

Fall 2021

## Aqueous Geochemistry

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# Geol 588 Aqueous Geochemistry

Tues & Thurs 1130-1245

Fall 2020

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**Instructor:** Dr. Dorothy Vesper

**Email:** [djvesper@mail.wvu.edu](mailto:djvesper@mail.wvu.edu)

**Course Web Site:** eCampus & various links therein (google drive mostly)

**Office hours:** Tuesday 3-4 & by appointment

**Office hours place:**

<https://tinyurl.com/DJV-OfficeHrs>  
(Passcode GEOL365F20)

**PURPOSE.** The purpose of this class is to provide graduate students with a strong theoretical background in inorganic, aqueous geochemistry for application in a wide range of research topics. My approach is to combine conceptual knowledge with quantitative skills in a cyclic fashion – to build independent understanding and “chemical intuition”. Ultimately, this class is about obtaining the problem solving skills to allow you to better analyze natural geochemical systems.

**STUDENT OUTCOMES:** Upon completion of this course students will be able to do the following:

1. Understand fundamental aqueous geochemistry of acid-base and oxidation-reduction systems
2. Derive chemical and mathematical expressions to analyze data and evaluate hypotheses
3. Use geochemical models MINTEQA2 and PHREEQC to solve problems
4. Interpret natural settings and test hypotheses using geochemical calculations and data
5. Construct effective graphics to illustrate data trends and predict chemical outcomes

## GRADING

Topics Covered	Problem Sets (%)	Exams (%)
Thermodynamics	15	10
Acid-base chemistry, carbonate dissolution, karst waters	15	15
Redox chemistry, coal mine drainage	15	15
Modeling project	15	none
<b>TOTAL</b>	<b>60 %</b>	<b>40 %</b>

Letter grades: A $\geq$ 90%; B $\geq$ 80%; C $\geq$ 70%; D $\geq$ 60% (strict cut-off, no rounding)

**Recommended Text:**

Benjamin, Mark M (2010) Water Chemistry. Waveland Press Inc. 668 p. (2<sup>nd</sup> edition is 2014 – either is okay)

**Alternative Texts and References:**

Kehew, Alan E (2001) Applied Chemical Hydrogeology. Prentice-Hall, Inc. 368p

Drever, James I (1997) The Geochemistry of Natural Waters. Surface and Groundwater Environments, Third Edition. Prentice Hall, Inc. 436p. This is the textbook I've used in the past but it is now out of print.

Langmuir, Donald (1997) Aqueous Environmental Geochemistry. Prentice-Hall, Inc. 600p.

Stumm, Werner and James J Morgan (1996) Chemical Equilibria and Rates in Natural Waters, 3<sup>rd</sup> Edition. John Wiley & Sons. 1022p

**Readings:** In addition to the text book there are numerous readings on Google Drive that I will direct you to over the course of the semester. (You have unlimited google drive space via your MIX account). You can get to the google drive via eCampus.

**Problem Sets:** This is a problem solving class. For that reason, the problem sets are designed to be challenging and not simply a re-do of examples done in class or in the text. I suggest that you start on each set early. If you wait to start until the night before the problem set is due, you probably won't be able to complete it in time. Any questions at all – come see me! A "Guideline for doing problem sets" will be handed out with the first assignment.

You are encouraged to work together on the problem sets. This means you can share ideas, help each other out, and check that you got to the same conclusions. However, this does not mean you can copy answers, materials or spreadsheets from each other. That constitutes plagiarism. Learn from each other but submit your own work. Duplicate spreadsheets and problems will be awarded zero's and be treated as academic integrity issues.

**Deadlines: *UNLESS otherwise specified....*** All problem sets are due at midnight on the specified day. The penalty for late assignments is 10% per day (that includes weekend days). No credit will be given for problem sets handed in after the graded assignments are returned.

I understand that "unseen events" can take place right now. I can be flexible with deadlines as long as you let me know ahead of time. The solution to the problem is, as if often is, communication.

**Exams:** There will 3 exams over the course of the semester – covering each of the major groups of topics. These will lag the topics somewhat so that there is sufficient time for you to review your returned problem set on that topic prior to the quiz. The purpose of these exams is to test your mastery of the basic fundamentals.

**WVU Academic Policies and Syllabus Statements.** Please review the information on course policies provided by WVU: <https://tlcommons.wvu.edu/syllabus-policies-and-statements#10>.

Topics include (1) Academic Integrity; (2) Academic Standards; (3) Accessibility; (4) Adverse Weather; (5) Attendance; (6) Campus Safety; (7) Inclusivity; (8) Incompletes; (9) Sale of Course Material; (10) Sexual Misconduct; and, (11) Student Evaluation of Instruction.

### **WVU COVID-19 Syllabus Statement**

WVU is committed to maintaining a safe learning environment for all students, faculty, and staff. Should campus operations change because of health concerns related to the COVID-19 pandemic, it is possible that this course will move to a fully online delivery format. If that occurs, students will be advised of technical and/or equipment requirements, including remote proctoring software.

