



# MH2057 Computational Thermodynamics 7.5 credits

## Termodynamisk modellering

This is a translation of the Swedish, legally binding, course syllabus.

If the course is discontinued, students may request to be examined during the following two academic years

## Establishment

The official course syllabus is valid from the autumn semester 2024 in accordance with the decision by the Head of the ITM School: M-2024-1162. Date of decision: 2024-06-14.

## Grading scale

A, B, C, D, E, FX, F

## Education cycle

Second cycle

## Main field of study

Materials Science and Engineering

## Specific prerequisites

For CMATD, at least 90 higher education credits in the main field of study Technology from programme syllabus for year 1-3.

## Language of instruction

The language of instruction is specified in the course offering information in the course catalogue.

## Intended learning outcomes

After passing the course, the student should be able to:

1. Explain important concepts in thermodynamic modelling
2. Use thermodynamic relationships for solution phases (solid phases, liquids and gas phase).
3. Model these phases with simple models and with sub-lattice formalism (Compound Energy Formalism).
4. Illustrate relationships between thermodynamic relations, Gibbs energy and phase diagrams.
5. Carry out analytical and numerical calculations of thermodynamic problems.

## Course contents

- Thermodynamic models for solid phases, liquids and gas phase
- Modelling of solid substitutional and interstitial solution, carbides, oxides and intermetallic phases
- Modelling of metallic melt systems and slags
- The connection between Gibbs energy and phase diagrams
- Readout of units such as chemical potential, running forces etc from molar Gibbs energy diagram
- Reference state and change of reference state and change of components
- Phase diagrams and equilibria
- Computer calculations of equilibria, phase diagrams, running forces etc
- Nomenclature of crystal structures
- Introduction to the Calphad methodology

## Examination

- INL1 - Assignment, 3.5 credits, grading scale: P, F
- TEN1 - Written exam, 4.0 credits, grading scale: A, B, C, D, E, FX, F

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

## Ethical approach

- All members of a group are responsible for the group's work.
- In any assessment, every student shall honestly disclose any help received and sources used.
- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.