Groundwater Flow and Solute Transport Modeling

GEOL 5030/4030
Spring, 2018
3 Credits

Dept. of Geology & Geophysics
University of Wyoming
Instructor: Ye Zhang

Grading: A/F (GEOL 5030) & S/U (GEOL 4030)
Lecture location: ESB1006
Lecture time: Tues + Thurs (9:35~10:50 am)
Office hours: Thurs (4:00~6:00 pm), GE 220
Email: yzhang9@uwyo.edu
Phone: 307-223-2292

Course Aims:
Movement of groundwater in the subsurface is responsible for a variety of environmental, engineering, and geological processes of importance. To evaluate them, mathematical modeling provides an essential quantitative tool. In recent years, increasing reliance is placed upon using computer simulations to make predictions of flow and transport in the subsurface, thus familiarity with the fundamental principles behind modeling is critical. This course presents an overview of the analyses of groundwater flow and solute transport using numerical modeling. The principles of the Finite Difference Method will be introduced. The following topics will be covered:

Modeling Overview
Mathematics Review
- *Differential Equations*
- *Scalar, Vector, Tensor*
- *Taylor Series & Finite Difference*
- *Error, Convergence, Stability*
- *Linear Algebra & Solutions*

Lumped Parameter Models
One-Dimensional Flow Modeling
- *Steady-state*
- *Transient*

Two-Dimensional Flow Modeling
- *Steady-state*
- *Transient*

Solute Transport Modeling
3D Flow and Transport Modeling (Groundwater Vista)
Advanced Topics (Optional & Topics may vary each year)
- *Tensor Analysis*
- *Upscaling*
- *Parameter Estimation*
- *Reactive Transport Modeling*

Learning Outcomes:
Students will learn how to derive and implement numerical approximations of ordinary and partial differential equations describing various subsurface flow and transport processes. They will learn how to construct models of flow and transport from 0 to 2 dimensions, for both steady-state and transient problems. They will understand the basic solution techniques including direct and iterative methods, as well as the distinction between matrix-based and matrix-free methods. They will write small computer codes using Matlab for simpler 1D to 2D problems, but will use a popular commercial software for three-dimensional flow and transport modeling.

Prerequisite:
Calculus I & II;

Geohydrology, <u>or</u> an equivalent introductory hydrology course, <u>or</u> instructor consent;

Matlab Programming language*

**This course emphasizes the fundamental development of mathematical models and their applications using computer simulations. Students are expected to write small computer codes, thus rudimentary skills in programming with Matlab are necessary. See two Matlab tutorials on my website (under Teaching): http://geofaculty.uwyo.edu/yzhang/ (it will take a few hours to complete).*

Attendance Policy:
Each student is expected to attend the lectures to fulfill the academic requirements. For participation in a University-sponsored activity or for unusual circumstances (personal hardship), an authorized absence may be issued to the student by the Director of Student Life or the Director's authorized representative. If a student produces the proof of absence, a makeup session can be arranged with the instructor. http://uwadmnweb.uwyo.edu/legal/Uniregs/ur713.htm

Course requirements:
This class is composed of 2 lectures per week. Students are expected to independently work out the class exercises, homework problems, lab projects, and exams. The instructor has developed a set of PowerPoint presentations as well as lecture notes for this class and will periodically post them in the course website via *Wyoweb*. The lecture notes however do <u>not</u> contain formula proofs, equation derivations and solutions to class exercises, so class attendance and participation are key to learning the materials.

Grading Policy:
In this course, emphasis is placed on the homework problems and lab projects due to the time-consuming nature of these assignments. The final grades will be given based on your homework, labs and term project (or exams). The appropriate percentage is shown:

Homework	42% (6% *x* 7 homework)
Lab/Project	40% (10% x 4 labs)
Term Project/Final Exam	18%

Note that each homework/lab/exam has a standalone grade of 100 points. When determining the final grade, these will be normalized reflecting the percentage distribution above. The final letter grade is given based on the numerical grade:

A	B	C	D	F
90-100	80-89	70-79	60-69	<60

The graduate students in the class will be graded using the +/- grading system; the undergraduate students will not. The undergraduate students will be given extra hints and help in homework and projects (e.g., code segments).

