ENVIRONMENTAL MODELLING: CHEMICAL AND PHYSICAL FUNDAMENTALS

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Elective course for Master Students of Industrial Ecology

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ENVIRONMENTAL MODELLING: CHEMICAL AND PHYSICAL FUNDAMENTALS

Course Structure

Lectures 24h
Tutorials 24h
Study visit 4h

ECTS 6

Examination method: written examination
oral presentation

- Homework assignments 1+1+1+1 credits
- Application examples (grouped) 1+1 credits

• 5 course parts covering different aspects

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Course parts

A) Basics of Environmental Modelling

B) Transport Processes

C) Bio/geo- chemical Reactions and Radioctivity

D) Application Examples

E) Element Cycles and Ecosystem Modelling

The course intends to give the student introductory knowledge and a broad overview of the quantification of important physical and bio/geo-chemical processes in natural system. Special attention is given to processes relevant for air /environmental and indoor/ quality problems and their modelling.

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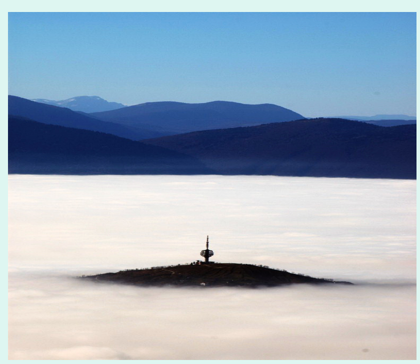
Goals:

- To gain understanding of the fate and transport of chemicals by quantifying their reactions and movement

- To determine chemical exposure concentrations to organisms and/or humans in the past, present, or future

- To predict future conditions under various loading scenarios or management action alternatives



Learning outcomes

After finishing the course, the student should be able to (1):

- *Describe the key concepts within Environmental Modelling, for example calibration, verification, validation, model error, 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 of numerically (using EXCEL or SIMILE or similar software) for steady-state and dynamic conditions;*
- *Explain the concepts of* ***advection, diffusion, and dispersion****; Choose appropriate modelling concept for bio/geo-chemical reactions (kinetic, equilibrium, stoichiometric);*
- *Make and interpret chemical equilibrium diagram, using MEDUSA/HYDRA or corresponding modelling tools, for the assessment of environmental problems;*

Learning outcomes - 2

- *Describe chemical equilibrium and predict its effects in water systems (acid-base equilibria, redox equilibria, complex formation equilibria, solubility, Henry's law equilibria);*
- *Mathematically formulate biochemical 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 corresponding modelling tool to solve simple reactive transport problems for ground or surface waters;*
- *Explain the key aspects of the bio/geo-chemical cycles and be able to evaluate the cycles in terms of turn-over-times;*

Learning outcomes -3

- *Put up, use and interpret a mathematical model for material cycling in ecosystems; and for the dynamical aspects of ecological systems*
- *Understand written descriptions of environmental models and on a basic level evaluate such models.*
- *Mathematically describe turbulent flows and applicate basic models of turbulence for environmental modeling*
- *Accustom the Finite Element anf Finite Volume Methods*
- *Understand and describe the measurement and behaviour of natural radionuclides in environment.*
- *Choose appropriate modelling concept for dispersion of radionuclides in the atmosphere.*

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Course Requirements and Examination

- Passed homework assignments (4 credits)
- Passed application examples (2 credits)

Course grading: marks *from 6 to 10*

Homework assignment A (covers *Basics of Environmental Modelling*)
Homework assignment B (covers *Transport Processes*)
Homework assignment C (covers *Bio/geo-chemical Reactions and Radioactivity*)
Homework assignment E (covers *Eco-Cycles, Ecosystem Modelling*)

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Teaching Methods

- Introduction: Overview
- Check list: Defines detailed aims/objectives
- Study Plan: Defines reading and exercises
- Sub-sections: Guide through Study Plan
- Examination: Defines requirements within the part
- Evaluation

Part A: Basics of Env. Modelling

- A1: The Scope of Environmental Modelling
- A2: Model Thinking: Finding Simplicity in Complexity (SIMILE, EXCEL)
- A3: Mass-Balances
- A4: Calibration and verification

- **Why model?**
- **How model?**
- **Basics of quantifications?**
- **When is the model good enough? How to improve the model? ....**

Part B: Transport Processes

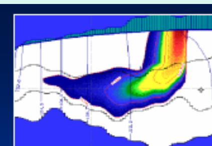
SIMILE
EXCEL

- B1: Advection, Diffusion and Dispersion
- B2: Transport models for Environmental Applications
- B3: Sediment transport
- B4: Suface water transport
- B5: Ground water transport

- Quantifying transport processes
- How choosing type of model
- Transport of solutes with surface and groundwater
- Transport of pollutants in air

Part B: Transport Processes

Advection-Dispersion Equation solved by MT3D

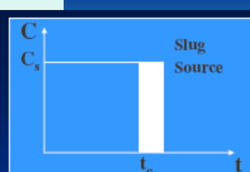


$$\underbrace{\frac{\partial}{\partial x_i}\left[D_{ij}\frac{\partial C}{\partial x_j}\right]}_{\text{Dispersion}} - \underbrace{\frac{\partial}{\partial x_i}(v_i C)}_{\text{Advection}} + \underbrace{\frac{q_s C_s}{\theta}}_{\text{Sink/Source}} - \underbrace{\lambda\left[C + \frac{\rho_b S}{\theta}\right]}_{\text{Reactions}} = \underbrace{R\left[\frac{\partial C}{\partial t}\right]}_{\text{Retardation}}$$

