Course Syllabus as of February 2, 2019
Geol 5450 - Geochemical Modeling, Spring 2019
Department of Geology and Geophysics, University of Wyoming

Instructor	
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Office Hours: Mon 3-4p, Tues 4-5p, Wed 3-4p, and by appointment	
Co-Instructor (for Phase Diagrams)	
Professor Ron Frost	Email: rfrost@uwyo.edu
Office Hours: by appointment	

Course Information: 2:45 - 4 pm Tues/Thurs in Room 1006. The first class is on Tuesday January 29 and the final class is on Thursday May 9. In addition we will meet for approximately 6 hours on Saturday February 2, 2019.

Prerequisites: GEOL 4777/5777 – Geochemistry of Natural Waters **OR** Geol 5610 – Geological Thermodynamics I **OR** GEOL 4490 – Geochemistry **OR** Consent of Instructor

Course Description: Modeling of geochemical processes in fluid-rock systems of the Earth's crust. Emphasizes development and application of conceptual models as well as quantitative numerical models. Reinforces and expands fundamental skills in aqueous and fluid-rock geochemistry to better understand geochemical processes and solve problems in fluid-rock systems. 3 credit hours. Limited to 10 students.

Course Objectives/Outcomes: In this course students will reinforce and expand fundamental skills in aqueous and fluid-rock geochemistry to better understand geochemical processes and solve problems in fluid-rock systems. Geochemical modeling skills will be developed as a tool to perform these functions and, in the process, to improve understanding of geochemistry in natural systems. Both conceptual and numerical models will be developed and employed. At the conclusion of this course students will be able to apply geochemical skills to a wide range of fluid-rock problems that include geothermal and hydrothermal systems, petroleum systems, environmental geology, geologic carbon sequestration, diagenesis, ore deposits, and contact metamorphic aureoles. In addition, students will develop geochemical problem solving skills as well as computer modeling skills prized by employers in a variety of geologic and engineering disciplines.

Primary Text: Craig M. Bethke, 2008, *Geochemical and Biogeochemical Reaction Modeling*, Cambridge University Press; 2 edition, ISBN-10: 0521875544, ISBN-13: 978-0521875547, 564 p.

Supplemental Books:

Drever, J.I. (1997) *Geochemistry of Natural Waters: Surface and Groundwater Environments*, 3rd ed. Prentice Hall, 436 pp.

Langmuir, D., 1997, *Aqueous Environmental Geochemistry*. Prentice Hall.

Krauskopf, K.B. and Bird, D.K., 1995, *Introduction to Geochemistry*, 3rd Ed. McGraw-Hill, Inc.

Nordstrom, D.K. and Munoz, J.L., 1985, *Geochemical Thermodynamics*. Benjamin Cummings Publishing

Stumm, W. and Morgan, J.J., 1996, *Aquatic Chemistry*, 3rd Ed. John Wiley & Sons.
Grenthe, I., and Puigdomenech, I., 1997, *Modeling in Aquatic Chemistry*, Nuclear Energy Agency.
Garrels, R.M., and Christ, C.L., 1982, *Solutions Minerals and Equilibria*, Freeman Cooper Co.
Anderson, G.M., and Crerar, D.A., 1993, Thermodynamics in Geochemistry: The Equilibrium Model, Oxford University Press.

Supplementary Literature (available on course website):

Garrels, R.M. and Thompson, M.E. (1962) A chemical model for sea water at 25°C and one atmosphere total pressure. *Am. J. Sci.* **260**, 57-66.
Helgeson, H.C., Garrels, R.M. and Mackenzie, F.T. (1969) Evaluation of irreversible reactions in geochemical processes involving minerals and aqueous solutions - II. Applications. *Geochim. Cosmochim. Acta* **33**, 455-481.
Steinmann, P., Lichtner, P.C. and Shotyk, W. (1994) Reaction path approach to mineral weathering reactions. *Clays Clay Miner.* **42**, 197-206.
Zen, E.-A. (1984) Construction of Pressure-Temperature Diagrams for Multicomponent Systems After the Method of Schreinemakers - A Geometric Approach: U.S. Geological Survey, 3rd edition, U.S. Government Printing Office, Washington D.C., 56p.

Computer Software: We will use the software code Geochemist's Workbench (abbreviated GWB) Standard 12.0 (https://www.gwb.com) which I will provide for use in the course. This software is provided on an academic teaching license and is restricted to coursework. If you use GWB for your research then you'll have to obtain and use an official copy. User's manuals for this software are included in the software as PDF files.

Course Requirements: In each class meeting we will typically spend time in lecture and on the computer. Reading and problem sets are listed in the course outline. Reading assignments include material from your modeling textbook and the software manuals as well as relevant geochemistry textbooks and primary literature. Reading assignments should be completed prior to the class period as they serve as supplemental material. Bring your questions to class. The Saturday session will be a full day's immersion into the software and its application to geochemistry.

