EES 4203 Phase Partitioning in the Environment

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e-Learning: All course material will be posted on e-Learning

Office Hours: Tuesdays and Thursdays: 9:30–11:30 a.m. or by appointment

Teaching Assistant: Stephanie Ishii

Textbook: *Environmental Organic Chemistry*, 2nd Edition, R. P. Schwarzenbach, P. M. Gschwend, and D. M. Imboden.

Reference Books: These books are on reserve at the Marston Science Library
Organic Chemistry, 2nd Edition, F. A. Carey.
Chemical and Engineering Thermodynamics, 3rd Edition, S. I. Sandler.
Four Laws That Drive the Universe, P. Atkins.

Prerequisites: CHM 2046

Credits: 4

Lecture Room and Times: 386 NEB, Tuesday and Thursday, 7–8th period (1:55–3:50 pm)

Relationship of course to Environmental Engineering Sciences program outcomes:
Successful completion of this course should increase the students':

(1) Ability to apply knowledge of math, science, and engineering;
(9) Knowledge of contemporary issues;
(13) Proficiency in chemistry.

The goal for this course is to understand the fate of organic pollutants in the environment by applying principles of organic chemistry and chemical thermodynamics. By the end of this course, students should be able to:

1. Categorize the reactivity of organic compounds based on attributes, such as structure and functional group chemistry;
2. Define and interpret the laws of thermodynamics;
3. Understand the relationship between chemical structure, molecular interactions, and thermodynamic functions;
4. Evaluate the partitioning of a pollutant between two different phases.

This course is divided into four Topics. The specific objectives of each Topic are described below.

Topic I Environmental Organic Chemistry

Specific objectives:

1. Learn basic principles of organic chemistry;
2. Identify hydrocarbon skeleton and major functional groups;
3. Classify chemical reactivity;
4. Explain the most important aspects of nucleophilic substitution reaction mechanisms.

Overview of phase partitioning (Chapter 1)

Organic Chemistry (Chapter 2)

Introduction to kinetic vs. thermodynamic control (Chapter 12)

Hydrolysis: Nucleophilic substitution reaction mechanisms (Chapter 13)

Topic II Introduction to Thermodynamics

Specific objectives:

1. Learn fundamental thermodynamic properties and variables;
2. Understand the four laws of thermodynamics.

Introduction

- Thermodynamic properties and variables

Conservation of Mass and Energy

- General balance equations
- Enthalpy
- First law of thermodynamics

Entropy

- Entropy balance
- Second law of thermodynamics
- Helmholtz free energy and Gibbs free energy

Topic III Chemical Thermodynamics

Specific objectives

1. Define intermolecular forces and give examples;
2. Explain the following thermodynamic functions: Gibbs free energy, enthalpy, entropy, chemical potential, fugacity, activity, and activity coefficient;
3. Calculate vapor pressure using phase diagrams, theoretical relationships, and experimental data;
4. Explain solubility in terms of enthalpy and entropy of solution.

Molecular Interactions (Chapter 3)

- Overview of molecular interactions
- Thermodynamic functions: Gibbs free energy, enthalpy, entropy, chemical potential, fugacity, activity, and activity coefficient
- Equilibrium partitioning constants

Activity Coefficient and Solubility in Water (Chapter 5)

- Equilibrium between pure material and aqueous solution
- Chemical structure and solubility
- Effect of temperature and solution composition on aqueous solubility

Topic IV Phase Partitioning in the Environment

Specific objectives

1. Calculate the partitioning of an organic compound between different environmental phases;
2. Describe how an organic compound released into the environment bioaccumulates.

Partitioning Between Organic Liquid and Water (Chapter 7)

Bioaccumulation (Chapter 10)

The following is a tentative schedule. All dates are approximate and subject to change.

Week	Tuesday	Thursday
January 5, 7	Start Topic I	
January 12, 14	Assign Homework 1	
January 19, 21	Homework 1 Due Assign Homework 2	End Topic I Return Homework 1
January 26, 28	Homework 2 Due Start Topic II	Return Homework 2
February 2, 4	EXAM Topic I	
February 9, 11	Assign Homework 3	
February 16, 18	End Topic II	Homework 3 Due
February 23, 25	Start Topic III Return Homework 3	EXAM Topic II
March 2, 4	Assign Homework 4	
March 9, 11	SPRING BREAK!	
March 16, 18		Homework 4 Due Assign Homework 5
March 23, 25	End Topic III Return Homework 4	Homework 5 Due
March 30, April 1	Start Topic IV Return Homework 5	EXAM Topic III
April 6, 8		Assign Homework 6
April 13, 15		Homework 6 Due
April 20, 22	End Topic IV Return Homework 6	No class Reading Day
April 29	FINAL EXAM 29B, 10:00 am – noon	

Attendance: Students are strongly encouraged to attend class. In-class participation is a component of your grade.

In-class Participation: In-class participation will include individual and group assignments, such as Reading & Lecture Questions and discussion of Online News from *Environmental Science & Technology* website.

Homework: There will be 1–2 homework assignments for each Topic. The assignments will be designed to reinforce concepts from the lecture and highlight the most important ideas for each Topic. *No late homework will be accepted.*

Exams: There will be 4 exams in this course; one exam for each Topic. Exams will be in-class and approximately one week after completion of the respective Topic.

Make-up Exams: Make-up exams are only given for medical reasons. A student may request a make-up exam if they cannot attend the scheduled exam for medical reasons. The student must contact the instructor before the exam to state that he/she will not be able to attend the exam.

Grade Distribution and Grading Scale:

20% In-class Participation	A: 95–100
30% Homework	A-: 90–94
50% Exams	B+: 87–89
	B: 83–86
	B-: 80–82
	C+: 77–79
	C: 73–76
	C-: 70–72
	D+: 67–69
	D: 63–66
	D-: 60–62
	E: <60

Students with Disabilities: Students requesting classroom accommodation must first register with the Dean of Students Office. The Dean of Students Office will provide documentation to the student who must then provide this documentation to the instructor when requesting accommodation.

Cell phones: Cell phones must be turned off at the beginning of class; use of cell phones during class is prohibited.

The Honor Code:
We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity. On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied:
"On my honor, I have neither given nor received unauthorized aid in doing this assignment."