

16:375:527 Spring Semester

Physicochemical Process Dynamics in Environmental Systems

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Description: This course covers fundamentals of process dynamics analysis and modeling in natural and engineered environmental systems. Major topics include chemical reaction thermodynamics and reaction kinetics, transport processes (advection and dispersion), molecular diffusion process at the particle scale, interphase mass transfer (rate and equilibrium), and reactor design. Reactions in homogeneous and heterogeneous systems, air stripping, gas-liquid absorption, liquid-solid adsorption processes and particle-particle interactions for water and air quality control are also discussed.

Objectives:

- Able to understand the fundamentals of a specific process (e.g., transport, chemical kinetics, mass transfer) and parameterize it from experimental tests;
- Able to analyze thermodynamics and kinetics of complex environmental reactions;
- Able to set up governing equations for describing major transport, mass transfer, and reaction processes in both natural and engineered systems;
- Able to define initial and boundary conditions and make appropriate assumptions to solve simplified governing equations for various engineering design and modeling applications;
- Able to design physicochemical process-based reactor systems for water and air quality control.

Grading:	Exam I + II	60%
	Term Paper + Presentation	25%
	Homework	15%

Textbook:

Environmental Systems and Processes: Principles, Modeling, and Design, by W.J. Weber, Jr., Wiley-Interscience, New York, 2001.

References:

Process Dynamics in Environmental Systems, by W.J. Weber, Jr. and F.A. DiGiano, John Wiley & Sons, Inc. New York, 1996.

Chemical Reaction Engineering, 3rd Ed, by O. Levenspiel, John Wiley & Sons, Inc. New York, 1999.

Mass Transfer Operations, 2nd Ed, by R. E. Treybal, McGraw-Hill, New York, 1996.

The Mathematics of Diffusion, 2nd Ed, by J. Crank, Pergamon Press Ltd., Oxford, 1975.

Transport Modeling for Environmental Engineers and Scientists, by M. M. Clark, John Wiley & Sons, Inc. New York, 1996.

- Notes:** 1) There will be seven (7) individual homework assignments during the semester. Each homework assignment is to be submitted at the beginning of class or on the designated deadline. Assignments submitted through e-mail or fax, in photocopied forms will not be accepted. ***There will be no credit given for late responses to assignments.***
- 2) There will be two equally-weighted close-book exams. If a student must miss an exam or a lecture due to illness or other extenuating circumstance, the instructor must be notified prior to the time of the examination or lecture.
- 3) Attendance at each lecture is ***required.***
- 4) Receiving or providing unauthorized assistance on examinations is prohibited, and reporting any violations observed is required. Additionally, the use of homework solutions completed by others (in either this semester or a previous semester) in preparing an assignment is not allowed. You are encouraged to discuss homework assignments with other students, but you must do all of your own work (writing, spreadsheets, graphs, tables, etc.).

Algorithm for Solving Environmental Engineering Problems

1. Draw a picture, label the knowns and unknowns;
2. State any required assumptions;
3. Identify boundary and initial conditions;
4. Write the full governing equations;
5. Simplify the governing equations based on assumptions;
6. Solve the equation algebraically;
7. Apply initial conditions and boundary conditions to determine the constants of integration;
8. Substitute in numerical values if required and solve for the unknown numerical solution.

Major Topics

Introduction to process dynamics analysis
Conservation of mass, energy and momentum
Continuity equation and plug flow reactor (PFR) systems
Mass balance based models: PFRs, CMBR and CMFRs
Dispersion process analysis
Reactor design
Diffusion processes
Interphase mass transfer and aeration process analysis
Intermolecular forces
Surface chemistry and particle-particle interactions
Chemical kinetics
Environmental catalysts
Sorption processes
Process dynamics analysis for complex systems
Term paper presentation

HOMEWORK FORMAT

The following items are required for your homework assignments. However, you will find that these items constitute a rational approach toward completing any engineering problem. Following this procedure will help you better understand your solution rationale when you refer back to the problem at a later date.

1. Always start a new problem on a new sheet
2. Write legibly. Print if necessary. If what you have written can't be read, you may not get full credit, even if the answer is correct.
3. If appropriate, draw a picture or schematic and label its important components, both knowns and unknowns.
4. List initially defined variables at the top of the page, giving definitions, values and units. Variables defined later should be prominently placed and identified in the solution derivation.
5. **STATE ALL ASSUMPTIONS**, including initial and/or boundary conditions. Making and stating your assumptions for peer review is a critical engineering/communication skill.
6. Write the full governing equation that you are basing your solution upon, then simplify that equation based upon the assumptions you have made. Indicate what your limits of integration, etc. represent.
7. Annotate, comment, or explain calculations. Add brief comments every few steps about what you're doing. A long list of equations is hard to follow, especially if there are errors. Often it helps to write "word" equations to clarify your objective. This also helps when you need to refer to your work at a later date.
8. **ALWAYS USE UNITS**. Include units on all numerical values and make sure that they are all consistent with the desired units of the final answer. Keeping track of units helps to solve a problem by identifying deficiencies or inconsistencies in the variables used to describe a system.
- 9 Always express your governing equation(s) and appropriate boundary and initial conditions completely in variable form before you substitute numerical values. It is often easier to leave all quantities as variables during intermediate steps and substitute numbers only during the very last steps.
10. If appropriate, plot your results. Plots should be done via computer (hand-drawn plots are not acceptable). If a question asks you to express a variable as a function of time, provide both the algebraic equation and a plot of the variable over time.
11. If a question asks you to compare two or more values, provide a brief discussion of why they are the same or different (i.e., do not simply state that they are equal or one is less than the other). The explanation should be brief but substantial (i.e., 1/4 of a page or so - enough to demonstrate your understanding of the concept.)
12. Circle or otherwise clearly label final answers. If you consistently do not circle your answers, you may not get full credit, even if the answer is correct.

