



# **ENGG\*6790 Special Topics in Environmental Engineering**

## **Geochemical Modelling**

Summer 2021

Section(s): S2

School of Engineering

Credit Weight: 0.50

Version 1.00 - August 05, 2021

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## **1 Course Details**

### **1.1 Calendar Description**

A course of directed study involving selected readings and analyses in developing knowledge areas of environmental engineering.

### **1.2 Course Description**

Geochemical modeling is a technique that enables understanding of geochemical phenomena based on fundamental principles of geochemistry coupled to physical observations and measurements. It can be used to predict the behavior of materials, fluids and solutions, the extent of chemical reactions and the reaction path that is followed, as well as to explain observed phenomena and to describe complex multi-phase elemental speciation and distribution. Geochemical modeling has traditionally been applied to systems in equilibrium, but has now extended to include kinetic modeling, biological modeling and transport modeling. Consequently, geochemical modeling has become a powerful tool in a number of research fields where geochemistry governs a natural process or is applied to produce a desired result.

This course will explore the thermodynamic underpinning of geochemical modeling, the inner workings of geochemical models, and will enable students to perform geochemical modeling of various systems and phenomena. Students will learn to use, and make use in projects, of the modeling software Visual MINTEQ and The Geochemist's Workbench.

This course will demonstrate the application of geochemical modeling for the study of several natural and engineered systems, including: water supply and treatment, groundwater flow and extraction, waste injection wells, recovery of oil from reservoirs, formation,

dissolution and alteration of minerals, biodegradation, and microbial populations. It will also cover several aspects of geochemistry (equilibrium and redox reactions, reaction kinetics, phase diagrams, surface complexation, activity and fugacity, the first and second laws of thermodynamics) and mineralogy (weathering, ageing, Ostwald ripening, leaching, polymorphs).

With the knowledge and skills gained in this course, students will be able to apply geochemical modeling in diverse engineering fields, such as Water and Wastewater Treatment, Groundwater Management, Oil and Gas Extraction, Solid Waste Storage, Site Remediation, Carbon Capture and Storage, (Bio)Hydrometallurgy, Chemistry of Building Materials, Fouling and Scaling, Geothermometry, and the Fate of Pollutants.

### 1.3 Timetable

**Lectures/Computer Labs:** Mondays and Wednesdays from 2:30PM to 05:20PM, online via WebEx.

### 1.4 Final Exam

No final exam is scheduled for this course. This course runs on an accelerated 6-weeks schedule of lectures, but the final project is due by Week 12 of the summer semester.

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## 2 Instructional Support

### 2.1 Instructional Support Team

<b>Instructor:</b>	Rafael Santos PhD, PEng
<b>Email:</b>	santosr@uoguelph.ca
<b>Telephone:</b>	+1-519-824-4120 x52902
<b>Office:</b>	THRN 2342
<b>Office Hours:</b>	Upon request.

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## 3 Learning Resources

### 3.1 Required Resources

#### Course Website (Website) (Website)

<https://www.courselink.uoguelph.ca>

Course materials, news, announcements, and grades will be regularly posted to the *ENGG\*6790\*S2 Special Topics in Environmental Engineering: Geochemical Modelling* Courselink site. You are responsible for checking the site regularly. **As per University regulations, all students are required to check their <mail.uoguelph.ca> e-mail account regularly;** e-mail is the official route of communication between the University and students.

#### Thermodynamics of Natural Systems (Textbook)

<http://search.ebscohost.com.subzero.lib.uoguelph.ca/login.aspx?direct=true&db=e000xna&AN=13live&scope=site>

Greg Anderson (2017), Cambridge University Press, Third Edition, eBook ISBN: 9781316796856.

The eBook of the Second Edition (2005) is currently (May 2021) available through the University of Guelph Library, via the above weblink.

### **The Geochemist's Workbench (Software)**

<https://www.gwb.com/>

The Standard Edition of The Geochemist's Workbench is accessible through the secondary remote access server

(<https://www.uoguelph.ca/engineering/it#Working%20From%20Home>) on machines 1 to 20 in THRN 2336.