Transport Mechanisms

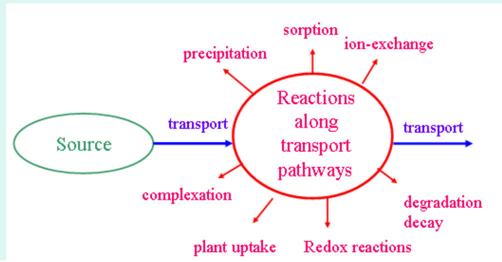
Advection

$$-\frac{\partial}{\partial x_i}(v_i C)$$



- Transport of dissolved solute at the same velocity of groundwater flow (t_c = Distance/v_i)
- The dominant mechanism for most practical plume migration problems
- MT3D calculates v_i using heads and K's from the MODFLOW modeling results

Part B: Transport Processes – in general

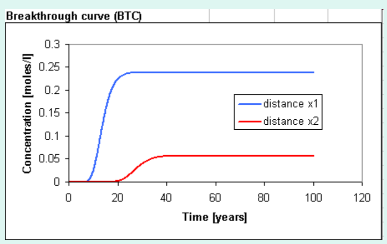


Conceptualise

SIMILE
EXCEL

$$C(x,t)=\frac{C_0}{2}\exp\left\{\left(\frac{x}{2\alpha_x}\right)\left[1-\sqrt{1+\frac{4\lambda\alpha_x}{v}}\right]\right\}erfc\left[\frac{x-vt\sqrt{1+\frac{4\lambda\alpha_x}{v}}}{2\sqrt{\alpha_x vt}}\right]$$

Formulate and solve



Solve
Analyse

Part C: Chemical Processes

SIMILE
MEDUSA

- C1: Bio/geo-chemical equilibria
- C2: Bio/geo-chemical kinetics
- C3: Sources and pathways of environmental radioactivity
- C4: Design and evaluation of environmental radioactivity models

- **How to quantify chemical reactions**
- **Occurance form(s)?**
- **Radioactivity and protection.**

Part D: Application examples

Part: Project work

Students choose their own theme(s):

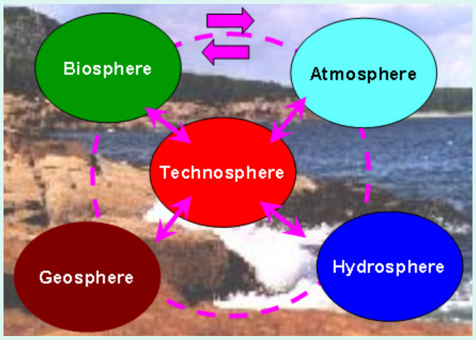
?

- Organic pollutants
- Trace metals
- CO_2 and global warming
- Own project related to quality
  of air and post- war pollution and radioactivity

The purpose of the project in Part D of the course is to get acquainted with a couple of Environmental Modelling applications. Focus will be on air quality modelling and environmental effects of the technosphere.

Part E: Element cycles and Eco system modelling

SIMILE



E1: Element cycles and global change

E2: Ecosystem modelling

E3: Ecological modelling

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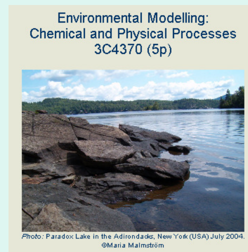
Course Homepage

http://www.mef.unsa.ba/ie/Program/MScProgram/tabid/154/Default.aspx

Master program: Industrial Ecology



KTH course page : http://www.ima.kth.se/im/3c4370

Course material is in English.

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Course Timetable

- ????

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Course Literature

- Schnoor J.L., Environmental Modeling: fate and transport of pollutants in water, air, and soil, 1996. ISBN 0471124362

- Baxter M., Radioactivity in the Environment, 2005. ISBN-13: 978 0 08 044300 3

- H K Versteeg & W Malalasekera: an Introduction to Computational Fluid Dynamics, 1995.ISBN 0-582-218845-5

- Extra material will be distributed at the starting meeting (also available through the course web site)

Meet our team !

Rajfa Musemić
Faculty of Mechanical Engineering UNI Sarajevo
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- Physical Engineering degree (Faculty of Natural Sciences, SA)
- MSc in Applied Mechanics of Continuum
- (Mechanical Engineering Faculty, SA)
- PhD In Applied Physics / Fluid Mechanics (Mechanical Engineering Faculty Ljubljana, SLO)
- Assoc Professor at Mathematics and Physics department (MEF) since 2004

Teaching:
- General Physics
- Mathematical Methods in Physics
- Physics 1 and Physics 2
- Technical Physics
- Modelling of transport processes
  - Turbulence /MSc course/

Research:
- Biophysics
- Solar energy, salt solar ponds
- Mathematical modeling of turbulence
- Turbulent Double-Diffusive Convection

Aida Šapčanin,
Faculty of Pharmacy UNI Sarajevo
ida@bih.net.ba

- Chemical Engineering degree (Faculty of Natural Sciences, SA)
- M.Sc in Analytical chemistry (Faculty of Natural Sciences, SA)
- Ph.D. in Analytical chemistry (Faculty of Natural Sciences, SA)

Teaching:
- Analytical Chemistry
- General Chemistry
- Inorganic Chemistry
- Organic and Biochemical Analysis

Research:
- Analysis of biological samples
- Antioxidant capacity
- Utilization of ORAC method in food chemistry
- Analytical methods in neuroscience

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- Question ?