Useful Sources of Process and/or Design Information

(updated Fall 2013)

American Water Works Association, Water Quality and Treatment, 5th ed., McGraw-Hill Book Company, New York, NY, 1999.

Balzhiser, Richard E. and Michael R. Samuels, Engineering Thermodynamics, Prentice-Hall, Englewood Cliffs, NJ, 1977.

Bennett and Meyers, Momentum, Heat and Mass Transfer.

CRC Handbook of Chemistry and Physics, 58th ed., McGraw-Hill Book Company, New York, NY, 1982.

Culp, Wesner and Culp, Handbook of Public Water Systems, New York, NY, 1986.

Cussler, E.L., Diffusion, Mass Transfer in Fluid Systems, Cambridge University Press, Cambridge, 1984.

Degremont, Water Treatment Handbook, 6th ed., Halsted Press, New York, NY, 1991.

Fair, Geyer and Okun, Water and Wastewater Engineering, John Wiley & Sons, New York, NY.

Henley, Ernest J. and J.D. Seader, Equilibrium-Stage Separation Operations in Chemical Engineering, John Wiley & Sons, New York, NY, 1981.

James M. Montgomery, Water Treatment Principles and Design, 2nd Edition, John Wiley & Sons, New York, NY, 2006.

Lyman, Warren J., William F. Reehl and David H. Rosenblatt, Handbook of Chemical Property Estimation Methods: Environmental Behavior of Organic Compounds, McGraw-Hill Book Company, New York, NY, 1982.

McCabe, Warren L., Julian C. Smith and Peter Harriott, Unit Operations of Chemical Engineering, 4th ed., McGraw-Hill Book Company, New York, NY, 1985.

Metcalf and Eddy, Inc., Wastewater Engineering: Treatment/Disposal/Reuse, 3rd ed., McGraw-Hill Book Company, New York, NY, 1991.

Perry, Robert H. and Cecil H. Chilton, Chemical Engineers' Handbook, 5th ed., McGraw-Hill Book Company, New York, NY, 1973.

Reid, Robert C., John M. Prausnitz and Bruce E. Poling, The Properties of Gases and Liquids. 4th ed., McGraw-Hill Book Company, New York, NY, 1987.

Reynolds, Unit Operations in Environmental Engineering, Brooks and Cole.

Sanks, Robert L., Water Treatment Plant Design for the Practicing Engineer, Ann Arbor Science Publishers, Ann Arbor, MI, 1978.

Schweitzer, Philip A. Handbook of Separation Techniques for Chemical Engineers, 2nd ed., John Wiley & Sons, New York, NY, 1987.

Stumm, Werner, Aquatic Surface Chemistry: Chemical Processes at the Particle-Water Interface, John Wiley & Sons, New York, NY, 1997.

Treybal, Robert E., Mass-Transfer Operations, 3rd ed., McGraw-Hill Book Company, New York, NY.

Verschueren, Karel, Handbook of Environmental Data on Organic Chemicals, Van Nostrand Reinhold Company, New York, NY, 1977.

Vesilind, P. Aarne, Treatment and Disposal of Wastewater Sludges, Ann Arbor Science Publishers, Ann Arbor, MI.

Weber, Walter J., Jr., DiGiano F.A., Process Dynamics in Environmental Systems, John Wiley & Sons, Inc., New York, NY, 1996.

Weber, Walter J., Jr., Physicochemical Processes for Water Quality Control, John Wiley & Sons, Inc., New York, NY, 1972.

U.S. EPA Design Manuals.

Water Pollution Control Federation Manuals of Practice.

Proceedings Annual Purdue University Industrial Waste Conference.

JOURNALS:

American Water Works Association, American Water Works Association.

Chemical Engineering Progress, American Institute of Chemical Engineers.

Chemical Engineering, McGraw-Hill, Inc.

Environmental Progress

Environmental Science and Technology, American Chemical Society.

Industrial Engineer Chemical Fundamentals, American Chemical Society.

Journal of Environmental Engineering

Research Journal of the Water Pollution Control Federation, Water Pollution Control Federation.

Water Environment and Technology, Water Pollution Control Federation.

Water Research, (Journal of the International Association on Water Pollution Research and Control), Pergamon Press.