Groundwater Flow and Solute Transport Modeling

GEOL 5030/4030
Spring, 2022
3 Credits

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

Grading: A/F or S/U (see week 1's lecture for more information)
Lectures: Online asynchronous
Office hours: Thursday (4:30~5:30 pm); https://uwyo.zoom.us/j/3072232292
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Course Objectives:
Movement of groundwater and dissolved solutes in the subsurface is responsible for a variety of environmental, engineering, and geological processes of importance. To evaluate these processes, mathematical modeling is an essential tool. In recent years, increasing reliance is placed upon using computer simulations to predict flow and transport in the subsurface in order to capture their spatiotemporal variability. To effectively utilize computer models as an aquifer management tool, familiarity with the fundamental principle behind numerical modeling is needed. This course presents an overview of the analyses of groundwater flow and solute transport using the Finite Difference Method. Problems solved range from 0-D to 3-D and steady-state to transient in simple as well as realistic model domains. Besides computer coding, popular software platform will also be utilized. 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)
One or more advanced topics (topics may vary each year)
- *Tensor Analysis*
- *Upscaling*
- *Parameter Estimation & Inverse Modeling*
- *Reactive Solute Transport Modeling*

Learning Outcomes:
Students will learn how to derive and implement numerical approximations of ordinary and partial differential equations describing subsurface flow and transport processes. They will learn to construct models of flow and transport from 0 to 3 dimensions, for both steady-state (i.e., time-invariant) and transient (i.e., time-dependent) problems. They will understand solution techniques including direct and iterative methods as well as the distinction between matrix-based and matrix-free methods. They will write computer codes with Excel and Matlab for simpler problems in regular (e.g., box) model domains. They will also learn a popular software for more complex modeling in 3-d.

Prerequisite:
- Calculus I & II;

- Geohydrology, or an equivalent groundwater hydrology course, or instructor consent;
- Matlab Programming language*

**This course emphasizes the fundamentals of computer modeling. Students are expected to write small computer codes, thus skills in programming with Matlab are necessary. See Matlab tutorials on my website (under Teaching): http://geofaculty.uwyo.edu/yzhang/.*

Textbook, Tools, Questions:
Textbook: the instructor has written a set of lecture notes. Course lectures and notes are thus key although below is a list of suggested readings:

- Introduction to groundwater modeling: finite difference and finite element methods, H. F. Wang and M. P. Anderson, 1995, Academic Press, 237 p.
- Applied Groundwater Modeling: Simulation of Flow and Advective Transport, M. P. Anderson and W. W. Woessner, 1992, Academic Press, 381 p.
- Applied Contaminant Transport Modeling, C. Zheng, G. D. Bennett, 2002, Wiley, 656 p.

Tools: ruler, pencil, eraser, calculator, scrap paper; for some problems, we use Excel. For others, modeling will be done using Matlab (or a programming language of your choice) or software.

Questions for instructor: (1) office hour (online); (2) email instructor to set up an appointment.

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 exercises, homework, projects, and exams. The instructor will post PowerPoint, lecture videos, and course notes on the Wyocourse class website. The lecture notes do not contain formula proofs, equation derivations, and solutions, which are covered during the lectures.

Grading Policy:
The final grade will be given at the appropriate percentages shown:

Homework*1	42% (6% *x* 7 homework)
Lab/Project	40% (10% x 4 labs)
Final Exam*2	18%

*1 Each homework/lab/exam has a standalone grade of 100 points.

*2 Advanced topics will not be tested in the final exam. 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

Concerning homework/lab/exams:

(1) For problems involving equations, provide your complete analysis rather than a single number.

(2) Be professional in presentations: if applicable, write down the units of the results and round off real numbers to 1 or 2 decimal points.

(3) Unless otherwise stated, upload all assignments to Wyocourse class website.
- With a few exceptions, most are due one week after they are assigned.

- All due dates are listed on Wyocourse website: if not handed in on time, each day it is delayed, 10 points will be taken out of the respective grade (100) of the assignment until no points remain.

- Given a valid proof-of-absence, the above due-date rule does not apply. Within a reasonable time (1 weeks), the student is expected to hand in the work or arrange with the instructor for a make-up exam. It is the student's responsibility to contact the instructor in a timely manner and in advance if possible, failing to do so will result in the forfeiture of the points.

