



Faculty of Health, Science and Technology
Chemistry

Syllabus

Chemistry calculation methods

Course Code:	KEGA51
Course Title:	Chemistry calculation methods <i>Kemins beräkningsmetoder</i>
Credits:	7.5
Degree Level:	Undergraduate level
Progressive Specialisation:	First cycle, has less than 60 credits in first-cycle course/s as entry requirements (G1F)

Major Field of Study:

KEA (Chemistry)
MAA (Mathematics)

Course Approval

The syllabus was approved by the Faculty of Health, Science and Technology 2022-01-31, and is valid from the Autumn semester 2022 at Karlstad University.

Prerequisites

Registered for 60 ECTS credits in Chemistry, with 30 ECTS credits completed, and upper secondary level Mathematics 4, or equivalent

Learning Outcomes

The aim of the course is for students to acquire basic knowledge and skills in chemistry calculation methods.

Upon completion of the course, students should be able to:

1. describe the meaning of the mathematical concepts derivative, differential equation, and integral for selected chemical systems,
2. use basic mathematical concepts in chemical kinetics,
3. use differential equations for selected chemical systems,

4. apply matrix algebra to solve linear equation systems in stoichiometry, kinetics, and spectroscopy,
5. apply polar coordinates and complex numbers in quantum chemistry,
6. explain and use vector analysis to describe dipole moments, force, and flow,
7. relate limit values and asymptotes to chemical systems,
8. describe and use basic statistics, error estimation, and regression analysis for chemical problems,
9. use computer-based methods to solve chemical problems,
10. give an account of and use graphical methods to solve chemical problems, and
11. discuss mathematical problems from the perspective of chemistry.

Content

Instruction is in the form of lectures, exercises, and seminars.

Some components are based on self-study, and it is important for students to be able to read and understand course literature in English.

The course includes a number of integrated parallel components focused on chemical kinetics, chemical reactions, quantum chemistry, spectroscopy, molecular description, statistics, and graphical methods. The following mathematical concepts and methods are covered:

- the definition and calculation principles of the derivative, derivatives of elementary functions, and implicit derivation
- increasing and decreasing functions, polar extremes, asymptotes, and limit values
- primitive functions, partial integration, and integration of elementary functions
- ordinary differential equations to describe the zeroth, first, and second order of kinetics and connected processes
- polar coordinates, complex numbers, linear equation systems, and matrix algebra
- computer-based methods for solving linear equation systems
- graphical methods, both manual and computer-based
- basic statistics, expected value, variance, probability, uncertainty, accuracy, error propagation, and significance

The mathematical concepts and methods are related in the course to calculation methods for chemical systems.

Reading List

See separate document.

Examination

Assessment is based on individual hand-in assignments and individual oral presentations in seminars.

If students have a decision from Karlstad University entitling them to Targeted Study Support due to a documented disability, the examiner has the right to give such students an adapted examination or to examine them in a different manner.

Grades

One of the grades Distinction (VG), Pass (G), or Fail (U) is awarded in the examination of the course.

Quality Assurance

Follow-up relating to learning conditions and goal-fulfilment takes place both during and upon completion of the course in order to ensure continuous improvement. Course evaluation is partly based on student views and experiences obtained in accordance with current regulations and partly on other data and documentation. Students will be informed of the result of the evaluation and of any measures to be taken.

Course Certificate

A course certificate will be provided upon request.

Additional information

The local regulations for studies at the Bachelor and Master levels at Karlstad University stipulate the obligations and rights of students and staff.