CIV ENV 367: Chemical Processes in Aquatic Systems

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MoWeFr 9:00 – 9:50 in Tech Room #A110
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Discussion: Th 12:30 – 13:50 in Tech Room #M177
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Abstract: The distribution and the cycling of chemical elements and their compounds in aquatic, soil and atmospheric environments are controlled by biotic (biological) and abiotic (chemical) processes. The purpose of this course is to introduce you to the theoretical framework needed for understanding and predicting the chemical composition of natural and engineered systems. This knowledge will be applied to investigate chemical processes using primarily a chemical equilibrium approach.

1 Course Objective

This course presents a method for solving simple and complex chemical equilibrium problems in aqueous solutions. The goal of the first classes is therefore focused on learning that method. Since it is an equilibrium based approach, a short review of chemical thermodynamics is presented. During this quarter we will then explore various processes taking place in environmental compartments with a focus on aquatic systems.

2 Course Outcomes

Upon completion of this course students will be able to:

- Understand the **"tableau" method** used for solving equilibrium problems.
- Master a computer program to find the solution of complex equilibrium problems.
- Derive and use chemical thermodynamics laws & principles to determine how equilibrium properties vary with T and P.
- Determine the pH of a variety of aqueous solutions, *i.e.*, containing multiple acid/base species, and gain a detailed understanding of the carbonate system.
- Compute the chemical speciation of metals in complex aqueous systems.
- Determine the composition of natural waters at equilibrium with various mineral phases.

For the engineering student, the course primarily supports the following ABET program outcome criteria:

(1) An ability to identify, formulate, and solve complex engineering problems by applying principles of Chemistry.

In addition it provides some support to address:

- (3) An ability to communicate effectively with a range of audiences
- (5) An ability to function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives
- (6) An ability to develop and conduct appropriate experimentation, analyze and interpret data, and use engineering judgment to draw conclusions
- (7) An ability to acquire and apply new knowledge as needed, using appropriate learning strategies

3 Class notes & Textbooks

No formal textbook is required. I have developed a series of notes as pdf slides that will be distributed through CANVAS in advance of our class meeting times. Classes will then be devoted to interactive Q&A as well as examples of problem solving.

If you see the need to refer to a textbook you will find below a list of books that I recommend, ranked by how they are related to the material presented in this course:

1. Principles and Applications of Aquatic Chemistry, *Morel F.M.M. and Hering J. (1993), Wiley.* [1]
2. Below is a list of other books that you may want to consider:
   (a) Aquatic Chemistry: Chemical Equilibria and Rates in Natural Waters, *Stumm W. and Morgan J. (1996), 3rded., Wiley.* [2]
   (b) Water Chemistry, *Benjamin M.M. (2015), 2nded, Waveland Press* [3]
   (c) Water Chemistry: An introduction to the Chemistry of Natural and Engineered Aquatic Systems. *Patrick L. Brezonik & William A. Arnold (2011) Oxford.* [4]
   (d) Aquatic Chemistry Concepts, *Pankow J.F. (2019), 2nded, CRC Press*[5]

4 Prerequisites – for undergraduates –

- General Chemistry: CHEM 132 or Accelerated/Advanced General Chemistry – CHEM 152/172.
- Thermodynamics: BMD ENG 250; CHEM ENG 211; CHEM 341 or equivalent, MECH ENG 222 is okay although it does not cover chemical thermodynamics!
- Computer Programming/Use: We will use freely available software that can be installed on various computing Operating Systems – OS.