- Reading assignments (posted under Wyocourse/File/Reading) require no turn-ins. Nor are they graded. The pdf can also be found after logging into UW's library or on the internet (try searching by the title of the paper).

(4) Students can discuss the problems with other, but please complete assignments independently. Copying other's work is considered cheating and no points will be given.

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 explained here: 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 "F" for the course. Plagiarism is considered a form of cheating: both students will lose the full points on the assignment.

Statement on Diversity:
The University of Wyoming values an educational environment that is diverse, equitable, and inclusive. The diversity that students and faculty bring to class, including age, country of origin, culture, disability, economic class, ethnicity, gender identity, immigration status, linguistic, political affiliation, race, religion, sexual orientation, veteran status, worldview, and other social and cultural diversity is valued, respected, and considered a resource for learning.

Disability Support:
The University of Wyoming is committed to providing equitable access to learning opportunities for all students. If you have a disability, including but not limited to physical, learning, sensory or psychological disabilities, and would like to request accommodations in this course due to your disability, , please register with and provide documentation of your disability as soon as possible to Disability Support Services (DSS), Room 128 Knight Hall. You may also contact DSS at (307) 766-3073 or udss@uwyo.edu. It is in the student's best interest to request accommodations within the first week of classes, understanding that accommodations are not retroactive. Visit the DSS website for more information at: www.uwyo.edu/udss.

Duty to Report:
UW faculty are committed to supporting students and upholding the University's non-discrimination policy. Under Title IX, discrimination based upon sex and gender is prohibited. If you experience an incident of sex- or gender-based discrimination, we encourage you to report it. While you may talk to a faculty member, understand that as a "Responsible Employee" of the University, the faculty member MUST report information you share about the incident to the university's Title IX Coordinator (you may choose whether you or anyone involved is identified by name). If you would like to speak with someone who may be able to afford you privacy or confidentiality, there are people who can meet with you. Faculty can help direct you or you may find info about UW policy and resources at http://www.uwyo.edu/reportit You do not have to go

through the experience alone. Assistance and resources are available, and you are not required to make a formal complaint or participate in an investigation to access them.

Student Resources:

- DISABILITY SUPPORT SERVICES: udss@uwyo.edu, 766-3073, 128 Knight Hall, www.uwyo.edu/udss
- COUNSELING CENTER: uccstaff@uwyo.edu, 766-2187, 766-8989 (After hours), 341 Knight Hall, www.uwyo.edu/ucc
- ACADEMIC AFFAIRS: 766-4286, 312 Old Main, www.uwyo.edu/acadaffairs
- DEAN OF STUDENTS OFFICE: dos@uwyo.edu, 766-3296, 128 Knight Hall, www.uwyo.edu/dos
- UW POLICE DEPARTMENT: uwpd@uwyo.edu, 766-5179, 1426 E Flint St, www.uwyo.edu/uwpd
- STUDENT CODE OF CONDUCT WEBSITE: www.uwyo.edu/dos/conduct

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

Tentative Schedule

**Traditional lecture dates are shown as a reference.*

Week 1 **1/18** **1/20**	**Introduction to the course.** *Course policy and modeling overview. What is groundwater flow and transport modeling? What kind of problems can numerical models solve? What is the overall modeling approach? What kind of skills can you acquire in this class?* ***Homework 1: due in 1 week.*** ***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 **1/25** **1/27**	**Modeling Overview** *Conceptual model, mathematical model, numerical model, computer model* *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).*
Week 3 **2/1** **2/3**	**Mathematics For this Class** *Differential Equations; Scalar, Vector, Tensor; Taylor Series & Finite Difference;* *Error, Convergence, Stability; Linear Algebra & Solutions (Direct vs. Iterative; Matrix-Based vs. Matrix-Free);* ***Homework 2: due in 1 week***
Week 4 **2/8** **2/10**	**Lumped Parameter Models (ODE)** *The Mass Balance Principle; Groundwater Stream Interaction;* *Numerical Solution; Euler's Method; Huen's Method; Runga Kutta Method;* ***Homework 3: due in 3 days*** ***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).* ***Due in 1 week.***
Week 5 **2/15** **2/17**	**One Dimensional Flow modeling: Introduction** *1D Steady-State Flow in Homogeneous & Heterogeneous Porous Media;* *Analytical vs. numerical solutions.* ***Homework 4 (****develop FDM solution by hand****): due in 1 week.***

