UNIVERSITY OF BORÅS

Introduction to Computational Modelling
Introduktion till datormodellering

7.5 credits
7.5 högskolepoäng

Ladok Code: 42RI07
Version: 1.2
Established by: Committee for Education in Technology 2015-12-18
Valid from: Spring 2016

Education Cycle: Second cycle
Main Field of Study (Progressive Specialisation): Chemical Engineering (A1N)
Disciplinary Domain: Technology
Prerequisites: Meets the admission requirements for the Masters programme in Resource Recovery (or equivalent).
Subject Area: Other Subjects within Technology
Grading Scale: Seven-degree grading scale (A-F)

Content

The course deals with thermodynamic properties like enthalpy, entropy and Gibbs energy. Furthermore treated reaction kinetics and molecular modeling, including molecular mechanics modeling, molecular dynamics modeling and Monte Carlo methods. Moreover, emphasis is placed on thermochemical modeling of processes related to resource recovery, eg combustion.

Learning Outcomes

After completing this course, students must be able:
1 Knowledge and understanding
1.1 Give an account of the basics of thermodynamics and chemical equilibrium,
1.2 Give an account of the basics of molecular dynamics and Monte Carlo methods,
1.3 Give an account of the basics of macroscopic modelling in a state of equilibrium,
2. Skills and abilities
2.1 Be able to confidently handle the theory and calculations in thermodynamics and chemical equilibrium,
2.2 Be able to confidently handle the theory and calculations in reaction kinetics,
2.3 Carry out a computer modelling project at the molecular or macroscopic level,
3. Judgement and approach
3.1 Understand the strengths and limitations of computer modelling as a tool in the industry.

Forms of Teaching

Teaching consists of lectures with exercise opportunities and project work.

The language of instruction is English.

Forms of Examination

The course will be examined through the following examination elements:

Exam
Learning outcomes:
Credits: 4
Gradingscale: Seven-degree grading scale (A-F)

Project work
Learning outcomes:
Credits: 3
Gradingscale: Fail (U) or Pass (G)

Learning outcomes:
Credits: 0.5
Gradingscale: Fail (U) or Pass (G)

The module exam determines the final grade which is issued when all components of the course are approved.

Student rights and obligations at examination are in accordance with guidelines and rules for the University of Borås.

Literature and Other Teaching Materials

Recommended literature:
Allen, M. P. & Tildesley, D. J. (1989). Computer simulation of liquids. Oxford: Clarendon
Cramer, Christopher J. (2004). Essentials of computational chemistry: theories and models. 2. ed. Chichester: Wiley
Materials distributed

Student Influence and Evaluation

The Head of Academy and course coordinator are responsible for ensuring that students are invited systematically and regularly to put forward their views on the course. The results of the evaluations will be reported back to the students and will form the basis for the future structure of the course.

Miscellaneous