

CEE 697K - ENVIRONMENTAL REACTION KINETICS
Fall Semester 2013

TuTh 2:30-3:45 (Mrst 15)

Course Description: CEE 697K: Environmental Reaction Kinetics. Environmental Engineers are increasingly called upon to analyze the speed of pollutant conversion in chemical and biological systems. These may be engineered systems such as water and wastewater treatment plants, or natural systems, such as lakes and aquifers receiving industrial pollution. This course examines the rates and kinetics of a range of chemical and biological systems important to Environmental Engineers. These systems are limited to the aqueous phase at atmospheric pressure and near ambient temperature. The fundamentals of kinetic theory are briefly covered. Mathematic simulation of kinetic systems and analysis of kinetic data are examined. Several case studies of importance in Environmental Engineering are explored in detail. Prerequisites are CEE 370, Chem 111, Chem 112 and CEE 680 or equivalent.

Textbook: Brezonik, P.L. Chemical Kinetics and Process Dynamics in Aquatic Systems, 1994, Lewis Publishers, Ann Arbor, MI.

References: Moore, J.W. and Pearson, R.G. Kinetics and Mechanism, 3rd Ed., 1981, J. Wiley & Sons., New York

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Objectives:

1. To become familiar with the fundamentals of chemical kinetics.
2. To learn how to design kinetic studies and interpret the results.
3. To understand the theoretical impacts of changes in physical, chemical and biochemical conditions on the anticipated rate of environmental processes, and
4. To gain detailed understanding of the kinetics of a few selected processes of significance to Environmental Engineers.

Prerequisites by Topic:

1. Basic understanding of environmental engineering and the significance of environmental parameters (e.g., CEE 370).
2. Knowledge of chemical equilibria in natural waters (e.g., CE 680).
3. Understanding of chemical and biological systems in Environmental Engineering (e.g., CEE 471)

- Goals:
1. To provide a fundamental understanding of the means by which kinetic models are formulated so that the students are able to adapt existing models to new situations.
 2. To provide the students with some direct exposure to kinetic models currently used in environmental engineering practice. This will equip them with the knowledge to apply such models to help with design and operation of treatment systems
 3. To instruct as to how kinetic data can be analyzed and interpreted
 4. To show how kinetic models may be calibrated, verified, and applied to environmental engineering problems.
 5. To further develop the students' skills at working in teams, and presenting results in the form of written engineering reports and oral presentations to clients or to the public.
 6. To acquaint the student with current issues in environmental kinetics; and to make them aware of the technical, political, ethical and sociological components of these issues.

Topics:

Reading:

- | | |
|---|--------------------|
| 1. Introduction | Pg 1-21 |
| 2. Rate Expressions | Pg 25-53 |
| a. Elementary Reactions | |
| b. Competitive Reactions | |
| c. Sequential Reactions | |
| d. Chain Reactions | |
| 3. Analysis of Kinetic Data | Pg 53-101 |
| a. Differential, Integral and Initial Rate Methods | |
| b. Dealing with Uncertainty | |
| c. Determining rate equations from proposed mechanisms | |
| d. Inferring mechanisms from rate equations | |
| e. Experimental Aspects | |
| 4. Mathematic Simulation of Chemical Reactions | (Scientist 2.01) |
| 5. Theoretical Aspects | Pg 109-162 |
| a. Temperature Dependence | |
| b. Properties of Water and Reactants | |
| c. Encounter Theory | |
| d. Transition State Theory | |
| e. Pressure Effects | |
| f. Ionic Strength Effects | |
| 6. Reaction Catalysis (non-enzymatic) | Pg 167-193 |
| 7. Environmental Engineering Case Studies | Pg 194-273 |
| a. Metals hydrolysis | |
| b. Hydrolysis of organics | |
| c. Chlorination | |
| d. Oxidation of Iron and Manganese | |
| e. Oxidation of Organic Compounds in Biological Systems | |
| 8. Enzyme Reactions | Pg 419-547 |
| 9. Linear Free Energy Relationships | Pg 553-634 |
| 10. Surface Reactions | Pg 292-325 & other |

Grading Criteria

Mid-term Exam	15 %
Final Exam	25%
Homework/projects/critiques	<u>60%</u>
	100%