

Water Quality Modeling: EAS 4803/8803

3 credit hours

Required Textbook: Chen Zhu and Greg Anderson, "**Environmental Applications of Geochemical Modeling**" Cambridge University Press, Cambridge, UK, ISBN 0 521 00577 9. www.barnesandnoble.com or www.half.com (?)

Other sources: J. I. Drever, "The Geochemistry of Natural Waters." C. M. Bethke, "Geochemical Reaction Modeling." Research papers to be suggested as we go along.

Instructor: Andrew G. Stack

Office Hours: 10-11 MWF or by appointment. Office is ES&T 3240. Phone: 404-894-3895.
E-mail: andrew.stack@eas.gatech.edu

Course Summary:

The focus of this course is to gain hands-on experience in modeling using the geochemical software packages commonly found in the environmental consulting industry. In addition to becoming familiar with these software packages, students will gain a better understanding of the governing geochemical principles pertaining to the movement and transformation of contaminants as well as other species in the subsurface through a series of applied case studies. The regulatory environment in which environmental consulting is done and implications for society are discussed as well.

Format:

The course will be a mixture of lectures, discussion and computer work. With a small class, hopefully we will get a large part of the computer modeling done in class. A large number of the homework exercises will be from the textbook, but some additions. Discussions will be based on issues facing large segments of society where geochemical modeling is being used (e.g., nuclear waste disposal, mining, current events, etc.). Graduate students will need to conduct a research project and give a brief presentation to the class. Hopefully you will be able to pick a project that will be useful with your own research. Grades will be based on the exercises, class participation and the presentation.

Course Material:

Background

- Needs for Water Quality Modeling
- Regulatory Framework (EPA drinking water standards, CERCLA and Superfund)
- Limitations on current models

Molecular Diffusion and Dispersion

- Basic Concepts: diffusion and dispersion.
- Heterogeneities and Scale Length
- Fractured versus porous flow

Case study: Yucca Mountain Nuclear Waste Repository

Equilibrium Speciation and Solubility Modeling

Review of thermodynamics and matrices

How speciation models work

Software package: MINTEQA2

case study: Sea water

case study: Uranium mill tailings pond

Surface Adsorption

Soil mineral surface composition

Linear distribution coefficient

Langmuir and Freundlich isotherms

Surface complexation models

case studies: mobility of radionuclides at Oak Ridge and Uranium Mills tailings

Impoundment

Reaction Path Modeling

Alkalinity titrations

case studies: Acid mine waste

Software packages: PHREEQC, PHRQPITZ

case studies: legacy contamination from bomb making, (nuclear) Waste Isolation Pilot Plant, and brines

Kinetics modeling

Review of kinetics

Software package: EQ3/6

case study: CO₂ sequestration as a solution for global climate change

Miscellaneous (if time permits)

Modeling mixing

case study: Tritium box model

Software package: NETPATH

case study: acid rain

case study: Black Mesa groundwater genesis

Honor Code:

Students in this class are expected to abide by the Georgia Tech Honor Code and avoid any instances of academic misconduct, including but not limited to:

1. Possessing, using, or exchanging improperly acquired written or oral information in the preparation of a paper or for an exam.

2. Substitution of material that is wholly or substantially identical to that created or published by another individual or individuals.
3. False claims of performance or work that has been submitted by the student.

That said, students are encouraged to help each other when getting the programs to run, but write-up is to be done individually!