In a face-to-face environment, our commitment to safety requires students, staff, and instructors to observe the social distancing and personal protective equipment (PPE) guidelines set by the University at all times. While in class, students will sit in assigned seats when applicable and wear the required PPE. Should a student forget to bring the required PPE, PPE will be available in the building for students to acquire. Students who fail to comply will be dismissed from the classroom for the class period and may be referred to the Office of Student Conduct for further sanctions.

If a student becomes sick or is required to quarantine during the semester, they should notify the instructor. The student should work with the instructor to develop a plan to receive the necessary course content, activities, and assessments to complete the course learning outcomes.

Details to get it done...

- We will have a seating chart and you will need to sit in your official seat in class. I will take attendance for all classes but it is not part of my grading process. Please remind me! (if my records aren't complete, we can end up ALL being quarantined)
- **MASKS** & distancing (if you need another or more masks, let me know. I can get help)
- Cleaning materials will be available for everything you may touch in class
- Bring your own handouts (I will post them on eCampus in advance, probably in OneNote)
- No eating or drinking in class
- Be on time for class – I am not allowed to begin until everyone is seated. So... if you're late you may not be allowed to join us. If you know you'll be late or absent, please email me ahead of time.
- Remember... noncompliance will result in a report to Student Conduct and penalties.

We're living in historic times. Let's do our best to keep each other safe. And to make sure we can keep meeting in person.

# Aqueous Geochemistry - Tentative Schedule of Topics

Fall 2020

*Water is H<sub>2</sub>O, hydrogen two parts, oxygen one, but there is also a third thing, that makes it water and no one knows what that is (D H Lawrence)*

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## INTRODUCTION AND BASIC TOOLS (~ 1 WEEK)

*I could scarcely sleep for the excitement the night after seeing the periodic table – it seemed to me an incredible achievement to have brought the whole, vast, and seemingly chaotic universe of chemistry to an all-embracing order. (Oliver Sacks)*

Introduction, syllabus, Chemistry Reunion, concentrations vs. (re)activity, the structure of water

Intro chemistry text; Benjamin 1; Berner & Berner

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## REACTIVITY & ENERGY CONTROLS (~ 2-3 WEEKS)

*... the determination of the energy states of substances, and how they change.. is fundamental to understanding what processes are possible and why they happen. (Anderson)*

Introduction to energetics and thermodynamics, activity-concentration relationships, Gibbs Free Energy calculations & derivations, solubility, ionic strength, disequilibrium

Benjamin 1-2

Anderson Ch 1-2 Thermo Philosophy

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## ACID-BASE SYSTEMS (~3 WEEKS)

*Gutta cavat lapidem: For water continually dropping will wear hard rocks hollow (Plutarch)*

Acids and bases, pH, speciation plots  
Carbonate waters – alkalinity, equivalence points, saturation indices, open and closed systems, PCO<sub>2</sub>-SiC relationships, carbonate solubility  
Applications in karst geochemistry

Benjamin 3-5, 7; White Ch 5 Carbonate Chem;

White Ch 7 Karst Waters White (1997) ThermoMin;  
Eby (2004) Buffer Capacity

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## REDOX-CONTROLLED SYSTEMS (~2 WEEKS)

*If redox species all came to equilibrium it would destroy life. Life depends on redox gradients and redox disequilibria (DK Nordstrom)*

Redox chemistry, balancing equations, half cells, Nernst equation, Eh as a master variable, Eh-pH diagrams; Natural Waters, field readings, redox couples

Benjamin 9; Kehew Ch 5 Redox in field; Barcelona et al (1989) when Eh works

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## WEATHERING PROCESSES (~2 WEEKS)

*Nothing on earth is so weak and yielding as water, but for breaking down the firm and strong it has no equal. (Lao-Tsze)*

Weathering, mineral stability diagrams;  
Watershed chemistry

Benjamin 6, 8, 10

Rose and Cravotta (1998) AMD Chem

BernerBerner1996 Ch 5 WorldRivers

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## MINTEQ, METALS, MISC. (~2 WEEKS OR AS TIME PERMITS)

*"When the water of a place is bad it is safest to drink none that has not been filtered through either the berry of a grape, or else a tub of malt. These are the most reliable filters yet invented. (Samuel Butler)*

MINTEQ in computer lab; Metal chemistry  
Analytical methods

Benjamin 8, 10

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**Comments on the schedule:** The schedule is tentative. Stay flexible and expect there to be some changes. I like to leave time for discussion, questions, and tangents that make sense.

LETTER	UPPERCASE	LOWERCASE	LETTER	UPPERCASE	LOWERCASE
Alpha	A	α	Nu	Ν	ν
Beta	B	β	Xi	Ξ	ξ
Gamma	Γ	γ	Omicron	Ο	ο
Delta	Δ	δ	Pi	Π	π
Epsilon	E	ε	Rho	Ρ	ρ
Zeta	Z	ζ	Sigma	Σ	σ
Eta	H	η	Tau	T	τ
Theta	Θ	θ	Upsilon	Υ	υ
Iota	I	ι	Phi	Φ	φ
Kappa	K	κ	Chi	Χ	χ
Lambda	Λ	λ	Psi	Ψ	ψ
Mu	M	μ	Omega	Ω	ω