COURSE SYLLABUS

Spring 2017

CHE 470 Analytical Chemistry of Pollutants / CHE 516 Environmental Chemistry

Location: 209 NORTON
Time: Tue/Thu, 9:30 AM - 10:50 AM
Instructor: Dr. Diana S. Aga
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Office Hours: Mon/Wed 1:00-2:00, or by Appointment

This course will focus on the role of *Analytical Chemistry* in investigating the fate and transport of chemical pollutants in the environment. This class will require students to submit an independent research paper at the end of the semester. We will discuss the fundamentals of environmental sampling, sample preparation, and trace analysis using modern instrumental techniques. Students will learn how to interpret mass spectra, generate calibration curves for trace analysis, and quantify contaminants from the chromatograms using various methods (e.g. standard addition, isotope dilution mass spectrometry, external versus internal curve, use of internal standards). Focus will be on the analysis of persistent organic pollutants, pesticides, heavy metals, pharmaceutical compounds, and other emerging contaminants in various environmental compartments. Topics will also include a discussion on the physico-chemical factors that affect the persistence, mobility, and distribution of pollutants in soil, water, atmosphere, and biota. We will be discussing recent research and review articles from the *Journal of Environmental Science and Technology* or other relevant journals to familiarize the students with current and emerging issues in environmental science. In addition, guest lecturers will be invited to present on-going research activities in their groups in order to familiarize the students with a wide range of environmentally-relevant topics. At the end of this course, the students will learn how to select the most activities appropriate analytical tool for a particular environmental investigation based on their knowledge of the chemical and physical properties of pollutants. Students will also gain knowledge on the impacts of chemical pollutants on wildlife, human health, and the environment as a whole.

Main References:

- Environmental Chemistry: A global perspective (2nd edition) by Gary W. vanLoon
- Environmental Chemistry (4th edition) by Colin Baird and Michael Cann
- Environmental Organic Chemistry, by Rene P. Schwarzenbach, et al.
- Journal of Environmental Science and Technology, and other relevant journals

Grade Distribution:

For Students Enrolled in CHE 470:

Quizzes, Homework, Class Activities	25%
2 Exams	40%
Journal articles / Seminar Questions	20%
Research Paper (written only)	15%

For Students Enrolled in CHE 516:

Quizzes, Homework, Class Activities	20%
2 Exams	40%
Journal articles / Seminar Questions	20%
Research Paper (50% written report and 50% class presentation)	20%

TOPICS

I. Physico-chemical Properties of Contaminants Affecting Fate, Transport, and Toxicity

In order to clearly understand the environmental chemistry and toxicology of chemical contaminants it is critical to have knowledge on the nature of their physico-chemical properties. For instance, physical properties of greatest importance are water solubility, vapor pressure, Henry's law constant (H), octanol-water partition coefficient (Kow), and the organic carbon-water partition coefficient (Koc). In addition, chemical properties that are likely to influence the persistence, mobility, bioavailability, and toxicity include the structural makeup of the molecules and are often associated with greater degrees of halogenation. Chemicals that are considered persistent organic pollutants like DDT (dichlorodiphenyltrichloroethane) and the chlordanes, PCBs (polychlorinated biphenyls), PBDEs (polybrominated diphenylethers), and polychlorinated dioxins and furans have physico-chemical properties that favor sufficiently high atmospheric concentrations, resulting in global redistribution by evaporation and atmospheric transport. In this course, we will devote some time to review basic concepts on molecular structures that influence the hydrophibicity or hydrophilicity of chemicals, and learn factors that affect a chemical's H, Kow, and Koc values. We will discuss how these parameters can be used to predict fate and transport of the chemical contaminants in the environment, and how they affect the bioavailability and toxicity of chemicals to humans and wildlife.

