Groundwater Flow and Solute Transport Modeling

GEOL 5030/4030 Dept. of Geology & Geophysics

Spring, 2026 University of Wyoming 3 Credits Instructor: Ye Zhang

Grading: A/F or S/U (see week 1's lecture for information) Lectures (Traditional): ESB 1006; Tues + Thurs (9:35~10:50 am)

Office hours: Thurs (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 Modelina

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 (GEOL 4444/5444), or an equivalent groundwater hydrology course, or instructor consent;
- Matlab Programming language*

This course emphasizes the fundamentals of computer modeling as applied to groundwater flow and solute transport. Students are expected to write codes, thus programming skills are required. Assignments can use another language rather than Matlab. See Matlab tutorials on my website (under Teaching): http://geofaculty.uwyo.edu/yzhang/.

Textbook, Tools, Questions:

Textbook: the instructor has written full lecture notes, so there is no required textbook. Course lectures and notes are key although below is a list of suggested readings:

- <u>Introduction to groundwater modeling: finite difference and finite element methods</u>, H. F. Wang and M. P. Anderson, 1995, Academic Press, 237 p.
- <u>Applied Groundwater Modeling: Simulation of Flow and Advective Transport</u>, 2nd Edition, M. P. Anderson, W. W. Woessner, R. J. Hunt, 2015, Academic Press, 650 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 <u>not</u> 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 42% (6% *x* 7 homework)
Lab/Project 40% (10% *x* 4 labs)

Final Exam 18% Reading assignments: 0%

* Each homework/lab/exam has a standalone grade of 100 points. When determining the course grade, these will be normalized reflecting the percentage distribution above. The course grade is given based on the numerical grade:

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

More information:

- (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 in the same week that 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.
 - Advanced topics discussed in lectures will not be tested in the final exam.
- Reading assignments (under Wyocourse/File/Reading) require no turn-ins nor are they graded. Most come from the Anderson et al. (2015), which gives excellent advice for building real world models, thus they complement the theoretical approach of this class. The full book can be downloaded from UW library.
- (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, <u>www.uwyo.edu/acadaffairs</u>
- 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

* spring semester, 2026

	Topics covered	Assignments: see Wyocourse for due dates for all submitted work
Week 1 1/20 1/22	Introduction: 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 Reading assignment: Overview of GW modeling: Andersonetal-2015-Chapter1.pdf
	Review of 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 1/27	Modeling Overview: Conceptual model, mathematical model, numerical model, computer model;	Reading assignments: Conceptual model: Andersonetal-2015-Chapter2.pdf
1/29	How do we model? 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).	Eqns, BC, Numerical models: Andersonetal-2015-Chapter3.pdf
Week 3 2/3	Mathematics For this Class: Differential Equations; Scalar, Vector, Tensor; Taylor Series & Finite Difference;	Homework 2
2/5	Error, Convergence, Stability; Linear Algebra & Solutions (Direct vs. Iterative; Matrix-Based vs. Matrix-Free);	
Week 4	Lumped Parameter Models (ODE)	Homework 3
2/10	The Mass Balance Principle; Groundwater Stream	
2/12	Interaction; Numerical Solution; Euler's Method; Huen's Method;	Project One : Lumped parameter flow and transport modeling & calibration for groundwater contamination at
	Runga Kutta Method	Nantucket Island, Massachusetts

Week 5 2/17	One Dimensional Flow modeling: Introduction 1D Steady-State Flow in Homogeneous & Heterogeneous	Homework 4
	Porous Media;	
2/19	Analytical vs. numerical solutions.	
Week 6	One Dimensional Flow modeling: Steady-State 1D Steady-State Flow (Direct Full matrix; Direct Banded Matrix; Iterative Gauss-Seidel); Computer Storage Issue	Reading assignment: Higher (2D to 3D) spatial dimensions: Andersonetal-2015-Chapter4.pdf
2/24	(how to compute the storage for different methods of matrix assemblages); Irregular grids;	(Sections 4.1 and 4.2)
2/26	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	One Dimensional Flow modeling: Transient	Reading assignment:
3/3 3/5	Motivation; FD discretization of spatial and temporal derivatives;	Higher (2D to 3D) spatial dimensions: Andersonetal-2015-Chapter4.pdf
3/5	FD Explicit Method; Write our first transient code implementing the explicit method.	(Sections 4.3-4.6)
Week 8	Stability Analysis; FD Implicit Method; FD Weighted	Homework 5
3/10	Formations;	
		Homework 6
3/12	Two Dimensional Steady-State Flow modeling Specified Head & No-Flow;	
Week 9 3/17 3/19	Spring break: no class	
Week 10 3/24	Two Dimensional Steady-State Flow modeling: Specified Head & Specified Flux;	Project Two: 2D Steady-State Flow Modeling in a Homogeneous Porous Medium
3/26	Darcy Flux; Steady state mass balance analysis.	Project Two B (Optional): 2D Steady-State Flow Modeling in a Heterogeneous Conductivity Field using a different matrix assemblage technique.
Week 11 3/31	Streamlines and velocity visualizations; Aquifer K heterogeneity.	Project Three : 2D Transient Flow Modeling in a Homogeneous Conductivity Field
4/2	Two-Dimensional Transient Flow modeling (Chp 7) Mathematical and FD Formations; Mass Balance;	Conductivity Floid
Week 12	Time-dependent specified-flux BC; Transient mass	Reading assignment:
4/7	balance analysis; hydraulic response time; solute response time; Project Three (An Optional Section): See description in this lecture.	Spatial discretization: Andersonetal- 2015-Chapter5.pdf (Sections 5.1-5.3)
4/9	No lecture: Please review Chp 5, 6, 7 for flow modeling & complete Project Three.	
Week 13	Solute Transport Modeling	Homework 7
4/14	Advection & Dispersion; Advection-Dispersion Equation (ADE);	
4/16	FD Formation for ADE (Explicit, Implicit, Weighted);	

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Week 14	Solute Transport Modeling	Reading assignments:
4/21	Discussion of Homework 7; ADE extension to higher	Parameter assignment & common
	dimensions;	modeling errors: Andersonetal-2015-
		Chapter5.pdf (Sections 5.4-5.7)
	Solute transport BC for high dimensional problems; mass	
4/23	fluxes;	Sources and sinks & common
		modeling errors: Andersonetal-2015-
		Chapter6.pdf
Week 15	Solute Transport Modeling	Project Four: 3D flow and streamline
	Particle tracking; An effective solute transport theory to	modeling with Groundwater Vista.
	represent missing K heterogeneity in the flow model.	_
4/28		Reading assignment:
	Three-Dimensional Flow Modeling	Guideline for Evaluating Ground-water
	Groundwater Vista (Version 9 Advanced)	Flow Models: 2004-Reilly-
4/30	(Harbaugh.pdf
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Week 16	Advanced Topic:	Reading assignments:
5/5	Geochemical & Reactive transport modeling*1	TransportModeling_Konikow_2011.pdf
		TransportModeling Molz 2015.pdf
5/7	Final Review & Wrap Up	
Week 17	Final Take-Home Exam: Monday, May 11*2	
Final's week		

^{*1}The advanced topic will give an overview of reactive transport modeling.

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^{*2} The date for the final exam is highlighted here: there is a typo in the video lecture.