Textbook:
Course lectures and notes are key though below is a list of suggested textbooks:
(1) <u>Introduction to groundwater modeling: finite difference and finite element methods</u>, H. F. Wang and M. P. Anderson, 1995, Academic Press, 237 p.
(2) <u>Applied Groundwater Modeling: Simulation of Flow and Advective Transport</u>, M. P. Anderson and W. W. Woessner, 1992, Academic Press, 381 p.
(3) <u>Applied Contaminant Transport Modeling</u>, C. Zheng, G. D. Bennett, 2002, Wiley-Interscience, 656 p.

Concerning homework/lab/exams:
Four points must be emphasized: (1) For problems involving equations, if appropriate, provide a complete analysis rather than a single number. (2) Be professional in your presentations. If applicable, write down the unit for your results and round off the final number to 1 or 2 decimal points. (3) You can discuss the problems with fellow students, but complete your assignments by yourself. Copying other's work is considered cheating and no points will be given. (4) Hand in the homework on time. Finally, please keep

all course materials (notes, exercises, homework/exams/labs) to yourself and do not share them with future students. They must, as you have, work to earn the credit.

Tools:
Some exercise and homework problems can be solved by hand or using Excel spreadsheet. For others, computer modeling will be done using Matlab.

Questions & Answers
Questions for the instructor: (1) during lecture; (2) office hour.

Policy on Late homework, make-up exams, grade of incomplete:
Policy for this class:

- Unless otherwise stated, each homework is expected to be handed in to the instructor in the beginning of the class one week after the homework is assigned; If not handed in on time, each day it's delayed, 10 points will be taken out of the total grade (100) of that homework until no points remain. For a few small assignment, the homework will be handed in by the next class (this will be stated in class).

- Unless otherwise stated, each Lab project is expected to be completed and handed in the beginning of the next lab.

If a student can provide valid proofs of absence, the above rules do not apply. Within a reasonable time (1 week), the student is expected to hand in the late homework/lab to the instructor or arrange with the instructor on a make-up exam. It is the student's responsibility to contact the instructor to make arrangement in a timely manner and in advance if at all possible, failing to do so will result in the forfeiture of the relevant points.

Grade of incomplete:
During the semester, if a student has suffered severe problems (e.g., serious physical or mental incapacitation) and cannot complete the course as a result, he/she may be issued an "I" (incomplete) grade. The UW policy on how to make up for this grade is:
http://uwadmnweb.uwyo.edu/legal/Uniregs/ur720.htm

Academic dishonesty:
As defined by UW, academic dishonesty is: "*An act attempted or performed which misrepresents one's involvement in an academic task in any way, or permits another student to misrepresent the latter's involvement in an academic task by assisting the misrepresentation."* UW has a time-tested procedure to judge such cases, and serious penalties may be assessed. Please refer to UW Regulation 6-802 for details: http://www.uwyo.edu/generalcounselsupport/clean%20uw%20regulations/UW%20Reg%206-802.pdf

In this class, if a student is caught cheating, he or she will not only lose the full point of the assignment/test, but may also be assigned a "F" for the course. Plagiarism is considered a form of cheating. Both students will lose the full points on the particular homework or lab assignments. However, when writing papers, a student may cite other's work, but proper attribution must be given.

Students with disability:
Please refer to the University Disability Support Service: http://uwadmnweb.uwyo.edu/UDSS/

Disclaimer:
The syllabus is subject to changes as deemed necessary by the instructor. If a significant change were to be made, all students will be informed of it and given appropriate reasons for such a change.