Course Assignments/Grading: The course will be graded on the basis of problem sets and phase diagram assignments (35% of grade) as well as a Term Project. The Term Project consists of a paper (50% of grade) and class presentations (15% of grade).

Term Project. Your term project is the most important part of this course. Everyone must complete a term project. The final products of this project will be a written paper and a class presentation. The project must consist of original work and can take the form of:

1) a research project conducted as part of a thesis, job, or other venue
2) an in-depth critical review of the literature of a topic related to the course content
3) a report on original field-based, theoretical or experimental research project undertaken solely for this course
4) a well-researched and documented proposal for a research, thesis, or dissertation project

Time Table for Term Project

February 7 – Lightening Science 1, present tentative title and thesis for your project
February 15 (noon) – project title and thesis due
February 22 (noon) - annotated bibliography due.

February 26 – Lightening Science 2, present data slides relative to your project.
March 1 (noon) - rough presentation outline due.
March 8 (noon) – rough paper outline due.
March 13 (noon) – detailed presentation outline due.
March 18 (noon) – detailed paper outline due. I won't read outlines outside office hours after this date.
April 9 – Lightening Science 3, present data slides relative to your project.
April 5 (noon) – draft presentation due.
April 12 (noon) - draft paper due. I will not read drafts outside of office hours after this date.
April 16 and 18 – Student Presentations (Status of Ongoing Project).
April 26 (noon) – near-final draft paper due.
May 7 and 9 – Final Student Presentations.
May 15 (noon) - Final paper due

Detailed information on the paper and presentations is provided in separate handouts.

Problem Sets. A total of seven problem sets will be assigned. No exams will be administered. I use standard percentages to assign grades (e.g., ≥ 90% = A, 80-89% = B, etc.). I do not grade on a curve. Work turned in late (without prior consent of the instructor) will be penalized at a rate of 10% per day. You are encouraged to work together on the problem sets, and seek help from people and sources in addition to me. However, each assignment should be your own work. Learning how things work, developing your own understanding of the problem, submitting solutions that represent your own thinking, and conscientious completion of the problem sets are important keys to success on understanding this material. Problem sets will be posted on the web by Monday noon of each week and due by noon on Friday of the following week. Problem sets will be submitted as PDF files via WyoCourses. Information regarding WyoCourses is provided on the last page of this syllabus.

Lightning Science Sessions. Three class sessions will be devoted to in-depth classroom discussion of each student's science. The goal of the first session is to focus attention on starting the term project. The goal of the second and third sessions is to share progress on individual research.

Phase Diagram Sessions. Six class sessions will be devoted to understanding the fundamentals of phase diagrams. Several problems and calculations will be assigned as part of these sessions.

Lecture Final Exam: None.

Attendance/Participation Policy: University sponsored absences are cleared through the Office of Student Life. If you plan to be gone at any time during the semester and your absence will be officially authorized by UW, please contact me beforehand so that we can work out some way for you to make up any assignments. Any absences from class as a result of illness will require proper documentation from your physician.

Classroom Behavior Policy: At all times, treat your presence in the classroom and your enrollment in this course as you would a job. Act professionally, arrive on time, pay attention, complete your work in a timely and professional manner, and treat all deadlines seriously. You will be respectful towards you classmates and instructor. Spirited debate and disagreement are to be expected in any classroom and all views will be heard fully, but at all times we will behave civilly and with respect towards one another. Personal attacks, offensive language, name-calling, and dismissive gestures are not warranted in a

learning atmosphere. As the instructor, I have the right to dismiss you from the classroom, study sessions, electronic forums, and other areas where disruptive behavior occurs. Electronic devices such as mobile phones should be set to silent. Laptops are allowed for note-taking purposes. No video or audio recording during class is allowed to protect the privacy of your fellow students.

Classroom 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.

Academic Dishonesty Policies: Example: "Academic dishonesty will not be tolerated in this class. Cases of academic dishonesty will be treated in accordance with UW Regulation 2-114. The penalties for academic dishonesty can include, at my discretion, an "F" on an exam, an "F" on the class component exercise, and/or an "F" in the entire course. Academic dishonesty means anything that represents someone else's ideas as your own without attribution. It is intellectual theft – stealing - and includes (but is not limited to) unapproved assistance on examinations, plagiarism (use of any amount of another person's writings, blog posts, publications, and other materials without attributing that material to that person with citations), or fabrication of referenced information. Facilitation of another person's academic dishonesty is also considered academic dishonesty and will be treated identically.

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.
Substantive changes to syllabus: All deadlines, requirements, and course structure is subject to change if deemed necessary by the instructor. Students will be notified verbally in class, on our WyoCourses page announcement, and via email of these changes.

