CE573 - ENVIRONMENTAL ORGANIC CHEMISTRY

Spring 2007

Lecture: 10:10 -11:00 am MWF 209 Hammond Building

Instructor: Dr. Bill Burgos Telephone: 863-0578

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Office Hours: 9:00-10:00am TTh, 3:30-5:00pm W, other times by appointment

Prerequisites: CE 475 Water Quality Chemistry (or equivalent aquatic chemistry course)

Description: This course focuses on prediction of the fate and transport of anthropogenic organic chemicals in aquatic environments. The course is divided into two major subjects: (1) physical transformations ($^{3}/_{4}$ content), and (2) chemical transformations ($^{1}/_{4}$ content). The physical transformations include sorption, volatilization, and uptake, the processes that control the distribution of organic chemicals between the phases of interest: water, soil, air, biota. The chemical transformations include hydrolysis, redox, and biologically-mediated reactions that control the breakdown of organic chemicals. Throughout both subjects, we will develop predictive relationships for the parameters that control the fate and transport of organic chemicals by developing a thorough understanding of the chemical structure of the organic chemicals.

Objectives: (1) Understand the basics of organic compound structure and its role in contaminant transformations; (2) Apply these basics to predict the fate and transport of these compounds; and (3) Solve problems of environmental importance.

Textbook: Environmental Organic Chemistry 2nd Ed (2003) R.P. Schwarzenbach, P.M. Gschwend

and D.M. Imboden, Wiley, New York, NY, ISBN 0-471-35750-2.

Relevant Textbooks and References:

Baum E.J. (1998) <u>Chemical Property Estimation: Theory and Application</u>. Lewis Publishers, Boca Raton, FL.

Chiou C.T. (2002) <u>Adsorption and Partition of Organic Contaminants in Environmental Systems</u>. Wiley, New York.

Lyman W.J., Reehl W.F., and Rosenblatt D.H. (1982) <u>Handbook of Chemical Property Estimation</u> <u>Methods: Environmental Behavior of Organic Compounds</u>. McGraw-Hill, New York (out of print).

MacKay D. (1992 to 1997) <u>Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals</u>, Lewis Publishers, five volumes for different classes of organic chemicals.

Boethling, R.S. and MacKay D. (2000) <u>Handbook of Property Estimation Methods for Environmental</u> and Health Science. CRC Press.

Montgomery J.H. (1996) Groundwater Chemicals Desk Reference. CRC Press, Boca Raton, Florida.

Schwarzenbach R.P., Gschwend P.M., and Imboden D.M. (1995) <u>Environmental Organic Chemistry: Illustrative Examples, Problems, and Case Studies</u>. Wiley-Interscience, New York.

Budavari S. et al. (1996) The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals, 12th Ed. Chapman & Hall.

Lide D.R. (1999) <u>CRC Handbook of Chemistry and Physics 1999-2000, 80th Ed.</u> Chemical Rubber Company Press

Course Web Page: The ANGEL course management system will be used to communicate with students, to post lecture notes, homework assignments (and solutions) and exams, and as a link to other relevant reference material. I expect that you will check the web page and your e-mail regularly, particularly before assignments are due.

Grading:

with final exam		without final exam	
5 Homework Assignments @ 10% each	50	5 Homework Assignments @ 10% each	50
3 Examinations @ 17% each	<u>51</u>	2 Examinations @ 25% each	<u>50</u>
Total	101	Total	100

Homework Assignments: Students are encouraged to try all suggested homework problems listed in the syllabus below. Additional homework problems will also be assigned. A smaller subset of problems will be collected five times over the semester. Homework assignments will be given to develop your problem-solving ability and likely will be the most effective means to learn the material. Solutions will be made available on the course web page on the due date for each assignment. No credit will be given for late problem sets. Collaboration is encouraged; however, be sure that you fully understand the concepts and problem-solving approaches to succeed on the exams.

Examinations: Exams #1 and #2 will be take-home, 24-hour open-book, closed-colleague exams. Exams #1 and #2 will posted on ANGEL at approximately 10am on the Th before they are due. Exams will focus on the most recent course material, however, any previous material covered in class may appear in Exams #2 and #3. Exam#3 will be optional. Exam #3 will be an in-class, 2-hour open-book, exam scheduled during the final exam period.

Disclaimer: Due to the variable and unpredictable pace of this course, the syllabus and grading formula are strictly tentative, and the instructor may add or subtract one homework assignment or one exam at his discretion. The final grading formula would then be adjusted accordingly. Due to my travel to research meetings, up to three class periods will likely be canceled over the course of the semester.

CE 573 COURSE SYLLABUS, Spring 2007:

Dates	Lecture Topics	Reading	Assignments
01/17 – 01/19	Introduction; Organic Chemistry Review	EOC - Ch 1, 2	Q2.2, 5, 7, 9, 10, 11, 13, 15, 18, 20; P2.1
01/22 – 01/29	Thermodynamics	EOC - Ch 3	Q3.2, 3, 4, 6, 9; P3.1 HW #1 (Ch 2 & 3) due F 01/26
01/31 – 02/09	Vapor Pressure	<i>EOC</i> - Ch 4	Q4.1, 3, 5, 8, 9; P4.1, 2, 4, 6 HW #2 (Ch 4 & 5) due F 02/09
02/12 - 02/19	Water Solubility	<i>EOC</i> - Ch 5	Q5.2, 3, 4, 6, 7; P5.1, 3, 5, 6, 8
	Exam #1 – Ch 1 - 5 posted Th 02/22 due Fr 02/23		
02/21 – 02/28	Air-Solvent, Air-Water Partitioning	EOC - Ch 6	Q6.3, 4, 6, 8; P6.1, 2, 3, 6
03/02 - 03/19 (no class 03/12-16)	Octanol-Water Partitioning	EOC - Ch 7	Q7.2, 3, 4, 7, 8, 9; P7.1, 2, 4, 6 HW #3 (Ch 6 & 7) due F 03/09
03/21 – 03/30	Sorption to Organic Matter	<i>EOC</i> - Ch 9	Q9.2, 3, 5, 8, 9, 10; P9.1, 3, 7 HW #4 (Ch 9 – 11) due F 03/30
04/02 - 04/06	Sorption to Biomedia	<i>EOC</i> - Ch 10	Q10.2, 5, 8, 9; P10.1, 2, 3
04/09 - 04/13	Sorption to Mineral Surfaces	EOC - Ch 11	Q11.3, 4, 7, 9, 10; P11.2, 5, 7, 9, 12
	Exam #2 – Ch 6, 7, 9 - 11 posted Th 04/12 due Fr 04/13		
04/16 - 04/20	Thermodynamics and Kinetics of Transformation Reactions	<i>EOC</i> - Ch 12	Q12.2, 4, 5, 7, 9, 10, 16; P12.1, 2, 3
04/23 - 04/27	Hydrolysis/Substitution Reactions	<i>EOC</i> - Ch 13	Q13.1, 4, 8, 9, 13; P13.3*, 2, 8 HW #5 (Ch 12 – 14, 17) due F 04/27
04/30 - 05/04	Redox Reactions	EOC - Ch 14 EOC - Ch 17	Q14.2, 4, 8, 10, 11; P14.1, 3, 5, 6 Q17.1, 3, 4; P17.1
finals week	Exam #3 in-class		