Students can obtain the Community Edition to install on their personal computers from The Geochemist's Workbench website (<https://community.gwb.com/>). The Community Version has limited capabilities, so is not a full replacement for the Standard Edition that will be used in lectures/labs.

### **Visual MINTEQ (Software)**

<https://vminteq.lwr.kth.se/>

Visual MINTEQ is a free geochemical modeling software that is less capable than The Geochemist's Workbench, but is still very powerful and intuitive to use.

Student can install it on their personal computer (Windows or Windows emulator required), or access it through the secondary remote access server

(<https://www.uoguelph.ca/engineering/it#Working%20From%20Home>) on machines 1 to 20 in THRN 2336.

## **3.2 Recommended Resources**

### **Geochemical and Biogeochemical Reaction Modeling (Textbook)**

<http://search.ebscohost.com.subzero.lib.uoguelph.ca/login.aspx?direct=true&db=e000xna&AN=22live&scope=site>

Craig M. Bethke (2008), Cambridge University Press, Second Edition, eBook ISBN 9780511372919.

The eBook is currently (May 2021) available through the University of Guelph Library, via the above weblink.

### **Some Fundamentals of Mineralogy and Geochemistry (Website)**

<http://railsback.org/FundamentalsIndex.html>

L. Bruce Railsback (2006-2017), Department of Geology, University of Georgia.

### **GWB Online Academy (Software)**

<https://academy.gwb.com/>

Resources to learn to use and troubleshoot The Geochemist's Workbench: manuals, tutorials, forum, faq.

### 3.3 Lecture (Notes)

Lecture Notes (slides and task handouts) and Pre-Recorded Lecture Videos will be posted on Courselink prior to the respective lectures. Some supporting information will also be occasionally posted on the Courselink site.

### 3.3 Projects (Other)

Project assignments will be posted on Courselink at an appropriate time according to the due date schedule given in this course outline.

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## 4 Learning Outcomes

The goal is to prepare students to apply geochemical modeling to solve open-ended engineering and research problems that consist of water-gas, water-mineral, water-microbe, or purely aqueous interactions under either equilibrium or non-equilibrium conditions. These situations are often encountered when performing engineering work in both the professional and academic settings. To this end, students will learn and experience how to:

### 4.1 Course Learning Outcomes

By the end of this course, you should be able to:

1. Selectively search and critically review scientific literature on a geochemical modeling topic of their choice.
2. Collect and analyze relevant information to perform geochemical modeling of a problem of their choice.
3. Knowledgeably use geochemical modeling software to correctly model a geochemical process under equilibrium and non-equilibrium conditions.
4. Comprehend the fundamentals of geochemistry, mineralogy and thermodynamics behind geochemical models.
5. Critique applications of geochemical modeling to various Engineering, Environmental Sciences and Earth Sciences applications.
6. Communicate the rationale used to construct and how to operate a geochemical model.

### 4.2 School of Engineering - Graduate Degree Learning Outcomes

Successfully completing this course will contribute to the following:

#	Outcome	Learning Outcome
1	Literacy	1, 2, 4
1.1	Information Literacy	1, 2, 4

#	Outcome	Learning Outcome
1.2	Quantitative Literacy	1, 2, 4
1.3	Technological Literacy	1, 2, 4
1.4	Visual Literacy	1, 2, 4
2	Global Understanding	1, 5
2.1	Global Understanding	1, 5
2.2	Sense of Historical Development	1, 5
3	Communication Skills	1, 2, 5, 6
3.1	Oral Communication	6
3.2	Written Communication	1, 6
3.3	Reading Comprehension	1, 2, 5
4	Professional and Ethical Behaviour	3, 5
4.2	Ethical Reasoning	5
4.5	Intellectual Independence	3
5	Critical and Creative Thinking	1, 2, 3, 4, 5, 6
5.1	Independent Inquiry and Analysis	1, 2, 3, 5
5.2	Problem Solving	2, 3
5.3	Creativity	2, 3, 6
5.4	Depth and Breadth of Understanding	1, 2, 3, 4, 5

## 5 Teaching and Learning Activities

Students will receive weekly instructions about the lecture/lab format each week. The course will be delivered online, and some portions will be pre-recorded on WebEx, and some portions will be hosted live on WebEx.