Week 6 **2/22** **2/24**	**One Dimensional Flow modeling: Steady-State** *1D Steady-State Flow (Direct Full matrix; Direct Banded Matrix; Iterative Gauss-Seidel); Computer Storage Issue (how to compute the storage for different methods of matrix assemblages); Irregular grids;* ***Coding exercise:** Solve the same 1D steady-state flow problem with three solution techniques: Direct Full matrix; Direct Banded Matrix; Iterative Gauss-Seidel. Verification with results of Week 5 assembled by hand.*
Week 7 **3/1** **3/3**	**One Dimensional Flow modeling: Transient** *Motivation; FD discretization of spatial and temporal derivatives;* *FD Explicit Method; Write our first transient code implementing the explicit method.*
Week 8 **3/8** **3/10**	*Stability Analysis; FD Implicit Method; FD Weighted Formations;* ***Homework 5: due in 1 week.*** **Two Dimensional Steady-State Flow modeling** *Specified Head & No-Flow;* ***Homework 6: due in 1 week.***
Week 9 **3/15** **3/17**	**Spring break: no class**
Week 10 **3/22** **3/24**	**Two Dimensional Steady-State Flow modeling** *Specified Head & Specified Flux;* ***Project Two****: 2D Steady-State Flow Modeling in a Homogeneous Porous Medium,* ***due in 1 week.*** *Darcy Flux; Steady state mass balance analysis.*
Week 11 **3/29** **3/31**	*Streamlines and velocity visualizations; Aquifer K heterogeneity.* ***Project Two B (Optional)****: 2D Steady-State Flow Modeling in a Heterogeneous Conductivity Field using a different matrix assemblage technique.* **Two-Dimensional Transient Flow modeling (Chp 7)** *Mathematical and FD Formations; Mass Balance;* ***Project Three****: 2D Transient Flow Modeling in a Homogeneous Conductivity Field,* ***due in 1 week****.*
Week 12 **4/5** **4/7**	*Time-dependent specified-flux BC; Transient mass balance analysis; hydraulic response time; solute response time;* ***Project Three (An Optional Section):*** *See description in this lecture.* **No lecture: Please: (1) review Chp 5, 6, 7 for flow modeling; (2) complete Project Three.**
Week 13 **4/12** **4/14**	**Solute Transport Modeling** *Advection & Dispersion; Advection-Dispersion Equation (ADE);* *FD Formation for ADE (Explicit, Implicit, Weighted);* ***Homework 7: due in 1 week.***
Week 14 **4/19** **4/21**	**Solute Transport Modeling** *Discussion of Homework 7; ADE extension to higher dimensions;* *Solute transport BC for high dimensional problems; mass fluxes;*
Week 15	**Solute Transport Modeling**

4/26	*Particle tracking; An effective solute transport theory to represent missing K heterogeneity in the flow model.*
4/28	**Three-Dimensional Flow Modeling** ***Project Four**: 3D flow and streamline modeling with Groundwater Vista, **due in 1 week.*** ***Reading assignment (no turn-in & no grade assigned):*** *Reilly T E & A W Harbaugh (2004) Guideline for Evaluating Ground-water Flow Models, USGS Scientific Investigations Report 2004-5038, pp. 37.*
Week 16 **5/3**	**Advanced Topics (I) Introduction to Parameter Estimation (Chp 10)** Forward Upscaling to find Equivalent Conducti vities; Tensor Analysis; Global versus local coordinate; **Advanced Topic (II) Introduction to Parameter Estimation (Chp 10)** *Indirect inverse methods; non-Linear regression (Effective Groundwater Model Calibration: With Analysis of Data, Sensitivities, Predictions, and Uncertainty, Hill and Tiedeman, 2007, Wiley-Interscience, 455p). Direct inverse methods* **Advanced Topic (III) *Geochemical and Reactive transport modeling*[*1]** **Final Review & Wrap Up**
Week 17 **Final's week**	*Final Take-Home Exam: Tuesday, May 10, 2022*[*2]

*1The advanced topic will give an overview of reactive transport modeling. The grayed-out topics in Week 16 will not be covered this Spring.

*2 The correct date for the final exam is highlighted here. There is a typo about the date in the video lecture.