Abstract: The distribution and the cycling of chemical elements and their compounds in the environment 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 aquatic 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 how to apply this method after a short review of chemical thermodynamics that is the foundation for equilibrium bases calculations. The method is then applied to various natural and engineered 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 Textbooks

- Supplemental Reading: Inorganic Chemistry for Geochemistry and Environmental Sciences: Fundamentals and Applications George w. Luther, III (2016) \(^1\)

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.
- Computer Programming/Use: We will use freely available software that can be installed on various computing operating systems – OS.

5 Grading

Final Grade = Homework (40%) + Group Project (20%) + Midterm (20%) + Final (20%)

- Homework (40%): 8 problem sets as per class weekly schedule, will be assigned on Fridays. Completed problem sets are due at the start of the class the following 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. Please do not be late handing out your weekly homework, penalties will apply – i.e., 10% grade reduction per late day.
- Group Project (20%): During this quarter, you will evaluate a solution that has been proposed and recently reviewed to address climate change through a geo-engineering approach. You will work in groups of 3 students, through the quarter, to write a document that will present your assessment of the solution proposed. During this quarter, you will report weekly on your progress as a group during the discussion section of the class.
- Midterm (20%): In class Midterm Exam 1 hour and 20 minutes long – open book, open notes, and computer use allowed – on Thursday November 1, 2018
- Final (20%): Final Exam – open book, open notes, and computer use allowed – Wednesday December 5, 2018 time TBD.

\(^1\)– Note: A book that you may want to acquire if you are envisioning doing your research in environmental inorganic chemistry –
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 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. I shall reserve the last 5-10 minutes of class time for Q&A when prompted at the beginning of a session. Attendance to lectures and recitations is mandatory, please let the instructors know in advance if, and why, you have to miss class.

7 Weekly Schedule

The following schedule is subject to change.

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<td>Week 1</td>
<td>Introduction, Conservation Principles</td>
<td>Chapter #1 &amp; 2</td>
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<td>Week 2</td>
<td>Chemical Equilibrium, Short review of Thermodynamics</td>
<td>Chapter #3 &amp; 4</td>
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<td>Week 3</td>
<td>Chemical Equilibrium, Solution Methods</td>
<td>Chapter #7</td>
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<td>Week 4</td>
<td>Acids &amp; Bases, pH</td>
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<td>Week 10</td>
<td>Course Review &amp; Project Discussions</td>
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<td>Final is on December 5 in room TBA at TBD p.m.</td>
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