Course Outline and Reading Assignments for Geol 5450: Geochemical Modeling

	Lecture Topic	Reading Assignments (Bethke 2008)	Reading Assignments (Users Manual)	Recommended review in Langmuir 1997 OR Drever 1997	Problem Set and/or Paper to Read
Tues Jan 29	Introductions and course mechanics. Geochemical models.	None	None	None	---
Thurs Jan 31	Geochemical models and equilibrium calculations	Preface, A note about software, Ch 1 & 3	---	Langmuir Chapter 1 Drever Ch 2	Garrels and Thompson (1962)
Saturday Feb 2	**Saturday Class** (GWB basics, phase diagrams, equilibrium)	Review Chapters 2, 4, 5, 6, 8, 11, 12, & 13	---	Langmuir Ch 7, 8, & 9 Drever Ch 10 & 12	---
Tues Feb 5	Equilibrium models / Databases	Chapter 8	Essentials Chapter 2.3; Reaction Modeling Appendix 1	Langmuir Chapter 1 Drever Ch 2	Problem Set 1 – Equilibrium Geochemistry
Thurs Feb 7	Lightening Science 1 / Databases	---	---	---	---
Tues Feb 12	Carbonate Chemistry	Chapter 15	Reaction Modeling Chapter 2	Langmuir Ch 3, 5, & 6 Drever Ch 3	Problem Set 2 – Carbonate Geochemistry
Thurs Feb 14	Carbonate Chemistry / Redox	Chapters 7 & 28	Essentials Guide Chapter 5	Langmuir Ch 11 & 12 Drever Ch 7 & 8	---
Tues Feb 19	Redox	---	---	---	Problem Set 3 – Carbonate Geochemistry and Redox Equilibria
Thurs Feb 21	Phase Diagrams 1	---	---	---	Zen (1984)
Tues Feb 26	Lightening Science 2 / Redox	---	---	---	Problem Set 4 – Redox Equilibria
Thurs Feb 28	Phase Diagrams 2	---	---	---	---
Tues Mar 5	No class	---	---	---	---

Thurs Mar 7	Phase Diagrams 3	---	---	---	---
Tues Mar 12	Large Datasets	---	Essentials Guide Chapter 3	---	Problem Set 5 – Large Datasets
Thurs Mar 14	No class	---	---	---	---
Tues Mar 19	**Spring Break**	---	---	---	---
Thurs Mar 21					
Tues Mar 26	No class	---	---	---	---
Thurs Mar 28	Phase Diagrams 4	---	---	---	---
Tues Apr 2	No class	---	---	---	---
Thurs Apr 4	Phase Diagrams 5	---	---	---	---
Tues Apr 9	Lightening Science 3 / Kinetics	Chapters 16 & 26	Reaction Modeling Guide Ch. 4 & 5	Langmuir Ch 2 Drever Ch 11	Problem Set 6 – Kinetics
Thurs Apr 11	Phase Diagrams 6	---	---	---	---
Tues Apr 16	Student Presentations (Status of Ongoing Project)	---	---	---	Assess student problems & solutions as a class
Thurs Apr 18		---	---	---	
Tues Apr 23	Kinetics	---	---	---	---
Thurs Apr 25	Kinetics	---	---	---	---
Tues Apr 30	Water-Rock Systems Exhibiting Extreme Geochemistry	Chapters 22, 24, 29, 30, 31, 32	---	Langmuir Ch 5 & 6 Drever Ch 3, 9, 13, & 15	Problem Set 7 – Water-Rock Systems Exhibiting Extreme Geochemistry
Thurs May 2	Water-Rock Systems Exhibiting Extreme Geochemistry	---	---	---	---

Tues May 7 Thurs May 9	Final Student Presentations	---	---	---	Graded

Phase Diagrams: The following topics will be covered.

February 21 – Phase Diagrams 1. Intro to phase diagrams. Gratuitous calculus. The phase rule, G vs. T and G vs. P diagrams. Schreinermakers' rules.

February 28 – Phase Diagrams 2. Schreinermakers, analysis of invariant systems. Two and Three component systems. Chemographic diagrams.

March 7 – Phase Diagrams 3. Four component systems and chemographic diagrams.

March 28 – Phase Diagrams 4. Degenerate four component systems.

April 4 – Phase Diagrams 5. Definition of chemical potential, m-m diagrams.

April 11 – Phase Diagrams 6. Activity – activity diagrams.

Online Resources: We will use *WyoCourses* for the online course platform to post announcements, reading material, course syllabus, etc. Consult this website regularly for announcements and other information. Students are automatically enrolled in this course website.

The developer of GWB operates an online forum (http://forum.gwb.com/. The forum shares comments and results and answer questions of general interest. The forum also serves as a bulletin board for posting announcements, bug notices, patches, and other current information about GWB.

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