Chemical Hydrogeology and Solute Transport: GLY-5828

Meeting time: T, Th 9:30 - 10:45
Meeting location: Academic Health Center (AHC) 5 357
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. (S)

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Office Hours: T, Th 11 am to noon, 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 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 transport parameters. Students should understand the density effects of solutes and temperature differences and be able to model solute transport with MODFLOW/MT3DMS or similar software.

Outline

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

            i. Excel 'tricks'
            ii. Python
                1. surface plots
                2. contouring
                3. gradient function
                4. quiver and stream 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)
    b. Diffusion Equation solutions
        i. Analytical solutions
        ii. Finite difference solution
        iii. Excel model
        iv. Mathematica
        v. 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. Kd, linear isotherm
    b. Koc
    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. Vapor phase diffusion
    a. Henry's law
    b. VLEACH/HYDRUS
13. 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 must submit a coherent report that explains the material presented. 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 and a minimum 5-page report on the results at the end of 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.

Text

None

Bibliography

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

Fetter; C.W., Thomas Boving, David Kreamer (2018) Contaminant Hydrogeology: Third Edition, Waveland Press.

Saez, A.E. and J.C. Baygents, (2015) Environmental Transport Phenomena, CRC Press, Boca Raton, FL

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.