I. Course Identity, Teaching Staff, and Logistics

Instructor: New hire with Prof. Mark Lonergan, email: swb@uoregon.edu, office: 435 LISB, Phone: 541-346-2543

Office hour: The instructor will hold two office hours per week, held in faculty office #. The times will be determined on the first day of lecture based on student availability. Meetings will also be available by appointment.

Format: A blend of lecture, active learning, in particular through think-pair-share activities, and project-based laboratory work (using the simulation software).

Credits: 2

Location: Klamath 107, Tuesdays and Thursdays 1:00-1:50 pm

Required course materials:


Access to a COMSOL Multiphysics will be provided by the Oregon Center for Electrochemistry as part of the course. Students must log into the license server via the internet to use the software on their own personal computer.

Students are expected to bring their own laptop to class to run COMSOL. If you don’t have access to a laptop, we will work to provide a University-owned basic laptop to use in class. Please discuss well ahead of time with the instructor.

Course website: Simulation project assignments, lecture notes, videos, and grades will be posted on the Canvas course site.

Pre/Co-requisite: Advanced Electrochemistry CH454/554
II. Course Description

In CH454/554 students learn the fundamental theoretical concepts underlying electrochemical systems and see one example of a simple computer simulation. In this course CH690, students will learn how to implement theoretical concepts in advanced computer simulations. For students simultaneously enrolled in both courses, the numerical simulations explored will track with theoretical concepts developed in the lecture course. Modern finite-element simulation software is widely used in engineering to predict system performance/properties or in science to understand complex system behavior. Students will use industry standard software suites to simulate basic electrochemical cells and devices. Focus will be on (1) understanding the math and physics principles underlying finite element numerical simulation, (2) constructing robust electrochemical models, including defining boundary conditions, interfaces, transport, kinetics, and thermodynamic model inputs, (3) applying numerical methods to solve electrochemical problems using computers, (4) and interpreting data from numerical simulations in the context of a simple physical picture to develop an electrochemical intuition.

III. Expected Learning Outcomes

- Understand math and physics principles underlying finite element numerical simulation.
- Learn how to construct robust electrochemical models, including defining boundary conditions, interfaces, transport, kinetics, and thermodynamic model inputs.
- Apply numerical methods to solve electrochemical problems using computers.
- Learn to interpret data from numerical simulations in the context of a simple physical picture to develop an electrochemical intuition.

IV. Estimated Student Workload

Course participants will attend laboratory sessions, perform assigned reading, attend open laboratory times and collect data, analyze data, and write professional quality reports. The table below shows the estimated workload.

<table>
<thead>
<tr>
<th>Activity</th>
<th>Estimated hours per term</th>
<th>Comments</th>
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</thead>
<tbody>
<tr>
<td>Laboratory Report Preparation</td>
<td>20</td>
<td>4 simulation reports, typically 6-8 pgs. with data per report</td>
</tr>
<tr>
<td>Literature Analysis</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lectures/Discussion</td>
<td>20</td>
<td>2 h / week</td>
</tr>
<tr>
<td>Simulation Work</td>
<td>40</td>
<td>4 h / week</td>
</tr>
<tr>
<td>Total hours:</td>
<td>80</td>
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V. How Grades Will Be Determined
The grades will be determined based on the following percentage breakdown of the final total score:

**Quality of simulation reports; data, analysis, and discussion will make up all your grade:**

- **Project 1:** 20%
- **Project 2:** 20%
- **Project 3:** 20%
- **Final Project:** 40%

Projects will be graded based on the quality of the project report. Reports are expected to be concise formal documents with professional quality graphs (including appropriate use of units), precise definition of the physics employed in the model, analysis and insightful discussion of the simulation data (~6-8 pages for each). Each project assignment is accompanied by a document outlining project expectations.

The final project is a longer simulation project. Several topics will be provided by the instructor on current topics (e.g. bipolar membranes, nanoelectrodes, fuel cells, etc.) and each student will select one of these topics to focus on.

- **A** = Clearly written, concise document, with high-quality figures. All required pieces of data are shown and discussed without major errors in the interpretation. Discussion uses simulation data in quantitative and/or specific ways and shows mastery of the principles underlying computer simulation of electrochemical phenomena.
- **B** = One or more issues with the items above.
- **C** = Multiple issues with quality of the written document and interpretation/discussion.
- **D** = Multiple issues and incomplete.

+/- grades will be applied consistent with the above criteria. A+ will be given for near-perfect reports with high quality data.

A+ course grades will be given to the top-performing students in the course, provided they reach >95%. Students earning >90% in the course will earn at least an A, >80% at least a B, >70% at least a C, and >60% at least a D. The instructor may curve the course to increase the letter grades for a given percentage score to account for variations in difficulty of the exam questions from year-to-year. Students with a given percentage score will not, however, earn a grade lower than that indicated above.

