CIV ENV 448: *Computational Chemodynamics* (Winter 2023)

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Mo&We 16:00-17:50 am in Tech. Room A110
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Course Overview: *"Declare the past, diagnose the present, predict the future"* . This statement by Hippocrates of Kos defines the needs of developing mathematical models to simulate the fate of chemical in the environment. The primary focus of this course is to present the mathematical and computational foundations to develop such models. Many models used to describe environmental systems are available, yet one needs to understand their basic building bricks/blocks upon which they are based. The course is designed to provide an overview of **numerical methods** and **computational tools** for developing and solving simple environmental models simulating chemical, biological and transport processes for understanding the fate of contaminants in the environment.

1 Course Objective

The objective of the course is to integrate and apply the knowledge and skills that you have acquired in previous courses – *i.e.*, the core of the MS/PhD program in Environmental Engineering, namely: CIV ENV 361-1, 367, 440 – Environmental Microbiology, Chemical Processes in Aquatic Systems, Transport Processes, and provide an introduction to surface chemistry. In this course you will develop/review mathematical "intuition/reflexes" coding skills for performing simulations based on various type of models. These skills have now become very valuable for working in an environmental consulting firm as well as doing independent investigations in a research group. It also builds on your prior exposure to computational methods using Python and the Jupyter notebook interface.

2 Course Outcomes

Upon completion of this course students will be able to:

1. Understand and master the basic principles that control the environmental fate of chemical compounds
2. Use numerical methods to perform equilibrium and dynamic calculations
3. Interpret the results of computer simulations
4. Use modeling approaches to simulate either linear or non-linear systems
5. Determine parameters using least-square methods in linear and non-linear cases
6. **Write JuPyteR notebooks** to code and document the fate of chemicals – pollutants, nutrients, tracers,... — in the environment.

3 Reading Material

- Reference Book: *Introduction to Systems Analysis* by Dieter M. Imboden and Stefan Pfenninger, Springer (2013). See CANVAS for the link to download a pdf version of this book.
- Other books are available as the one above for the Northwestern community on Springer Verlag. Will demonstrate in class how to get them.
- **Supplemental Readings**: Scientific contributions – published papers in scientific journals – will be added to CANVAS during the course of this class. Based on the analysis of these papers, models will be constructed and simulations performed.

4 Computer Programming/Use

- All the computational part will be conducted by developing JuPyteR notebooks using Python as the programing language. Please make sure that the Anaconda/Conda complete distribution of Python is still present on your computer, if not then download it again from `https://www.anaconda.com/download/`. Please install the current version of Python 3.X – I am currently working with Python 3.9, but earlier one should work as well. Python is "free software"/freeware and provides many graphical possibilities, as you must know by now.
- Other programming tools previously used can be useful, notably ChemEql.

5 Grading

Final Grade = Problem Sets(40%) + Midterm (30%) + Final project (30%)

- **Participation to all classes in person is mandatory**, as you will work in groups during class on some simple assignments. The session on Wednesday will be dedicated in part to discussing the papers, as we advance during the course. In this course, I want to promote discussions about the different ways to write and document code. I know that everyone is not at the same level hence "coming to class", asking questions is important, proposing solutions, and debugging the code of others is how one learns.
- Problem Sets (40%): Up to 4 problem sets will be given through the course.
- Midterm (30%): After the first five weeks of classes, a take home Midterm will be distributed on Wednesday and due the following Monday.
- Final project (30%): *The code that you always wanted to write but never dare to start!*

6 List of Topics Covered

The following list, and its order, is subject to change, depending on how well we can progress through the quarter. I am also open to any ideas about topics that you would like to cover in this course about various computational approaches.

Topics	**Material Expected to be Covered**
Topic # 1	Introduction: A few words about "Chemodynamics" and mathematical models
Topic # 2	Computing Chemical Equilibria: *i.e.,* Besides ChemEql, review of chemical speciation models and how they work.
Topic # 3	Application: Equilibrium Modeling, solving for non-linear systems using the Newton-Raphson method.
Topic # 4	Surface Complexation Models: Solving for the Poisson-Boltzmann equation & the assumptions behind SCMs
Topic # 5	Finding parameters: Using least-square approaches to determine parameters from experimental data.
Topic # 6	Box Models & Well Mixed-Reactors: A first look at linear chemical cycles
Topic # 7	Environmental Kinetics & Reaction Pathways and solving non-linear reaction networks
Topic # 8	Some solutions methods for the Advection–Diffusion–Reaction (ADR) equation
Topic # 9	Microbe/Substrate Modeling: Solving for Monod type kinetics
Topic # 10	Ecological Models: Predator-Prey & Food Webs