[1]– Note: This is the last edition of the book that describes and uses the tableau method in details, a new version may soon be published ! –

[2]– Note: The book that is still considered as the reference in the field because of the range of processes that it describes. The authors in this edition use the tableau method –

[3]– Note: A book covering many aspects of water chemistry, using also some aspects of the tableau method as well as other approaches –

[4]– Note: The second and revised version of this book is to be released on September 30, 2022. I think that Chapter 7, dealing with the solution of equilibrium problems, has been rewritten and uses now the tableau method,... at least that was the intention of one of his authors –

[5]– Note: A recent book about aquatic chemistry, it does not use the tableau method to explore equilibria but provides computational approaches written in MATLAB and Simulink –

5 Grading

Final Grade = Homework (40%) + Midterm (30%) + Project (30%)

- Homework (40%): 8 problem sets as per class weekly schedule, will be assigned on Fridays. Completed problem sets are due at the end of the day on Friday(*i.e.*, just before midnight on Friday, seven days later). You may work with other class members for the purpose of solving the homework problems. However, you are responsible for generating your own and independently written solutions for grading **under the form of Jupyter notebooks**. Please do not be late handing out your weekly homework, penalties will apply – *i.e.*, 10% grade reduction per late day.
- Project (30%): During this quarter, we will discuss various environmental issues that are related to chemical processes taking place in aquatic systems. For example: how to control atmospheric CO_2 through geo-engineering approaches, ocean acidification, how to mitigate corrosion or clogging in water distribution systems, what is the fate of metals in aquatic systems, the formation of flocs in drinking water treatments, nutrient release and algal blooms. For your project, you will develop a notebook describing the topic of your choice and present an analysis of the processes at play based on **computing relevant chemical equilibria**.
- Midterm (30%): It is programed, for now, to take place on October 27^{th}

6 Additional Information

- **Computer Use:** Short computer programs will be written in Python using the Jupyter notebook interface that will provide you with a convenient and *"elegant"* platform for merging text – markdown – and code. For this purpose please download the Anaconda distribution – instructions will be provided on CANVAS. To perform more complicated calculations you will also use the computer program ChemEql – that you will have to download, with its manual, from the EAWAG/ETH, Zürich/Dübendorf, CH website. ChemEql uses the solution method that is at the core of this course.
- **Class Participation:** It is important that you ask questions in class to clarify the concepts discussed, and also the potential problems that you have with the material. If we have to move parts of the course online, short videos – 10 minutes – will demonstrate how to proceed with setting up example problems and class time will be devoted to Q&A as well as solving and discussing problems in breaking rooms. Please turn on video and microphones during class sessions – unless you are in a room with surrounding noise. Attendance to lectures and recitations is mandatory, please let the instructors know in advance if, and why, you have to miss class.
- **Accessibility Statement:** Northwestern University is committed to providing the most accessible learning environment as possible for students with disabilities. Should you anticipate or experience disability-related barriers in the academic setting, please contact AccessibleNU to move forward with the university's established accommodation process, email: accessiblenu; phone: +1 (847) 467-5530. If you already have established accommodations with AccessibleNU, please let me know as soon as possible, preferably within the first two weeks of the term, so we can work together to implement your disability accommodations. Disability information, including academic accommodations, is confidential under the Family Educational Rights and Privacy Act.
- **Class Recordings:** This class, or portions of this class, may be recorded in order to accommodate for any disruption(s) caused by the health issues related to the still on-going COVID-19 pandemic. These recordings will be shared only with students enrolled in the course. Portions of recordings in which students are visible will be deleted at the end of the end of the Fall 2022 term. I will communicate to you how you can access the recordings.
- **Diversity and Inclusion:** This course is a place where you will be treated with respect, and everyone is welcomed, *i.e.*, students of all backgrounds, beliefs, ethnicities, genders, gender identities, gender expressions, national origins, religious affiliations, sexual orientations, ability, and other visible and non-visible

differences. All members of this course are expected to contribute to a respectful, welcoming and inclusive environment for every other member of the class.

7 Weekly Schedule

The following list the concepts and the different parts of aquatic chemistry that will be discussed during this quarter. This schedule is subject to change given the current sanitary conditions.

Lecture	**Topics/Sections**
Week 1	Introduction, The Method – *i.e.,* the tableau method –
Week 2	Chemical Equilibrium: Short review of Thermodynamics
Week 3	Acids & Bases, pH
Week 4	The Carbonate System: Alkalinity
Week 5	The Carbonate System
Week 6	Metal Ions & Complexation Reactions
Week 7	Dissolution & Precipitation
Week 8	Oxidation & Reduction
Week 9	Project Discussions
Week 10	Course Review & Project Discussions