

KEMM27, Chemistry: Chemist's Modelling Tools, 15 credits

Kemi: Modellverktyg för kemister, 15 högskolepoäng

Second Cycle / Avancerad nivå

Details of approval

The syllabus was approved by Study programmes board, Faculty of Science on 2007-04-12 and was last revised on 2007-04-12. The revised syllabus applies from 2007-07-01, autumn semester 2007.

General Information

The course is an optional second-cycle course for a degree of Master of Science in Chemistry and is a compulsory course for a degree of Master of Science in Organizing Molecular Matter.

Language of instruction: English and Swedish

When necessary, the course in full is given in English.

Main field of studies

Organizing Molecular Matter

Chemistry

Depth of study relative to the degree requirements

A1N, Second cycle, has only first-cycle course/s as entry requirements

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Learning outcomes

The aim of the course is to provide general knowledge of applied mathematics specialising in chemical problems. The course also aims to familiarise the students with the various computer-based mathematics programmes.

On completion of the course, students shall be able to

- use vector analysis for calculating gradients, applying Gauss and Stokes theorems, and perform vector operations in curvilinear coordinate systems, with applications to molecular problems
- demonstrate familiarity with and use the most common transcendental functions
- formulate and solve application problems with the help of linear algebra in matrix representation

- use numerical analysis programmes for solving simple problems and producing plots
- perform the most common manipulations used for the integral calculation and solution of simple differential equations
- formulate and solve ordinary and partial differential equations, particularly diffusion problems, with the help of transform tables
- carry out simple series expansions, particularly the Taylor expansion
- solve simple problems within the Fourier analysis

Course content

Lectures: Basic theory and overview of illustrative examples.

Exercises: Exercises in practical calculating and problem-solving.

Computer laboratory work: Exercises in the use of mathematical analysis programmes.

Course design

Teaching comprises lectures and compulsory exercises treating theoretical aspects and practical calculation. The lecture block is followed by a compulsory block of computer laboratory work. These are presented orally and in writing.

Assessment

The course is assessed with a written examination. A re-sit examination is offered soon after the examination to students who do not pass.

Subcourses that are part of this course can be found in an appendix at the end of this document.

Grades

Marking scale: Fail, Pass, Pass with distinction.

To be awarded Pass on the whole course, students must pass the examination, pass the laboratory work and computer exercises.

The examination grades are: Pass with Distinction, Pass or Fail. Grades for the compulsory components are: Pass or Fail.

The final grade for the course is determined by the result of the examination.

Entry requirements

To be eligible for this course students must have basic eligibility and at least 90 higher education credits in completed Science courses, including:

- 45 credits of completed courses in Chemistry, including KEM103 General Chemistry 3 15 credits, or
 - 90 credits in physics, including FYS023 Physics 3: General Course 30 credits,
- and

- MAT015 Mathematics for Scientists 1 15 credits or MAT131 Mathematics 1 Alpha 15 credits

Equivalent knowledge that has been gained in another way also provides eligibility for the course.

Subcourses in KEMM27, Chemistry: Chemist's Modelling Tools

Applies from H13

- 0703 Chemist's Modelling Tools, 13,0 hp
Grading scale: Fail, Pass, Pass with distinction
- 0704 Chemist's Modelling Tools, Compulsory Elements, 2,0 hp
Grading scale: Fail, Pass

Applies from H07

- 0701 Chemist's Modelling Tools, 15,0 hp
Grading scale: Fail, Pass, Pass with distinction
- 0702 Chemist's Modelling Tools, Compulsory Elements, 0,0 hp
Grading scale: Fail, Pass