II. Fundamentals of Environmental Sample Preparation and Analysis

Scientist's understanding of the environment depends highly on their knowledge of the identities and quantities of pollutants in water, air, soil and biological systems. Therefore, it is of utmost importance that environmental scientists and engineers are at least familiar with the fundamental concepts of sampling and chemical analysis, so that state-of-the art techniques can be properly employed. New and improved analytical techniques have enabled detection of pollutants at much lower levels, and at a vastly increased data throughput. The challenge therefore lies on the overwhelming data analysis and interpretation of results that could lead to meaningful conclusions. Hence, the quality and choice of analyses is much more important than the number of analyses performed, because more carefully planned analyses would yield more useful information. In this section of the course, general aspects of environmental chemical analysis, and the major techniques and instrumentation used in organic and inorganic analysis will be discussed. In addition, the advantages and limitations of each technique will be emphasized in order for the students to learn how to choose the proper instrumentation to answer a specific environmental problem.

The following topics will be included:

- Basic concepts of quantitative analysis (standard curves, standard addition, internal standards, isotope dilution, quality assurance, quality control)
- Modern techniques in sample preparation:
    1. Accelerated solvent extraction (ASE)
    2. Solid phase extraction (SPE)
- Spectroscopic analysis (UV-Vis spectroscopy, atomic absorption spectroscopy)
- Chromatographic analysis: liquid chromatography (LC), gas chromatography (GC)
- Derivatization of analytes to make them amenable to instrumental analysis
- Mass spectrometry (LC/MS, GC/MS, inductively coupled plasma/mass spectrometry)
- Metal analysis and speciation

III. Chemical Pollution in the Aquatic Environment

Waterborne toxic chemicals pose a great threat to the safety of water supplies in developing and industrialized countries alike. Sources of chemical contamination include wastes from industrial chemical production, metal plating operations, and pesticide runoff from agricultural lands. Understanding the sources, interactions, and effects of water pollutants is essential for controlling pollutants in an environmentally safe and economically acceptable manner. Most importantly, understanding of water pollution and its control depends upon basic knowledge of aquatic environmental chemistry. That is why this course will cover principles of aquatic chemistry, sediment-water interactions, and other factors involved in the reactions, transport, and effects of chemical pollutants. Specifically, we will focus our discussion on the environmental chemistry, fate, and sources of halogenated industrial chemicals (e.g. PCBs, PBDEs), endocrine disrupting chemicals (e.g. estrogens and other hormones), personal care products (e.g. triclosan and musks), pharmaceutical compounds (e.g. antibiotics and other drugs), and pesticides (e.g. atrazine) that have been detected in the aquatic environment due to their large usage and persistence.

IV. Analysis and Treatment of Selected Contaminants, and Identification of their By-products

Some chemical pollutants may be degraded in the environment, but the degradation product is not necessarily less toxic than the parent compound. For example, abiotic degradation of pharmaceuticals due to exposure to sunlight might produce photodegradation products that have significant biological activity, as has been observed for the photodegradates of robenidine, an anticoccidial drug used in poultry. Therefore, it is important to consider the transformation pathways and identify by-products of chemical degradation of pollutants. Persistent degradation by-products of contaminants require consideration for risk assessment because the effects resulting from exposure to a mixture of parent compound and its by-products may be quite different from what could be observed based on toxicity tests using only a single compound. In addition to degradation by-products, chemical derivatives may also form during abiotic treatment (such as chlorination, ozonation, or ultraviolet [UV] exposure) employed in disinfection and/or advanced oxidation processes in water treatment. In most of the investigations reported to date, the efficiency of pharmaceutical removal during water treatment is determined by measuring the disappearance of the parent compound, but not the formation of by-products. Little attention has been given to the identification, let alone quantification, of transformation products formed during water treatment. Consequently, available information on the environmental fate and occurrence of excreted pharmaceutical metabolites formed during drug metabolism in humans and animals are scarce. Hence, this portion of the course will cover analysis of specific examples of contaminants and their degradation products in the environment. Modern techniques used in the identification of unknown degradation by-products of chemical contaminants will be discussed.