**VI. Course Schedule and Assignments**

**Assigned reading:** Weekly reading are given after each topic.
**Week 1**

**Class 1:** Introduction to numerical simulation and finite element methods. COMSOL installation.
**Class 2:** Introduction to COMSOL Multiphysics Interface; practice building model geometry and defining boundary conditions.


**Week 2**

**Class 1:** Building an electrochemical model with radial symmetry.
**Class 2:** Start simulation model for “Project 1: Electroanalytical electrochemistry with finite and semi-infinite boundary conditions” in class.


**Week 3**

**Class 1:** Continue Project 1: Electroanalytical electrochemistry with finite and semi-infinite boundary conditions”.
**Class 2:** Continue Project 1: Electroanalytical electrochemistry with finite and semi-infinite boundary conditions”.


**Week 4**

**Class 1:** Discussion/lecture: transport of “dilute” species and applications of the Nernst-Plank-Poisson Equations: current flow in electrolytes and ionomer membranes
**Class 2:** Start simulation model for “Project 2: Ion-selective membranes: Donnan Equilibria and Transport.” in class.

**Reading:** Electrochemistry Module User’s Guide. COMSOL 2018. Chapter 4: Chemical Species Transport Interfaces, pg 148-183 and 198-199.

Project 1 due.

**Week 5**

**Class 1:** Continue simulation model for “Project 2: Ion-selective membranes: Donnan Equilibria and Transport.”
**Class 2:** Continue simulation model for “Project 2: Ion-selective membranes: Donnan Equilibria and Transport.”

**Reading:** Electrochemistry Module User’s Guide. COMSOL 2018. Chapter 4: Chemical Species
Transport Interfaces, pg 148-183 and 198-199.

**Week 6**
**Class 1:** Lecture/discussion on modelling electrochemical reactions.
**Class 2:** Start simulation model for “Project 3: Cyclic Voltammetry and Reaction Mechanisms.”


Project 2 due.

**Week 7**
**Class 1:** Continue simulation model for “Project 3: Cyclic Voltammetry and Reaction Mechanisms.”
**Class 2:** Select final project topic from approved list of current topics of interest (e.g. electrodeposition in 3D, fuel cells, bipolar membranes, nanoelectrodes). Start planning modelling strategy. Collaboration is encouraged.

**Reading:** Selected chapters or primary literature related to the final project topic.

**Week 8**
**Class 1:** Continue working on final project with input from instructor and teaching assistants.
**Class 2:** Continue working on final project with input from instructor and teaching assistants.

**Reading:** Selected chapters or primary literature related to the final project topic.

**Week 9**
**Class 1:** Continue working on final project with input from instructor and teaching assistants.
**Class 2:** Continue working on final project with input from instructor and teaching assistants.

**Reading:** Selected chapters or primary literature related to the final project topic.

**Week 10**
**Class 1:** Continue working on final project with input from instructor and teaching assistants.
**Class 2:** Continue working on final project with input from instructor and teaching assistants.

**Reading:** Selected chapters or primary literature related to the final project topic.

**Finals Week**

**Wednesday:** Final project due.

VII. Course Policies
Late or missed work will not generally be accepted without prior approval.

Project reports must be your own work. You may share data across the class (with citation) if it strengthens the quality of the report but the analysis and discussion of the data in the report must be your own work.

There will be a zero-tolerance policy for plagiarism in laboratory reports.

Academic Misconduct: The University Student Conduct Code (available at conduct.uoregon.edu) defines academic misconduct. Students are prohibited from committing or attempting to commit any act that constitutes academic misconduct. By way of example, students should not give or receive (or attempt to give or receive) unauthorized help on assignments or examinations without express permission from the instructor. Students should properly acknowledge and document all sources of information (e.g. quotations, paraphrases, ideas) and use only the sources and resources authorized by the instructor. If there is any question about whether an act constitutes academic misconduct, it is the students’ obligation to clarify the question with the instructor before committing or attempting to commit the act. Additional information about a common form of academic misconduct, plagiarism, is available at https://researchguides.uoregon.edu/citing-plagiarism.

Accessibility: The University of Oregon is working to create inclusive learning environments. Please notify me if there are aspects of this course that result in disability related barriers to your participation. For more information or assistance, you are also encouraged to contact the Accessible Education Center, Suite 360 Oregon Hall, 346-1155 or uoaec@uoregon.edu; website: http://aec.uoregon.edu/content/about

A graduate employee (GE) will serve as a teaching assistant for this course. The GE’s responsibilities will include assisting in the implementation of the project component of the course, including supervising students completing the projects and obtaining/distributing materials needed for the project. The GE may assist with grading, and will also be available for general assistance in preparing project reports, completing homework assignments, and preparing for exams. Should graduate students enrolled in the course perceive the course as leading to any conflict of interest, privacy concerns, or unfairness related to having a GE in the above role please contact the instructor to discuss paths of recourse. If the GE is involved in grading assignments, graduate students may request that a faculty member, not the GE, grade their assignments. To do this please make the request in writing via email to the instructor.