



Course Syllabus: Aquatic Chemistry - EnSE 202

Division	Biological and Environmental Sciences & Engineering Division
Course Number	EnSE 202
Course Title	Aquatic Chemistry
Academic Semester	Fall
Academic Year	2019/2020
Semester Start Date	08/25/2019
Semester End Date	12/10/2019
Class Schedule (Days & Time)	01:00 PM - 02:30 PM Sun Wed

Instructor(s)				
Name	Email	Phone	Office Location	Office Hours
Himanshu Mishra	himanshu.mishra@kaust.edu.sa	+966128082110	4276, 4, Al-Jazri (bldg. 4)	Please speak with the instructor after the class

Teaching Assistant(s)	
Name	Email
Adair Gallo Junior	adair.gallojunior@kaust.edu.sa

Course Information

<p>Comprehensive Course Description</p>	<p>EnSE 202 is a core course in the Environmental Science and Engineering program. It provides a thorough understanding of the fundamentals of water chemistry to our incoming cohorts of students from engineering, chemistry, biology, hydrology, and so on. EnSE-202 administers active learning approaches, wherein lectures are not mere monologues from the instructor. Instead, students learn by asking and answering questions and helping each other through friendly discussions. The course also helps students develop quantitative problem-solving skills.</p> <p>A significant component of the course is the Individual Term Project, which students are encouraged to pick based on their MS/PhD thesis research. The expected outcome is a concise 2-page report with significant emphasis on scientific writing and a polished 15 minutes talk followed by an intense 15-minute Q&A session, evaluated by the class and the instructor.</p> <p>Key topics discussed in EnSE202 include:</p> <ol style="list-style-type: none"> 1. Introduction to aquatic chemistry: Molecular picture of water and its interfaces, ways to express concentrations in liquid- and gas-phases, e.g. molarity, normality, equivalent mass, ppm, ppb, ppt, TDS, TIC, DOC, TOX, and CaCO₃ 2. Chemical equilibrium: activity coefficients, Debye-Hückel theory, Davies model 3. Chemical Kinetics: First-, second-, pseudo first- and higher-order reactions; Temperature dependence of rate constants, Opposing reactions, parallel reactions, consecutive reactions, unimolecular decomposition, Oscillating reactions. 4. Acids and Bases: autodissociation of water; dissociation of strong acids/bases, dissociation of weak acids/bases—speciation as a function of pH, multiprotic weak/strong acids/bases, log C-pH plots. 5. Introduction to Phreeq C software 6. Gas-Liquid Equilibrium: Henry's law, Gas-dissolution and aqueous phase speciation and equilibrium pH 7. Miscellaneous topics: Ideal gas theory, solubility products, Langmuir adsorption isotherms, transition state theory, surface tension, wetting of rough surfaces... <p>Suggested reference book: Water Chemistry, Mark Benjamin (11nd Edition)</p>
<p>Course Description from Program Guide</p>	<p>Chemistry of processes in aquatic systems. Natural water composition, characteristics and analysis (inorganic and organic composition, ionic balance, pH, conductivity, turbidity), acids and bases, carbonate system, chemistry of metals, precipitation, redox chemistry.</p>
<p>Goals and Objectives</p>	<p>EnSE 202 is a core course in the Environmental Science and Engineering program. It provides a thorough understanding of the fundamentals of water chemistry to our incoming cohorts of students from engineering, chemistry, biology, hydrology, and so on. EnSE-202 administers active learning approaches, wherein lectures are not mere monologues from the instructor. Instead, students learn by asking and answering questions and helping each other through friendly discussions. The course also helps students develop quantitative problem-solving skills.</p> <p>A significant component of the course is the Individual Term Project, which students are encouraged to pick based on their MS/PhD thesis research. The expected outcome is a concise 2-page report with significant emphasis on scientific writing and a polished 15 minutes talk followed by an intense 15-minute Q&A session, evaluated by the class and the instructor.</p> <p>Key topics discussed in EnSE202 include:</p> <ol style="list-style-type: none"> 1. Introduction to aquatic chemistry: Molecular picture of water and its interfaces, ways to express concentrations in liquid- and gas-phases, e.g. molarity, normality, equivalent mass, ppm, ppb, ppt, TDS, TIC, DOC, TOX, and CaCO₃ 2. Chemical equilibrium: activity coefficients, Debye-Hückel theory, Davies model 3. Chemical Kinetics: First-, second-, pseudo first- and higher-order reactions; Temperature dependence of rate constants, Opposing reactions, parallel reactions, consecutive reactions, unimolecular decomposition, Oscillating reactions. 4. Acids and Bases: autodissociation of water; dissociation of strong acids/bases, dissociation of weak acids/bases—speciation as a function of pH, multiprotic weak/strong acids/bases, log C-pH plots. 5. Introduction to Phreeq C software 6. Gas-Liquid Equilibrium: Henry's law, Gas-dissolution and aqueous phase speciation and equilibrium pH 7. Miscellaneous topics: Ideal gas theory, solubility products, Langmuir adsorption isotherms, transition state theory, surface tension, wetting of rough surfaces... <p>Suggested reference book: Water Chemistry, Mark Benjamin (11nd Edition)</p>
<p>Required Knowledge</p>	<p>basic chemistry (concepts of moles, Avagadro number) basic mathematics (calculus, algebra, logarithm scale)</p>
<p>Reference Texts</p>	<p>Water Chemistry, Mark Benjamin (11nd Edition) The instructor will provide additional reading material.</p>

