Chemistry 4000B
Foundations of Chemical Kinetics
Fall 2021

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Course web site:	http://people.uleth.ca/~roussel/ C4000foundations
Class:	Mondays and Wednesdays from 10:30 to 11:45 In person: E640 Online: Zoom link to follow
Office hours:	Thursdays and Fridays from 10:00 to 11:00 In person: SA9414 Online: Zoom link to follow

Course prerequisites

The prerequisites are **Chemistry 2740** (Physical Chemistry) and **Math 1410** (Linear Algebra). If you lack this background, please see me so we can discuss your situation.

What this course will be about

In your past studies, you would have encountered the law of mass action and the consequent concept of a rate constant. In this class, we will ask ourselves why chemical kinetics is (mostly) governed by the law of mass action, and why the rate constants for various processes have the values they do. In other words, we will explore the fundamental physical theory underlying chemical kinetics.

The course will be organized into two parts. In part I, we will focus on gas-phase reactions, while part II will explore the theory of reactions in solution. Since molecules in the gas phase are far apart most of the time, the theory of gas-phase chemical reactions is somewhat simpler than the theory of reactions in solution. Somewhere along the way, I will also sneak in one of my favorite topics, the stochastic theory of chemical reactions, which is one way to conceptualize the transition from the statistical world that molecules inhabit to the deterministic world of the beaker.

I do some of my research with pen and paper, but a lot of theoretical chemistry requires computer calculations. I believe we should teach the field as it is rather than stick to things that can be done analytically. I will therefore show you how to do computer calculations based on the theory we are learning whenever possible. Because this is a new twist to a course that I haven't taught for some time, I am not entirely sure what software we will

be using throughout the term. So far, I am planning to introduce the use of Gaussian (for quantum chemical calculations) and of Matlab (or its free cousin Octave) for numerical computations. I will provide instruction as the need arises. The same software will be used for the assignments as in class.

Course delivery

This course will be offered both in person in the computer lab E640 and online. I initially scheduled this course in a computer lab to enable students to try things out as I explain how to do them. We will have to see how this works out for the remote students. It is possible that the course will mutate towards a more lecture-oriented style than I had originally intended as the term progresses.

In case there are connection problems or students have to miss classes, **the classes will be recorded**. Recordings will be available only to members of the class until the end of term, and will be deleted shortly after the final exam. The link to access the videos will be sent to you by email shortly after the first class.

All of the software we need will either be available in the computer labs, or there is a free version you can use at home. For commercial software available only on campus, there is the possibility of using lab computers from home if that is more convenient for you. The details on how you accomplish this act of technological magic are here: `https://uleth.sharepoint.com/sites/computer-lab-resources/SitePages/accessing-labs.aspx` (Note that this won't work unless you have UofL login credentials.)

Office hours

I will hang out in my office and on Zoom during my office hours. I may occasionally need to cancel an office hour, which is part of the reason I am scheduling two hours per week. I will try to give you as much notice as possible if this becomes necessary. I am also willing to meet at other times, especially if I have to cancel an office hour, of if you need to speak to me privately.

Note that I will provide you with different Zoom links for the class and for my office hours. This is necessary since classes are being recorded while office hours are not.

Textbook

I am writing a textbook for this course because existing textbooks don't cover the range of topics I would like to teach you. I will be emailing you chapters as I complete them, hopefully at least a few days ahead of the corresponding lecture. Note that the chapters I am sending you are **for your use only** and are **not to be redistributed by any means, physical or electronic**.

Email

Important information will frequently be communicated to the class via email. It is **your responsibility** to keep an eye on your email during the term.

Grading scheme

Evaluation	Date(s) assigned	Date(s) due	Weight
Assignments	Sept. 22, Oct. 6, Nov. 3 & 24	Sept. 29, Oct. 13, Nov. 17, Dec. 1	$4 \times 10\%$
Take-home midterm	Oct. 20	Oct. 27	20%
Take-home exam	Dec. 8	Dec. 15	40%

Assignments and exams submitted after the published deadline will normally earn a mark of zero. In exceptional cases, a short extension may be granted, or the assignment may be waived. In the latter case, the weight of the assignment will be redistributed over other course components. Students who find themselves unable to complete an assignment due to exceptional circumstances should notify me as soon as possible.

Assignments and exam answers will be submitted electronically. In some cases, I may want to see computer files (e.g. Gaussian input/output files, or Matlab/Octave scripts) in addition to your written answers. Detailed instructions on submission will be provided with the assignments.

The following are the maximum cut-off points for each of the letter grades:

A+	90%
A	85%
A−	80%
B+	77%
B	73%
B−	70%
C+	67%
C	63%
C−	60%
D+	55%
D	50%

In other words, if you get at least 80%, you will get at least an A−. I reserve the right to change these cutoffs downward in the event that two (or more) students with very similar marks straddle a boundary, so for instance if one student gets 79.8% and another has 80.1%, they would both get an A− since similar performances should earn similar grades.

Collaboration

My main concern is that your assignments and exams should reflect your understanding of the material, not another student's. It is understood that you may need to talk to me

or to classmates in order to sharpen your grasp of the material as you work through an assignment. But you should write up your own assignment in your own words. Please don't share files and especially don't share the text of your answers with each other. It's glaringly obvious when that has happened. **The penalties for attempting to pass off someone else's work as your own can be severe. You are better off taking an honest zero on a question than copying someone else's work.** If you have any doubts about what constitutes appropriate conduct, you are strongly encouraged to talk to me.

The take-home midterm and final exam, unlike the assignments, **must** be based on individual work **unaided** by any other person. If you have questions about the exam or the material as you are working on either the midterm or final, direct them to me.

Learning in Covid times

Our ability to continue with in-person learning depends strongly on everyone living by the rules the University has developed. I would ask you to be respectful of each other and to act in such a way as to minimize the risk that you will pass on an infection should you be (probably unknowingly) exposed to the virus. The rules around infection control are changing on an almost daily basis. Just a few hours before I sat down to write this, the Province reimposed a mask mandate requiring masks "in all indoor public spaces and workspaces" with some exceptions for employees "in work stations" and schools. Does that include students who can socially distance in a computer lab at a university? Course instructors? We don't know yet. In any event, it is likely that the public health guidance will evolve over the term. I will keep you informed of any changes and of their implications for our class as I learn of them.

If at any time you feel uncomfortable about your safety in the computer lab, let me know and I will see what I can do to address your concerns. You also have the fallback option of joining the class through Zoom, which you can avail yourself of at any time for any reason. I am happy for you to learn in whatever way is most comfortable for you.

For those attending in person, please keep the following in mind:

- The University generally **requires** you to wear a mask covering the nose and mouth in classes and in all public spaces inside University buildings, with a very few common-sense exceptions (e.g. for eating). You may be exempted from this requirement in this class *if* we can space out sufficiently in the computer lab, but be aware that this exemption could change at any time.

- You must be free of Covid symptoms to come to campus. The hybrid model facilitates your staying at home if you have any doubts about your health while still keeping up with the class. Note that, while there is no specific mandate for other illnesses, I would encourage you to stay at home if you suspect you have any communicable disease such as a cold or flu.

- You **must** either have received **two vaccine doses** or have **tested negative for Covid within the past week** to come to campus. This information must be provided to the University before you can attend campus. The uLethbridge Safe app is the easiest way to handle this requirement.