The lecture schedule below is given week-by-week in a tentative fashion. Some modules maybe be anticipated or delayed depending on the pace of lectures.

Weblinks to pre-recorded lectures will be posted on CourseLink on a weekly basis, and students can watch them at any time thereafter. Live sessions each week will always be scheduled during the regularly scheduled lecture periods. To take into account the duration of the various recordings, the duration of live sessions will typically be shorter than the allocated lecture duration (e.g. 50 minutes live and 120 minutes free time). Students are encouraged to

use the remainder of scheduled lectures (free time) to watch recordings or to work on their assignment and project.

When following lectures, students should be prepared to perform exercises using Visual MINTEQ or The Geochemist's Workbench. Hands-on practice is crucial for gaining familiarity with the lecture concepts and operation of the software.

Outside of lecture times, students are encouraged to read assigned chapters from the required textbook (Thermodynamics of Natural Systems) and practice/review end-of-chapter problems, and to spend time operating the geochemical modeling software to gain the level of proficiency required for the final project.

## 5.1 Lecture

### Week 1

#### Topics:

Introduction to Geochemical Modeling:

- Module 1: Basics of (Inorganic) Water Chemistry
- Module 2: Introduction to Geochemical Modeling

### Week 2

#### Topics:

Fundamentals of Geochemistry, Part 1:

- Intro
- Module 3: The First Law of Thermodynamics
- Module 4: The Second Law of Thermodynamics
- Module 5: Geochemical Data
- Module 6: Aqueous Solution Chemistry
- Module 7: Fugacity and Activity
- Module 8: Equilibrium Chemistry

### Week 3

#### Topics:

Fundamentals of Geochemistry, Part 2:

- Module 9: Rock Water Systems
- Module 10: Redox Reactions
- Module 11: Phase Diagrams

- Module 12: Affinity and Extent of Reaction

#### **Week 4**

##### **Topics:**

Modeling Geochemical Equilibrium, Part 1:

- Module 13: Using the Geochemist's Spreadsheet (GSS)
- Module 14: Reactions
- Module 15: Diagrams
- Module 16: Redox Disequilibrium
- Module 17: High Salinity Fluids

#### **Week 5**

##### **Topics:**

Modeling Geochemical Equilibrium, Part 2:

- Module 18: Geochemical Buffers
- Module 19: Fluid Mixing and Scaling
- Module 20: Surface Complexation

#### **Week 6**

##### **Topics:**

Modeling of Geochemical Equilibrium, Part 3:

- Module 21: Geothermometry
- Module 22: Injection Wells

Modeling Time-Dependent Geochemical Reactions:

- Module 23: Reaction Kinetics
- Module 24: Biodegradation
- Module 25: Microbial Populations

## **5.2 Other Important Dates**

- i) Classes begin: Monday 17th May 2021.
  - ii) Holiday: Monday 24th May 2021.
  - iii) Classes conclude: Thursday 24th June 2021 (Monday schedule in effect).
  - iv) Last day to drop S21 Summer Session (6-week) courses: 24th June 2021.
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## 6 Assessments

### 6.1 Marking Schemes & Distributions

Additional assignments (task handouts) will be given throughout the term but they will not be graded. Consider them as formative.

The midterm exam will be open book (subject to restrictions to be informed by the instructor).

Name	Scheme A (%)
Literature Review	20
Midterm exam	30
Project Model Presentation	20
Project Model Report	30
Total	100

### 6.2 Assessment Details

#### Midterm exam (30%)

**Date:** Wed, Jun 9, 2:30 PM - 5:20 PM, Online

**Learning Outcome:** 4

Exam questions will cover lecture materials and exercises from Modules 1 to 5 and 9 to 12.