Method of evaluation	25.00% - Midterm exam 10.00% - Homework /Assignments 25.00% - Final exam 40.00% - Course Project(s)
-----------------------------	--

Nature of the assignments

-Problem sets

-Mid-terms

-Individual Term Projects:

-Reading scientific literature,

-Scientific writing (a 2-page concise report)

-Class presentation (15 minutes followed by a 10-15 minutes Q&A session)

The Instructor will help the students identify the term projects. A partial list of tentative projects follows:

-How are global CO₂ concentrations coupled/related to the pH of the oceans and the global temperature?

-Despite high humidity, why does it not rain at KAUST?

-Why/how does low salinity water injection enhance oil recovery in some (carbonate) oil reservoirs? See work by Ali Yousouf and Firoozabadi

-Based on thermodynamics, what is the minimum amount of work that must be done to desalinate water (Assume initial concentration= 50,000 ppm NaCl and final 0.5 ppm NaCl)? What room does it leave for improving current water desalination technologies? See Elimelich's work

-Why do rates of several chemical reactions differ depending on whether they take place "in water" versus "on-water"? See articles by Sharpless, Marcus, Coyne & Butler, and Beattie on 'catalysis on-water'

-What are the key differences between water inside biological cells and isotonic water? For example, describe in terms of diffusion and structuring of water and the role of the hydrophobic interaction. See Ninham's work

-How do the following properties of ions compete in their relative binding to hydrophobic interfaces (e.g. air, oils): hydration energy, size, charge density...? Go in depth, look for analytical and/or empirical trends. See Kim Collins work; See Geissler's work

-How do desert plants prevent the loss of water under extreme heat?

-Why do some salts release heat (exothermic) when dissolving in water while others absorb heat (endothermic)? Think in terms of hydration energy and entropy loss of water

-What drives the rise of water in trees and plants? See Stroock's work

-How do some plants, e.g. Medusa and Venus Flytrap, perform tactile sensing and motion via osmotic pressures? Works of Mazzolai and Mahadevan

-How does the size of hydrophobic solutes in water impact (hydrophobic) interactions between them? See Chandler's and Amotz's work

-What is a good technique to quantify the diffusion of water molecules in bulk water? Describe a physical model to explain the underlying physics. See Songi Han and NMR literature

-What is a good technique to quantify the diffusion of protons in bulk water? Describe a physical model to explain the physics. See Eigen's work and Bonn's work..

-How do clouds generate electrical potential difference?

-Why does a water drop falling through air become negatively charged? On the other hand, it is generally

positively charged if collected after passing through a tube made of PTFE or PMMA. See Galembeck's work, Diaz's work and Whitesides's work..

-Why do leaves and flowers not burn out under intense heat, for example during summer season at KAUST, if the plants are well-watered?

-How do some insects walk on water?

Course Policies

I do not mind students missing classes as long as they perform well in the exams and the final presentation/report.

Students may discuss concepts, but must not copy solutions to problems, e.g., in problem-sets.

Class/course projects are a terrific way for you to apply the concepts that you learn in the course to a problem of mutual interest; you are most welcome to pick a topic (surrounding physical/chemical properties of water) that interests you and/or aligns with your MS/PhD research at KAUST. You will also learn how to write concise scientific documents.

EnSE202 is taught "actively", which means that students will be freely answering and asking questions and discussing concepts among each other, and having a good time! Active learning has been demonstrated to be more effective than the standard "one-way" discourses.

Additional Information

Class ethic:

Bring crazy ideas; Ask lots of questions; Have fun; THINK!!

The Class/course project carries much significance in this course. Thus, it is crucial to start working on your topic as early as possible. Sometimes, students change their projects too. The instructor and TA will host Class Project Clinics to assist students.

The finale of the course will entail talks by the students on their Projects followed by Q&A from the audience.

Class project report (details):

The instructor will assist students in improving their writing and summarizing their reports.

