DRAFT Syllabus for CHEM:5107
Electrochemistry

Spring 2019

Wednesday 18:30 to 21:10, PC C129 16 January to 1 May 2017

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Office Hours: TBD in W358 PBB and after class first in PC C129 and then W358 PBB

1 Purpose:

This course is intended to provide an introductory but thorough background in electrochemistry. Fundamentals, methods, and kinetics will be covered. Means for modeling electrochemical systems by explicit finite difference computer simulations and Laplace transforms will be introduced. (The course can be taken for 2 or 3 hrs credit. The 2 hr version includes all material covered in the 3 hr version except for the computer simulation. Precomp chemistry graduate students in chemistry should register for 3 hr.)

2 Text and Reserve Materials:

Bard and Faulkner, Electrochemical Methods, 2nd Ed., Wiley 2001, (ISBN 0-471-04372-9) is on sale in campus bookstore or online. A solution manual is also available, but not required (ISBN 0-471-40521-3). The solutions to the suggested problems below are provided in the solution manual, a copy of which is available in my labs in CB. Problems marked in bold are not in the solution manual but are on the course web page at icon.uiowa.edu. There is other supplemental materials on the webpage. The review article by Faulkner is a nice introduction, comparable to Chapters 1 to 4 in the text.

3 Course Topics:

Chapter	Topic	Suggested Problems	Evaluation
Fundamentals (about 4.5 lectures)			
1	Introduction	1,3,5,7,9	Take home exam: Due **TBD**
2	Potentials and Thermodynamics of Cells	1a,e,4a,d,6,8, 10a,12,14a,c,16	
3	Kinetics of Electrode Processes	3a,5a,11,13	
4	Mass Transport	1,3,**4**	
13.1-13.3	Double Layers	2,6	
Step and Sweep Methods, Modeling, and Reactions (about 3.5 lectures)			
5, App. A	Potential Step Methods, Laplace Transforms and Microelectrodes	**1,**2,4,6,8a,b,10,14,16,18, A1,A3,**A4**,A5a	LT problem & 5 min presentations **TBD**
7.3.5	Square Wave Voltammetry		
6	Potential Sweep Methods	2,4,6,8,10,12a	
12	Homogeneous and Heterogeneous Reactions	1,3,5,**8**,11,**12**	
13.7	Effect of Double Layer on Electrode Reactions	12	
Computer Simulations (about 1 lecture)			
App. B	Computer Simulation	B1,B3,B4	Sim (3 hr only): presentations & report **1 May**
Selected Methods and Systems (about 3 lectures, includes hydrodynamic methods and bulk electrolysis + ∼2 more topics)			
9	Hydrodynamic Methods (Rotating disk voltammetry)	3,**4**,5,7,9,**10**	Data Analysis of Literature Paper due **TBD**
11;13.5;13.6	Bulk Electrolysis and Thin Layer	**10**,11,**12**,13; 13.8,13.10,13.14	
14	Modified Electrodes	2,6	
15	Instrumentation	2,4,12	
16.4	Scanning Electrochemical Microscopy	2,4	
17,18	Spectrochemical & Photoelectrochemical Methods	2	
	Power Sources and Industrial Electrochemistry		

4 Prerequisites:

CHEM: 3110 and 3120 or 4171, or equivalent, or permission

5 Office Hours:

TBD in W358 PBB and after class first in PC C129 and then W358 PBB. Please arrange appointments by email and refrain from just stopping by.

6 Web Page:

There is a class web site on ICON (http://icon.uiowa.edu/). This includes syllabus, handouts, supplemental material, and messages to the class. Points for assignments will be available on ICON. Please check ICON for updates that may contain clarifying information.

7 Assignments:

The grading of the course is divided into three parts.

- **Fundamentals**: This covers the basic physical chemistry of electrochemistry and charged interfaces. Fundamentals of mass transport, electron transfer, kinetics, and thermodynamics are used to assess every electrochemical system and process. It will be presented solely in lecture format. Mastery of this material will be judged by an analysis of an electrochemical system during a take home exam.
  - **Exam:** A system will be analyzed quantitatively for thermodynamics, electrode kinetics, and mass transport. Exam is open book/ notes. An old exam is posted on ICON that illustrates types of information that will be covered in lecture and exam. Exam will be take home.
- **Step and Sweep Methods, Modeling, and Reactions:** This covers the two most common voltammetric methods, potential step and cyclic voltammetry. Application of the methods to various cases from simple Nernstian (fast electron transfer) cases to more complex reaction mechanism will be covered. Lectures will also cover some of the various homogeneous electrochemical reaction mechanisms. Laplace transforms will be used to evaluate voltammetric responses.