#### Literature Review (20%)

**Due:** Tue, Jun 22, 11:59 PM, Courselink Dropbox

**Learning Outcome:** 1

Perform and critically review scientific literature on geochemical modeling efforts done on a topic of the student's choice, either related to their graduate research or the project model they will prepare.

#### Project Model Presentation (20%)

**Date:** Wed, Aug 4, 5:00 PM, Courselink Dropbox

**Learning Outcome:** 6

Students will present their geochemical models prepared in The Geochemist's Workbench, explaining the rationale used to construct the model, the source and quality of the data



inputted to the model, assumptions and simplifications made, limitations of the model, and the results obtainable from the model.

### **Project Model Report (30%)**

**Due:** Wed, Aug 4, 5:00 PM, CourseLink Dropbox

**Learning Outcome:** 2, 3, 5

This "technical note" style report will discuss the modeling topic chosen, the procedure to build the model, the modeling results and their applications, and should be integrative of lecture topics covered in the course.

"Technical notes" are short articles published in some journals that emphasize an interesting result or a new perspective. You should follow the style described by the journal *Catena* for a technical note (except that you can, and should, include more figures and/or tables).

## **7 Course Statements**

### **7.1 Course Grading Policies**

**Missed Assessments:** If you are unable to meet an in-course requirement due to medical, psychological, or compassionate reasons, please email the course instructor. See the graduate calendar for information on regulations and procedures for Academic Consideration:

[https://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/sec\\_d0e2225.shtml](https://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/sec_d0e2225.shtml)

**Accommodation of Religious Obligations:** If you are unable to meet an in-course requirement due to religious obligations, please email the course instructor at the start of the semester to make alternate arrangements. See the graduate calendar for information on regulations and procedures for Academic Accommodation of Religious Obligations:

[https://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/sec\\_d0e2261.shtml](https://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/sec_d0e2261.shtml)

**Passing grade:** In order to pass the course, students must obtain an overall grade of 65% or higher on the aggregate of all the course work outlined in Section 6.1.

**Late Submissions:** Late submissions (> 1 hour) will be penalized if there are no acceptable compassionate or medical grounds. A 10% penalty per day (including weekends) will be applied for reports/assignments submitted between 1 and 120 hours late. Reports received more than 120 hours (five days) late will be assigned a grade of zero.

## **8 School of Engineering Statements**

### **8.1 Instructor's Role and Responsibility to Students**

The instructor's role is to develop and deliver course material in ways that facilitate learning for a variety of students. Selected lecture notes will be made available to students on

Courselink but these are not intended to be stand-alone course notes. Some written lecture notes will be presented only in class. During lectures, the instructor will expand and explain the content of notes and provide example problems that supplement posted notes. Scheduled classes will be the principal venue to provide information and feedback for tests and labs.

## 8.2 Students' Learning Responsibilities

Students are expected to take advantage of the learning opportunities provided during lectures and lab sessions. Students, especially those having difficulty with the course content, should also make use of other resources recommended by the instructor. Students who do (or may) fall behind due to illness, work, or extra-curricular activities are advised to keep the instructor informed. This will allow the instructor to recommend extra resources in a timely manner and/or provide consideration if appropriate.

## 8.3 Lab Safety

Safety is critically important to the School and is the responsibility of all members of the School: faculty, staff and students. As a student in a (computer) lab course you are responsible for taking all reasonable safety precautions and following the lab safety rules specific to the lab you are working in. In addition, you are responsible for reporting all safety issues to the laboratory supervisor, GTA or faculty responsible.

# 9 University Statements

## 9.1 Email Communication

As per university regulations, all students are required to check their e-mail account regularly: e-mail is the official route of communication between the University and its students.

## 9.2 When You Cannot Meet a Course Requirement

When you find yourself unable to meet an in-course requirement because of illness or compassionate reasons please advise the course instructor (or designated person, such as a teaching assistant) in writing, with your name, id#, and e-mail contact. The grounds for Academic Consideration are detailed in the Undergraduate and Graduate Calendars.

