



MJ286V Environment Modeling: Chemical and Physical Fundamentals 7.5 credits

Miljömodellering: kemiska och fysiska processer

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

Course syllabus for MJ286V valid from Autumn 2007

Grading scale

P, F

Education cycle

Second cycle

Main field of study

Language of instruction

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

Intended learning outcomes

The course intends to give the student introductory knowledge and a broad overview of the quantification of important physical and (bio) geochemical processes in natural systems. Special attention is given to processes relevant for current water quality problems and their modelling. After finishing the course, the student should be able to

- Describe the main aims and parts of water quality modelling;
- Describe the key concepts within Environmental Modelling, for example calibration, verification, validation, robustness, model error, oscillation, discretisations, and to distinguish between deterministic and stochastic models;
- Identify dominant processes and carry out sensitivity analyses;
- Mathematically formulate mass-balances for environmental modelling purposes and for simple system solve those analytically or numerically (using EXCEL or SIMILE or similar modelling tools) for steady-state and dynamic conditions (difference equations/differential equations);
- Explain the concepts of advection, diffusion, and dispersion; The student should also be able to formulate these transport processes mathematically and explain their effects on pollutant transport in various natural systems;
- Use dimensionless numbers to choose appropriate model (plug-flow, completely mixed, compartmentalised box model) and for simple cases formulate the model mathematically;
- Predict the key features of breakthrough curves for non-reactive and reactive substances and explain how these are affected by the dominant transport and chemical processes and their model parameterisation;
- Choose appropriate modelling concept for (biogeo)chemical reactions (kinetic, equilibrium, stoichiometric);
- Make and interpret chemical equilibrium diagram, using MEDUSA/HYDRA or corresponding modelling tools, for the assessment of environmental problems;
- Describe chemical equilibrium and predict its effects in natural and anthropogenically affected water systems (acid-base equilibria, redox equilibria, complex formation equilibria, solubility, equilibria, Henry's law equilibria)
- Mathematically formulate (biogeo)chemical kinetics using empirical rate laws, Arrhenius' and Michael-Menten relations, and predict the time evolution of concentration of substances in environmental systems;
- Mathematically couple simple chemical reactions (e.g. sorption and first order decay) with physical transport phenomena;
- Use PHREEQC (or corresponding modelling tool) to solve simple reactive transport problems for ground or surface waters;
- Explain the key aspects of the biogeochemical cycles and be able to evaluate the cycles in terms of turn-over-times, steady-state and dynamics;
- Put up, use and interpret a mathematical model for material cycling in ecosystems
- Put up, use and interpret a mathematical model for the dynamical aspects of ecological systems, including logistic growth, carrying capacity, and oscillations;
- Use the course content to solve modelling problems within environmental chemistry;
- Understand written descriptions of environmental models and on a basic level evaluate such models.

Course contents

Preliminaries of environmental modelling and mathematical quantification. Basic definitions and principles of model development. General formulation of mass balance laws. Material transport. Geochemical equilibrium. Reaction kinetics and dynamic fundamentals of equilibrium reactions. Geochemical master variables. Geochemical intensity and capacity. Fate of inorganic and organic pollutants. Examples of modelling water quality changes, global and local element cycles, and ecosystem dynamics.

Disposition

The course is based on distance learning. Preferably you need to visit KTH minimum 1 time, but additional, voluntary meetings will be arranged.

The course is examined through homework assignments and application exercises, with an obligatory oral presentation. Interactions with fellow students and the teacher is through an internet course platform.

The course language is English and the course runs at a speed of 20 hours of studies per week.

Specific prerequisites

Completed upper secondary schooling within Natural Sciences including very good results in Mathematics, Physics and Chemistry (corresponding to Maths D, Physics B and Chemistry A for Swedish applicants) you must also state knowledge of English.

University studies in Environmental or Geosciences or Environmental Management are required.

Course literature

Preliminary J.L Schnoor Environmental Modeling Course compendium

Equipment

Computer with internet connection + MS Office + Netscape or Internet Explorer or equivalent. Other software to be used in the course will be available on the internet or via the course platform.

Examination

- INL1 - Assignment, 1.0 credits, grading scale: P, F
- INL2 - Assignment, 1.5 credits, grading scale: P, F
- INL3 - Assignment, 1.5 credits, grading scale: P, F
- INL4 - Assignment, 0.5 credits, grading scale: P, F

- PRO1 - Project, 1.0 credits, grading scale: P, F
- PRO2 - Project, 2.0 credits, grading scale: P, F
- RED1 - Report, - credits, grading scale: P, 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.

The course is examined through homework assignments project work. Oral presentation of the project or one of the homework assignments will be required.

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.