Formatting:

- 2 pages max. (shorter the better)
- Font: Times New Roman, Size: 12
- Single spacing
- Narrow margins

References:

- Please use a bibliography software such as Endnote (Please see the TA for assistance, if needed)
 - › You are expected to cite at least 5 relevant papers (this would reading > 5 papers)
 - › Bibliography format: ACS (American Chemical Society – in-built in EndNote)
 - › If an article has more than 4 authors, you can refer to them as “XYZ et al.”, where XYZ is the last name of the first author.
 - › Suggested reading for scientific writing:
 - › Book: Strunk and White’s ‘Elements of Style’
 - › Plaxco’s article, entitled “The art of writing science”
 - › Platt’s article entitled “Strong Inference”

The Class Project Report should be structured as follows:

- Title:** a focused question; avoid broad/general questions, such as “What causes water pollution”
- Introduction:** One sentence on the significance of the field – it should be comprehensible to any scientist; Two sentences narrowing down to your Class Project – understandable to someone from the field; One sentence clearly stating the problem you seek to address – understandable to an expert.
- Hypotheses/Mechanisms/Rationale behind experiments:** Summarize your hypotheses, or mechanisms, or the rationale behind your experimental/theoretical work. This section could have a figure.
- Results:** Present your literature review and/or experimental/theoretical work - explain your findings. This section could have figures.
- Discussion:** Did they prove/disprove the above-mentioned hypotheses? This section could have figures.
- Conclusion:** A summary of your quest to answer the Question. What issues still remain unanswered? List new questions, if any, that emerged from your work, and how they should be addressed
- References (at least 5).

Tentative Course Schedule

(Time, topic/emphasis & resources)

Week	Lectures	Topic
1	Sun 08/25/2019 Wed 08/28/2019	(THE DATES AND TOPICS LISTED BELOW ARE NOT FINAL. BUT THEY SHOULD GIVE PROSPECTIVE STUDENTS A CLEAR IDEA OF THE OVER-ALL CONTENT OF THE COURSE IS) Space inside the lattice of water; Various ways to express concentrations: molarity, normality, ppm, ppb, ppt Examples
2	Sun 09/01/2019 Wed 09/04/2019	Various ways to express concentrations: TOC, DIC, TDS, TOX Various ways to express concentrations: TOC, DIC, TDS, TOX
3	Sun 09/08/2019 Wed 09/11/2019	Examples on Conductivity and mole fraction; Activity and activity Coefficients; Relative Humidity--water concentrations? Standard States, Examples on calculating activities Refresher on electrostatics: basics of electrostatics-electrical fields, electrical potentials
4	Sun 09/15/2019 Wed 09/18/2019	Refresher on electrostatics: basics of electrostatics-Gauss's law, Poisson-Boltzman eqn. Poisson-Boltzman equation and its solution leading to Debye length + Derivation of the Debye-Huckel model
5	Sun 09/22/2019 Wed 09/25/2019	No Class (Saudi National Day) Energy and Mass Balances: mass conservation
6	Sun 09/29/2019 Wed 10/02/2019	Energy and Mass Balances: first and second law of thermodynamics Reaction Kinetics: Rates of reactions; Orders of Zeroth, 1st, 2nd, 3rd, oscillating reactions; Rate limiting steps, catalysts
7	Sun 10/06/2019 Wed 10/09/2019	Reaction Kinetics: Rates of reactions; Orders of Zeroth, 1st, 2nd, 3rd, oscillating reactions; Rate limiting steps, catalysts Acid-salt equilibria#1(i) Autoionization of water; Strong acids and bases; Weak acids and bases: pKa - pH dependence; Weak acids + salts: concentrations
8	Sun 10/13/2019 Wed 10/16/2019	Acid-salt equilibria#1(i) Autoionization of water; Strong acids and bases; Weak acids and bases: pKa - pH dependence; Weak acids + salts: concentrations Introduction to Phreeqc
9	Sun 10/20/2019 Wed 10/23/2019	Review of concepts prior to the Exam Midterm (Concentrations, Activity, Kineics, Acid-Base equilibria, Gas-liquid equilibrium, Energy & Mass Balances)
10	Sun 10/27/2019 Wed 10/30/2019	No class (break) Midterm solution, Clinic for the Final Presentations (Reports due a week before the talk)
11	Sun 11/03/2019 Wed 11/06/2019	Water thermodynamics: Cp, sensible and latent heat, intro to thermal desalination Gas-liquid equilibrium: Henry's constants, Gas-liquid-pH equilibrium
12	Sun 11/10/2019 Wed 11/13/2019	Misc. Lecture: Pollutants and water treatment Misc. Lecture: (i) Surface Tension, (ii) Contact angles, (iii) Laplace Pressure, (iv) Wetting of rough surfaces
13	Sun 11/17/2019 Wed 11/20/2019	Misc. Lecture: (i) Surface Tension, (ii) Contact angles, (iii) Laplace Pressure, (iv) Wetting of rough surfaces Misc. Lecture
14	Sun 11/24/2019 Wed 11/27/2019	Final Exam FINAL PRESENTATIONS
15	Sun 12/01/2019 Wed 12/04/2019	Final Presentations (if any) Course over. Misc. Lecture
16	Sun 12/08/2019	Misc. Lecture

Note

The instructor reserves the right to make changes to this syllabus as necessary.