Geology 4/528
Physical Geochemistry
SpringQuarter

Professor: Dina L. López
210 Clippinger Laboratories
Phone: 593-9435
e-mail:lopezd@oak.cats.ohiou.edu

Office Hours:
Class:

Course Outline

Week	Lecture	Computer Exercises
1	**Review of thermochemical principles** 1. Enthalpy and Entropy 2. Gibbs free energy, chemical potential, and the equilibrium constant 3. Equilibrium calculations: pure solids and liquids, mixtures of solids and liquids, gases, solutes. 4. The effect of changes in temperature and pressure on the equilibrium constant 5. Exercises	Review of computer programs to calculate the chemical speciation of water. Exercises
2	**Adsorption-desorption reactions** 1. Properties of sorbent materials: particle size, surface area, surface charge, surface-site density 2. Cation exchange capacity 3. Sorption isotherms and the distribution coefficient 3.1 Freundlich Adsorption Isotherm 3.2 Langmuir Adsorption Isotherm 3.3 Comparison between the Adsorption isotherm models	Computer program to simulate reaction path in aqueous geological systems (e.g. PHREEQCI). Exercises I
3	4. Ion-exchange type models and concepts 5. Electrostatic Adsorption models 5.1 Diffuse-layer and constant capacitance models 5.2 Triple-layer model 6. Adsorption models and contaminant transport modeling	Computer program to simulate reaction path in aqueous geological systems (e.g. PHREEQCI). Exercises II.

4	**Redox reactions: Iron and sulfur geochemistry** 1. Review of redox reactions theory 2. Iron geochemistry 2.1 Stability constant of aqueous complexes 2.2 Eh-pH diagrams 3. Sulfur geochemistry 3.1 Acid-base reactions	Introduction to Inverse modeling I
5	3.2 Redox reactions 4. Iron-sulfur redox geochemistry 4.1 Occurrence and solubility of Fe(II) sulfide minerals 4.2 Eh-pH diagrams 5. Acid mine waters	**First mid-term,**
6	**Stable isotopes: Hydrogen and oxygen** 1. Isotopic composition of water molecules 2. Isotopic fractionation 3. Mass balance equations 4. Fractionation of reacting systems	Introduction to Inverse modeling II
7	5. The meteoric isotope line, effect of temperature, amount effect, continental effect, altitude effect. 6. Tritium as a short term age indicator	Introduction to forward modeling I
8	**Transport processes of chemical species: advection, dispersion, and molecular diffusion** 1. Advection and diffusion 2. Dispersal in flow 3. Molecular diffusion: basic equations and diffusion coefficient 4. Diffusion in water, gases and solids 5. Thermal diffusion	**Second mid-term,**

9	**Origin of petroleum and coal** 1. Diagenesis of organic matter 2. Catagenesis of organic matter 3. Metagenesis and metamorphism **Modeling the generation of petroleum and coal** 1. Determining kinetic parameters for oil generation 2. Variations in kinetic parameters with kerogen type. 3. A graphical method for modeling the oil and gas window	Introduction to forward modeling II
9	**Migration of oil** 1. Oil-field waters 2. Porosity of shales, carbonates and evaporites 3. Oil expulsion 4. Mechanisms of primary migration and secondary migration 5. Petroleum traps and seals.	
		Final Exam

Course Administration

Homework (quantitative and analytical exercises) will be assigned every week or two and must be turned in on time.

A report will be required after each computer lab session.

Two mid-quarter exams and one final exam will be given. The three exams are equally weighted. 60% of the final exam will cover the last 2 weeks of class and 40% will cover the first eight weeks. The mid-quarter exams and the final exam will include questions about the laboratory exercises.

Graduate students will be assigned an additional term paper. The topic for the paper will be chosen by the student from a list given by the instructor. For the grading of homework and tests, graduate students will be required to show a higher level of understanding and problem solution's skills.

Grading:

Mid-quarter exam I	20%
Mid-quarter exam II	20%
Final exam	20%
Homework and computer exercises	40%
Total	100%

For undergraduate students, the final grade will be given by the Total. For graduate students, this Total will be 80% of the final grade, the term paper will make up the remaining 20%. Letter grades will be assigned at the end of the quarter according to the statistical distribution of total points.

Student Regulations

Attendance policy: Attendance will be taken each day, and will be used as a subjective evaluation criterion in the determination of the final grade. Students are expected to attend lectures and laboratories. If there is a legitimate reason for absence from lecture or laboratory, students should notify the instructor in a timely fashion. Written excuses are not necessary.

Cheating policy: Students caught cheating will be dropped from the course with a grade of F.

Reference Books

No specific textbook will be required for this class, the instructor will prepare class notes and will assign additional readings to the students.
The following texts are considered as reference books:

Langmuir, D., 1997. *Aqueous Environmental Geochemistry*. Prentice Hall, 600 pp.

Hunt, J.M., 1996. *Petroleum Geochemistry and Geology*, 2nd Edition, W.H. Freeman and Company, 743 pp.

Lerman, A., 1988. *Geochemical Processes Water and Sediment Environments*, John Wiley and Sons, Inc., 481 pp.

Bethke, C. M., 1996. *Geochemical Reaction Modeling, Concepts and Applications*. Oxford University Press, 397 pp.