
Valid From: Aug 1, 2021	Subject group: NA9
Version: 1	Specialised in: A1N

Intended Learning Outcomes (ILO)

After a successful course, the student shall:

Knowledge and understanding

- show familiarity with concepts in chemical thermodynamics including the computational thermodynamics
- show familiarity with thermodynamic treatment of interface/surface
- show familiarity with applications of chemical thermodynamics which is required in the advanced courses within the program.

Skills and abilities

- demonstrate skills of (chemical) thermodynamic calculation
- demonstrate the ability to explain the interfacial phenomena in the materials processes.

Judgement and approach

- demonstrate the ability to apply thermodynamic approach to materials processes
- demonstrate the ability to explain the phenomena in the manufacturing processes with the knowledge in chemical thermodynamics.
- demonstrate an understanding of the deviation from the thermodynamic equilibrium from kinetics viewpoint, especially for the phase transformation.

Contents

The course includes:

- Basic theoretical knowledge in chemical thermodynamics, application of chemical thermodynamics and interfacial physical chemistry.
- Calculation of thermodynamic equilibrium (Gibbs energy, van't Hoff isotherm, Ellingham diagram)
- Calculation of activity and activity coefficient (Wagner's equation, Henrian and Raoultian standards, thermodynamic treatment of the solutions)
- Thermodynamic treatments of the surface/interface (Gibbs dividing surface, Guggenheim model, Nucleation) and interfacial phenomena in the high-temperature system.
- Thermodynamic treatments of the phase and phase diagram (Gibbs energy change, phase rule,

etc.).

- Calculations using a thermodynamic calculation software and a multiphysics simulation software (Lab activities).

- Thermodynamics and sustainability (CO₂ emission).

The course contains the following elements:

- Lectures on the advanced thermodynamics, i.e. chemical thermodynamics and

thermodynamics of interface, and its application (some examples in the actual processes).

- Exercises on the chemical thermodynamic calculation.

- Laboratory sessions on chemical thermodynamics.

Type of instruction

Lectures.

Exercises.

Laboratory sessions

The teaching is conducted in English.

Prerequisites

Passed courses at least 90 credits within the major subject Mechanical Engineering, 15 credits Mathematics, and completed course in Materials and Manufacturing, 7,5 credits, proof of English proficiency is required (or the equivalent).

Examination and grades

The course is graded 5,4,3 or Fail.

Registration of examination:

Name of the Test	Value	Grading
Assignments	2 credits	U/G
Written Examination [†]	4 credits	5/4/3/U
Laboratory work	1.5 credits	U/G

[†] Determines the final grade of the course, which is issued only when all course units have been passed.

Course literature

The literature list for the course will be provided one month before the course starts.

Recommended literatures:

- T. Matsushita and K. Mukai, Chemical Thermodynamics in Materials Science – From Basics to Practical Applications –, Springer, 2018.