Syllabus for Geochemical Kinetics (EAS 6212)

L1105 ES&T: TuTh 1:35-2:55 pm

I. Instructor

Dr. Martial Taillefert
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II. Course Material

Course material will be based on class notes, handouts, and assigned readings. There are no textbooks for the course, but the following books will be used regularly:

- **Bernard P. Boudreau. 1997. Diagenetic Models and their Implementation: modelling transport and reactions in aquatic sediments. Springer.**
- **Kenneth A. Connors. 1990. Chemical Kinetics. The study of reaction rates in solution. VCH Publishers Ltd.**
- **Antonio Lasaga. 1997. Kinetic Theory in the Earth Sciences. Princeton Series in Geochemistry.**
- **Jerald L. Schnoor. 1996. Environmental Modeling: Fate and transport of pollutants in water, air, and soil. Wiley.**
- **Werner Stumm and James J. Morgan. 1996. Aquatic Chemistry. Chemical equilibria and rates in natural waters. Wiley.**

III. Grading

One mid-term and one final: 50%
Homeworks: 25%
Project Report: 25%

IV. Course Outline

1. Introduction to Geochemical Kinetics

- Kinetics vs. thermodynamics
- Notion of time and applications of kinetics in geochemistry
- Elementary and overall reactions

2. Mechanisms and Rates of Simple and Complicated Reactions

- Rate equations and stoichiometric equations
- Sequential reactions, parallel reactions, and rate-determining step
- Integrated rate equations
- Experimental determination of reaction orders
- Application of kinetics in geochemical and biological processes

3. Theory of chemical kinetics

- The Arrhenius Equation
- Collision theory
- Transition state theory

4. Kinetics at the solid-water interface

- Adsorption
- Dissolution
- Aggregation
- Nucleation and crystal growth

5. Reactor kinetics

- Batch reactors
- Continuous-Flow Stirred-Tank Reactors (CSTR)
- Plug Flow Reactors (PFR)

6. Reactive transport

- The conservation equations
- Advection and diffusion
- Chemical reactions and transport
- Governing equations for the transport of multiple reactive species
- Boundary conditions
- Diagenetic equations
- Analytical and numerical solutions

V. Project

The project consists of developing a mathematical model or conducting significant kinetic calculations on a data set from the literature or from the student's own research. The model or calculations can either be used to review parts of a published paper that includes such efforts or to discuss the student's own data. The paper (double-spaced with a 12 font) should be no longer than 20 pages including figures and references, but not the script(s) of the calculations which should be included in appendix. The project has to be approved by the instructor during week 9.

VI. Tentative Timeline