Tentative Schedule

Week 1 **1/22 (Mon)**	**Introduction to the course.** *What is modeling? What kind of problems can models solve? What is the overall approach in modeling? What kind of skills can you acquire in this class?* ***Homework 1*** ***Review: Darcy's Law & Groundwater Flow Equations*** *Detail on equation derivations will be given in Geohydrology (GEOL 4444/5444), thus we give an overview only: general Flow EQ; 2D Planeview Flow; other simplifications.*
Week 2 **1/29**	**Modeling Overview** *Which Equation to solve? How do we specify boundary condition (Specified Head, Specified Flux, Mixed) for BVP? Analytical Versus Numerical Solutions; Common Numerical Methods; Definitions relevant to the Finite Difference Method (FDM); How to check the validity of numerical solutions; Model Calibration & Uncertainty; Homogenization (optional).* **Mathematics For this Class** *Differential Equations; Scalar, Vector, Tensor; Taylor Series & Finite Difference; Error, Convergence, Stability;*
Week 3 **2/5**	**Mathematics For this Class** *Linear Algebra & Solutions (Direct vs. Iterative; Matrix-Based vs. Matrix-Free)* ***Homework 2*** **Lumped Parameter Models (ODE)** *The Mass Balance Principle; Groundwater Stream Interaction; Analytical Solution;*
Week 4 **2/12**	**Lumped Parameter Models (ODE)** *Numerical Solution; Euler's Method; Huen's Method; Runga Kutta Method;* ***Homework 3*** **Lumped Parameter Models (ODE)** ***Project One****: Lumped parameter flow and transport modeling & calibration for groundwater contamination at Nantucket Island, Massachusetts (we'll use class time to discuss this project).*
Week 5 **2/19**	**One Dimensional Flow modeling** *1D Steady-State Flow (Homogeneous Media & Heterogeneous Media)* ***Homework 4*** *Numerical solution techniques (Direct Full matrix)*
Week 6 **2/26**	**One Dimensional Flow modeling: Steady-State** *1D Steady-State Flow (Direct Banded Matrix; Iterative Gauss-Seidel); Computer Storage Issue (how to compute the storage for different methods of matrix assemblages); Irregular grids;* **One Dimensional Flow modeling: Transient** *1D Transient Flow (FD Explicit);*
Week 7 **3/5**	**One Dimensional Flow modeling: Transient** *1D Transient Flow (FD Implicit)* *1D Transient Flow (FD Weighted Formations); Stability Analysis;* ***Homework 5***
Week 8 **3/12**	**Spring break (no class)**
Week 9 **3/19**	**Two Dimensional Steady-State Flow modeling** *Specified Head & No-Flow; Specified Head & Specified Flux* ***Homework 6***

Week 10 **3/26**	*General BC; Flux calculation; Mass Balance; Streamlines and Velocity visualizations;* ***Project Two**: 2D Steady-State Flow Modeling* ***Project Two B (Optional)**: 2D Steady-State Flow Modeling in a Heterogeneous Conductivity Field (a DIFFERENT matrix assemblage technique is used; we'll use some class time to work on this project).*
Week 11 **4/2**	**Two Dimensional Transient Flow modeling** *Mathematical and FD Formations; Mass Balance;* ***Project Three**: 2D Transient Flow Modeling in a Homogeneous Conductivity Field.*
Week 12 **4/9**	**Solute Transport Modeling** *Advection & Dispersion;* *Derivation of the Advection-Dispersion Equation (ADE);* *FD Formation for ADE (Explicit, Implicit, Weighted);* ***Homework 7***
Week 13 **4/16**	**Solute Transport Modeling** *ADE extension to higher dimension; Groundwater Pathline Generation & Particle Tracking; An effective solute transport theory to represent geological heterogeneity. Reactions and transport (optional)*
Week 14 **4/23**	**3D Modeling of Flow and Transport using Groundwater Vista** ***Project Four**: 3D modeling with Groundwater Vista (since Groundwater Vista is installed in ESB 1006, we'll use class time to work on this project). Students interested in installing this software on their own PC may contact Dr. James Rumbaugh [jrumbaugh@groundwatermodels.com]. His company may offer you a student discount.* ***Homework 8 (reading assignment):*** *Reilly T E & A W Harbaugh (2004) Guideline for Evaluating Ground-water Flow Models, USGS Scientific Investigations Report 2004-5038, pp. 37.* **Advanced Topics (I) Introduction to Parameter Estimation for Groundwater Models (Chp 10; Optional)** *Forward Upscaling to find Equivalent Conductivities; Tensor Analysis; Global versus local coordinate;*
Week 15 **4/30**	**Advanced Topics (II) Introduction to Parameter Estimation for Groundwater Models (Chp 10; Optional)** *Inverse Methods based on Non-Linear Regression (Effective Groundwater Model Calibration: With Analysis of Data, Sensitivities, Predictions, and Uncertainty, Hill and Tiedeman, 2007, Wiley-Interscience, 455pp.).* **Final Review and Wrap Up**
Week 16 **5/7**	*Final Take-Home Exam.*