

# Chemical Hydrogeology and Solute Transport: GLY-5828

Meeting time: 5:00-6:30 pm T, Th

Meeting location: PC-323

Course Level: Graduate 5828

Sections: 1

## **Course Catalogue Description**

GLY 5828 Chemical Hydrogeology and Solute Transport (3). Quantitative analysis of hydrologic, geologic, and chemical factors controlling water quality and the transport and fate of organic and inorganic solutes in the subsurface. Prerequisites: GLY 5827. (S)

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Department: Earth Sciences

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Office Hours: T, Th 1 to 3 pm, walk-in, and by appointment (best to arrange via e-mail)

## **Course Objectives**

Students should have thorough familiarity with various concentration units in use. They should understand the concepts of relative concentration, pore volume, and Peclet number. Students should know the difference between the dispersion coefficient and the dispersivity and know how to estimate the dispersivity. They should be familiar with the three major adsorption isotherms utilized in porous media solute transport and know how to estimate the linear distribution coefficient from tabulated data. Students should be able to mathematically state initial and boundary conditions pertinent to a given physical solute transport problem. Students should be able to derive the governing equations for solute transport in porous media and derive finite difference expressions for their solution. Students should be able to numerically solve the convection-dispersion problem for any boundary and initial conditions. They should be capable of inversely modeling solute transport problems to obtain the transport parameters. Students should understand the density effects of solutes and temperature differences and be able to model solute transport in MODFLOW/MT3DMS.

## **Outline**

1. Review
  - a. Math
    - i. Calculus
      1. Slopes
      2. Derivatives
      3. Partial derivatives
      4. Numerical derivatives
  - b. Tools
    - i. Excel 'tricks'

- ii. Matlab
      - 1. surface plots
      - 2. contouring
      - 3. gradient function
      - 4. quiver plots
    - iii. Mathematica
  - c. Ground Water
    - i. Flux and Darcy's Law
    - ii. Average pore water velocity
    - iii. Boundary value problems
    - iv. Numerical solution
- 2. 1-D Chemical Transport
  - a. Diffusion Equation
    - i. Derivation of PDE for 1-D Diffusion
    - ii. Boundary conditions
      - 1. Constant concentration boundaries (Dirichlet BC)
      - 2. No flux boundaries (Neumann BC)
    - iii. Initial conditions (Heaviside functions)
    - iv. Analytical solutions
    - v. Finite difference solution
    - vi. Excel model
    - vii. Mathematica
    - viii. Diffusion in porous media
- 3. Dispersion
  - a. Mechanisms
  - b. Poiseuille flow/Taylor dispersion
  - c. Estimating dispersion
    - i. Peclet number correlations
    - ii. Scale correlations
- 4. Convection Dispersion Equation
  - a. Derivation of PDE for CDE
  - b. Boundary and initial conditions
  - c. Analytical solutions
  - d. Peclet, column Peclet (Brenner), and grid Peclet numbers
  - e. Finite difference solution
    - i. Numerical dispersion
    - ii. Grid Peclet number
  - f. Excel model
  - g. Mathematica
  - h. Inverse modeling of solute transport; CXTFIT/STANMOD
- 5. Retardation
  - a.  $K_d$ , linear isotherm
  - b.  $K_{oc}$
  - c. Freundlich isotherm
    - i. Linearizing Freundlich isotherms
  - d. Langmuir isotherm

- e. Measuring isotherms
  - i. Solid/solution ratio
- f. Sorption kinetics
- g. Anion exclusion
- 6. Zero and first order decay and production
- 7. 2- and 3-D analytical solutions
- 8. Particle Tracking/Pathline Models
- 9. MT3D/STANMOD
- 10. Two-Region Model
- 11. Two-Site Model
- 12. FADE
  - a. Levy flights and distributions
- 13. CTRW
- 14. Vapor phase diffusion
  - a. Henry's law
  - b. VLEACH
- 15. Solute and temperature-coupled density-driven flows

### ***Assignment Dates***

Weekly assignments will be handed out on Thursday and will be due the following Tuesday.

### ***Performance Measures, Grading/Attendance Standards***

**Attendance:** Participation in classroom instruction and computer exercises is critical to successful completion of this course. More than 3 unexcused absences will result in one letter grade reduction.

**Homework:** Homework assignments will be given weekly and will generally consist of short reports on specific exercises usually including modeling and comparison with analytical solutions. English, spelling, units, significant figures, quality of graphics, accuracy of analysis, and quality of evaluation will all be considered in grading the homework. You are encouraged to work together to develop your understanding, but you must complete all assignments yourself; copying the work of others (including from the Internet) is unacceptable and will result in a grade of F for the course. Late homework will be reduced 25% for each late day. These assignments will account for 1/2 of your grade.

**Quizzes:** 1/8 of grade. 10-minute quizzes will be administered weekly or as appropriate following completion of the homework assignment. The sum of all quiz grades will be weighted to account for 1/8 of your overall course grade.

**Examinations:** 1/8 of grade each. One mid-term and one final examination will focus on concepts, theory, derivations, and practical computations associated with solute transport. Examinations will be based on lecture, homework, and quiz material.

**Projects/Presentations:** An in-class presentation of a final project consisting of a solute transport modeling effort will constitute 1/8 of your grade. Your presentation will be graded on content and professional quality. You will submit a one page description of your project concept early in the semester. Individual and group projects are possible, but equal effort (and a regular full presentation) is expected from each group project participant. Presentations will be at the end of the semester.

### ***Policy for make-up work***

In general, there will be no make-up for homework, quizzes, examinations, and presentations.

### ***FIU's statement of academic misconduct policy***

"Florida International University is a community dedicated to generating and imparting knowledge through excellent teaching and research, the rigorous and respectful exchange of ideas, and community service. All students should respect the right of others to have an equitable opportunity to learn and honestly to demonstrate the quality of their learning. Therefore, all students are expected to adhere to a standard of academic conduct, which demonstrates respect for themselves, their fellow students, and the educational mission of the University. All students are deemed by the University to understand that if they are found responsible for academic misconduct, they will be subject to the Academic Misconduct procedures and sanctions, as outlined in the Student Handbook."

### ***Text***

None

### ***Bibliography***

Anderson M.P. and Woessner, W. (1992) Applied Groundwater Modeling: Simulation of Flow and Advective Transport, Academic Press.

Toride N., Leij, F.J. and van Genuchten, M. Th. (1995) The CXTFIT Code for estimating transport parameters from laboratory or field tracer experiments. Research Report No. 137, U.S. Salinity Laboratory, USDA-ARS, Riverside, CA.