  Mastery of this section is done by solving a unique Laplace transform problem and by computer simulation (for the 3 hr course).
  - **Laplace Transform Assignment:** Each student will be given a unique Laplace transform to solve and all students will present their analyses in class. The written solutions and a 5 minute in class presentations are due in class the same day.
  - **Computer Simulation** (for those taking the 3 hour version only): Modeling of electrochemical mechanisms and systems is done by computer simulation. For the 3 hour version, students will develop a simulation to model potential step and cyclic voltammetry. Each student will be given an electrochemical mechanism to computer model; this will include sample data to fit by simulation for that mechanism. How to develop a simulations and the rudiments of Visual Basic will be covered in class but the assignment is completed outside of class. This will take more than a few hours, so allow sufficient time. There is an extensive handout on ICON. A written report and 8 minute presentation are due during the last class**.**
- **Methods and Systems**: Various electrochemical methods and systems will be covered in survey.
  - **Literature Analysis:** Mastery of this section will be demonstrated by writing a short review of a paper on a method, system, or electrochemical topic of your choice. Choose a paper in the literature on either a sweep or step method that contains data. The objective is to repeat the authors' analyses complete with graphs and statistics and comment on how your analyses compare. Provide a copy of the paper, your analysis (including error bars), and your comments on the quality of the authors analysis. Provide well formed plots and data tables for your analysis. The paper should be between 500 and 1000 words and include images, at least two plots with statistics made by the student, and at least two equations. Papers that include combination of two different voltammetric methods will be given +10 points in the grading. Papers that evaluate heterogeneous electron transfer kinetics will also garner a + 10 points bonus.
- There is no final exam.

8 Grading:

The grade will be assigned based on the two or three hour class.

For the two hour class: as follows: exam (40%), Laplace transform problem (30%), and literature analysis (30%).

$$Grade = \frac{40\ Exam\ + 30\ Laplace + 30\ Literature\ Analysis}{100}$$

For the three hour version, exam (35%), Laplace transform problem (15%), and literature analysis (15%). and simulation and report (35%).

$$Grade = \frac{35\ Exam\ + 15\ Laplace + 15\ Literature\ Analysis + 35\ Sim\&Report}{100}$$

There is no final.

9 For 3 hour Course: Details on Computer Modeling of Mechanism:

In explicit finite difference simulations, the computer mimics the physical behavior of the electrochemical system by incorporating mass transport, electron transfer, and homogeneous chemical reactions. Each student will develop a computer simulation for an assigned mechanism. The assigned mechanism will be different for each student. The simulation will be developed in three steps.

1. Write a basic simulation for potential step for reversible (Nernstian), quasi-reversible, and irreversible heterogeneous kinetics. This will demonstrate the coupling between mass transport and electron transfer in establishing the voltammetric response.
2. Modify this simulation to generate cyclic voltammograms for the three cases of heterogeneous kinetics.
3. This step introduces the impact of different homogeneous kinetic schemes on the voltammetric response. Each student will be provided with a mechanistic scheme that they will simulate for homogeneous kinetics. Cyclic voltammetric data at several scan rates will be provided. The data will be fitted with the student's simulation and the rate constants reported.

Only the third simulation will be submitted for grading. Each student will present their simulation and fitting during the last class.

A detailed handout of how to establish the explicit finite difference simulation is on the webpage. Appendix B in Bard and Faulkner is also about simulations. Handouts are also available on ICON for using Visual Basic inside of Excel. Any computer language maybe used to develop the simulation. We will do some development and simple programming on laptops during class.

Use dimensionless parameters throughout.

10 Manners and Administrative Details

Computer Access: Most problem will best be done using a spreadsheet. You will need access to a computer with a spreadsheet program. If you are not familiar with spreadsheets (e.g., Excel), best to get started learning.

Attendance: Except for the exam and in class reports, attendance is neither taken nor required. Audits have some constraints.

Cell Phones, Pagers, and Other Audible Devices: Please turn off all audible alarms during class.

Academic Fraud: Cheating is not tolerated in this class. If you are found to be cheating, I will pursue the maximum possible penalties for cheating. Plagiarism and any other activities when students present work that is not their own are academic fraud. Academic fraud is a serious matter and is reported to the departmental DEO and to the Associate Dean for Undergraduate Programs and Curriculum. Instructors and DEOs decide on appropriate consequences at the departmental level while the Associate Dean enforces additional consequences at the collegiate level. See the CLAS Student Academic Handbook.