Undergraduate Calendar - Academic Consideration and Appeals

<https://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-ac.shtml>

Graduate Calendar - Grounds for Academic Consideration

<https://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/index.shtml>

Associate Diploma Calendar - Academic Consideration, Appeals and Petitions

<https://www.uoguelph.ca/registrar/calendars/diploma/current/index.shtml>

## 9.3 Drop Date

Students will have until the last day of classes to drop courses without academic penalty. The deadline to drop two-semester courses will be the last day of classes in the second semester.

This applies to all students (undergraduate, graduate and diploma) except for Doctor of Veterinary Medicine and Associate Diploma in Veterinary Technology (conventional and alternative delivery) students. The regulations and procedures for course registration are available in their respective Academic Calendars.

Undergraduate Calendar - Dropping Courses

<https://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-drop.shtml>

Graduate Calendar - Registration Changes

<https://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/genreg-reg-regchg.shtml>

Associate Diploma Calendar - Dropping Courses

<https://www.uoguelph.ca/registrar/calendars/diploma/current/c08/c08-drop.shtml>

## 9.4 Copies of Out-of-class Assignments

Keep paper and/or other reliable back-up copies of all out-of-class assignments: you may be asked to resubmit work at any time.

## 9.5 Accessibility

The University promotes the full participation of students who experience disabilities in their academic programs. To that end, the provision of academic accommodation is a shared responsibility between the University and the student.

When accommodations are needed, the student is required to first register with Student Accessibility Services (SAS). Documentation to substantiate the existence of a disability is required; however, interim accommodations may be possible while that process is underway.

Accommodations are available for both permanent and temporary disabilities. It should be noted that common illnesses such as a cold or the flu do not constitute a disability.

Use of the SAS Exam Centre requires students to book their exams at least 7 days in advance and not later than the 40th Class Day.

For Guelph students, information can be found on the SAS website

<https://www.uoguelph.ca/sas>

For Ridgetown students, information can be found on the Ridgetown SAS website

<https://www.ridgetownc.com/services/accessibilityservices.cfm>

## 9.6 Academic Integrity

The University of Guelph is committed to upholding the highest standards of academic integrity, and it is the responsibility of all members of the University community-faculty, staff, and students-to be aware of what constitutes academic misconduct and to do as much as possible to prevent academic offences from occurring. University of Guelph students have the responsibility of abiding by the University's policy on academic misconduct regardless of

their location of study; faculty, staff, and students have the responsibility of supporting an environment that encourages academic integrity. Students need to remain aware that instructors have access to and the right to use electronic and other means of detection.

Please note: Whether or not a student intended to commit academic misconduct is not relevant for a finding of guilt. Hurried or careless submission of assignments does not excuse students from responsibility for verifying the academic integrity of their work before submitting it. Students who are in any doubt as to whether an action on their part could be construed as an academic offence should consult with a faculty member or faculty advisor.

Undergraduate Calendar - Academic Misconduct

<https://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-amisconduct.shtml>

Graduate Calendar - Academic Misconduct

<https://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/index.shtml>

## 9.7 Recording of Materials

Presentations that are made in relation to course work - including lectures - cannot be recorded or copied without the permission of the presenter, whether the instructor, a student, or guest lecturer. Material recorded with permission is restricted to use for that course unless further permission is granted.

## 9.8 Resources

The Academic Calendars are the source of information about the University of Guelph's procedures, policies, and regulations that apply to undergraduate, graduate, and diploma programs.

Academic Calendars

<https://www.uoguelph.ca/academics/calendars>

## 9.9 Disclaimer

Please note that the ongoing COVID-19 pandemic may necessitate a revision of the format of course offerings and academic schedules. Any such changes will be announced via CourseLink and/or class email. All University-wide decisions will be posted on the COVID-19 website (<https://news.uoguelph.ca/2019-novel-coronavirus-information/>) and circulated by email.

## 9.10 Illness

The University will not normally require verification of illness (doctor's notes) for fall 2020 or winter 2021 semester courses. However, requests for Academic Consideration may still require medical documentation as appropriate.

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