Special Requirements for Students with Disabilities: Please contact me immediately if you have a disability that may require some modification of seating, testing or other class requirements so that appropriate arrangements may be made. A student seeking academic accommodations should first register with Student Disability Services and then meet privately with the course instructor to make particular arrangements. See www.uiowa.edu/~sds/ for more information.

Chemistry Department Contact Information: Students in need of additional information may contact staff in the Chemistry Center (335-1341) during normal business hours.

Complaints: Students with a suggestion or complaint should first visit the instructor and then the departmental DEO. Complaints must be made within six months of the incident. See the CLAS Student Academic Handbook.

CLAS The College of Liberal Arts and Sciences is the administrative home of this course and governs matters such as the add/drop deadlines, the second-grade-only option, and other related issues. Different colleges may have different policies. Questions may be addressed to 120 Schaeffer Hall or see the CLAS Student Academic Handbook [www.clas.uiowa.edu/students/academic_handbook/index.shtml].

Harassment: Sexual harassment subverts the mission of the University and threatens the well-being of students, faculty, and staff. All members of the UI community have a responsibility to uphold this mission and to contribute to a safe environment that enhances learning. Incidents of sexual harassment should be reported immediately. See the UI Comprehensive Guide on Sexual Harassment at www.uiowa.edu/~eod/policies/sexual-harassment-guide/index.html for assistance, definitions, and the full University policy.

Weather: In severe weather, class members should seek appropriate shelter immediately, leaving the classroom if necessary. The class will continue if possible when the event is over. (Operations Manual, IV.16.14. Scroll down to e. h. and i.) If the University remains open but I determine the weather is too severe, I will send an email from ICON. Please make sure to have a valid address on ICON.

11 Information Required by CLAS: Teaching Policies & Resources — Syllabus Insert

Administrative Home: The College of Liberal Arts and Sciences (CLAS) is the administrative home of this course and governs its add/drop deadlines, the second-grade-only option, and other policies. These policies vary by college (https://clas.uiowa.edu/students/handbook).

Electronic Communication: Students are responsible for official correspondences sent to their UI email address (uiowa.edu) and must use this address for all communication within UI (Operations Manual, III.15.2).

Accommodations for Disabilities: UI is committed to an educational experience that is accessible to all students. A student may request academic accommodations for a disability (such as mental health, attention, learning, vision, and physical or health-related condition) by registering with Student Disability Services (SDS). The student should then discuss accommodations with the course instructor (https://sds.studentlife.uiowa.edu/).

Nondiscrimination in the Classroom: UI is committed to making the classroom a respectful and inclusive space for all people irrespective of their gender, sexual, racial, religious or other identities. Toward this goal, students are invited to optionally share their preferred names and pronouns with their instructors and classmates. The University of Iowa prohibits discrimination and harassment against individuals on the basis of race, class, gender, sexual orientation, national origin, and other identity categories set forth in the University's Human Rights policy. For more information, contact the Office of Equal Opportunity and Diversity (diversity.uiowa.edu).

Academic Honesty: UI is committed to making the classroom a respectful and inclusive space for all people irrespective of their gender, sexual, racial, religious or other identities. Toward this goal, students are invited to optionally share their preferred names and pronouns with their instructors and classmates. The University of Iowa prohibits discrimination and harassment against individuals on the basis of race, class, gender, sexual orientation, national origin, and other identity categories set forth in the University's Human Rights policy. For more information, contact the Office of Equal Opportunity and Diversity (diversity.uiowa.edu).

CLAS Final Examination Policies: The final exam schedule for each semester is announced around the fifth week of classes; students are responsible for knowing the date, time, and place of a final exam. Students should not make travel plans until knowing this final exam information. No exams of any kind are allowed the week before finals (https://clas.uiowa.edu/faculty/teaching-policies-resources-examination-policies).

Making a Complaint: Students with a complaint should first visit with the instructor or course supervisor and then with the departmental executive officer (DEO), also known as the Chair. Students may then bring the concern to CLAS (https://clas.uiowa.edu/students/handbook/student-rights-responsibilities).

Understanding Sexual Harassment: Sexual harassment subverts the mission of the University and threatens the well-being of students, faculty, and staff. All members of the UI community must uphold the UI mission and contribute to a safe environment that enhances learning. Incidents of sexual harassment must be reported immediately. For assistance, definitions, and the full University policy, see https://osmrc.uiowa.edu/.

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Reacting Safely to Severe Weather: In severe weather, class members should seek appropriate shelter immediately, leaving the classroom if necessary. The class will continue if possible when the event is over. For more information on Hawk Alert and the siren warning system, visit the Department of Public Safety website.