Chemistry 5000/7000B
Foundations of Chemical Kinetics
Fall 2021

Instructor:	Marc R. Roussel
Offices:	SA9414
Phone:	403-329-2326
Email:	`roussel@uleth.ca`
Course web site:	`http://people.uleth.ca/~roussel/C4000foundations`

Class:	Mondays and Wednesdays 10:30 to 11:45 Mountain time 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

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	$4 \times 6\%$
Take-home midterm	Oct. 20	Oct. 27	12%
Take-home exam	Dec. 8	Dec. 15	24%
Term paper			
—Topic selection and bibliography		Oct. 1	5%
—Detailed outline		Oct. 29	10%
—Final paper		Dec. 17	25%

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.

Term paper

You will be required to write a paper on a topic of your choice with one of the following themes:

- A topic relating to the physico-chemical foundations of chemical kinetics
- A topic in molecular chemical dynamics, including experimental approaches
- A review of a specific application area of theoretical kinetics

You can either write a paper on a topic not covered in class, or you can provide additional depth to an area we will cover in class. A topic related to your thesis research may be appropriate, but I would not want your paper to rehash something you have already done in a research context.

As a *rough* guide, here are the topics I intend to cover this term (subject to revision): transition-state theory, RRKM theory, master equations, diffusion-influenced reactions, Kramers theory, Marcus electron-transfer theory, theory of heterogeneous kinetics.

Your work on the term paper will proceed in three phases: First, you will select a topic and identify relevant reading materials. Second, you will write a detailed outline of your paper. Finally, you will write the paper itself.

Topic selection and bibliography

This document should give a draft title for your term paper, a brief description of your topic (one to two paragraphs) and a list of sources you have identified for this topic. You should list at least five books (indicating the relevant chapters if the whole book is not relevant to your topic) or peer-reviewed journal articles relating to your topic that provide at least some of the information you will need for your term paper.

The following are some possible sources of term paper topic ideas:

- Books on chemical kinetics and dynamics—yes, I'm suggesting you take a trip to the Library!
- *Annual Review of Physical Chemistry*
- *International Reviews in Physical Chemistry*
- *Chemical Reviews*
- *Accounts of Chemical Research*
- *ChemTexts*

Other resources may be useful depending on your interests. Consult me if you want additional advice.

You are encouraged to talk to me about your topic before you do too much work identifying resources. The point of this part of the exercise is to make sure that you start off with a good topic for which you will be able to find relevant source material. By the time you submit your topic and bibliography, you should feel confident about your choice. Getting to that point may require that you discuss your direction with me well in advance of the deadline.

The references in your bibliography should be given in the style used by the ACS (American Chemical Society) journals. If you use EndNote, BibTeX, or any of a number of other citation managers, then you can automatically generate references in the ACS style by choosing the appropriate output filter. This is much easier (and less error-prone) than hand-formatting your bibliography, and is strongly encouraged.

Detailed outline

The detailed outline will list the sections of your paper and outline (i.e. lay out in point form) the major points you plan to make in each section. For each point, you should list the source(s) you will use in support.

The point of this exercise is twofold: First and most obviously, it will help you get your ideas in order, and will give me a chance to provide some feedback before you produce the final paper. Almost as importantly, it will help you avoid a subtle form of plagiarism in which you end up copying the plan of someone else's paper (or of a major section of a paper), in the sense of presenting the same ideas, perhaps using slightly different words, in exactly the same order as someone else has done. Developing a detailed outline should alert you to this danger. If a large part of your term paper is entirely based on one source, you probably haven't done enough background reading, and you should make sure that you aren't just replicating someone else's thoughts in slightly different words. Ask yourself what questions you need to answer in order to understand your topic, and set up an outline in which you answer those questions in an order that makes sense to you (and hopefully to another reader). It will probably be different than any single source you have read.

Outlines will be judged based largely on their logic. It should be clear, after reading your outline, what major question or important point you want to address. Moreover, it should be clear how you plan on attacking your subject and what sources of information you will use in support of your points. At this stage, you may already have identified additional useful sources beyond those presented at the topic selection stage. By all means incorporate those into your outline.

Final paper

Your final paper should include at least 2500 words (not counting the references), but may be longer if necessary. It should include at least 10 references to books (or chapters therein) or peer-reviewed journal articles (and not the just 5 starter references required at the time of topic selection). Even if you cite multiple chapters within a book, each book only counts as one reference unless the book is an edited volume with different authors for each chapter, in which case the individual chapters can be counted as separate sources.

The paper will be graded by the following criteria:

Rubric	**Weight**
Topic clearly defined	5%
Major ideas clearly identified and discussed	35%
Internal logic and technical correctness	30%
Appropriate use of references	10%
Grammar, style	20%

If you have any questions about these grading criteria, then please talk to me.

You should write your paper as if it will be read by another member of the class, i.e. someone who has some basic background in the physical sciences (basic physics, introductory kinetics, etc.) plus the material covered in the course. Such a reader should be able to learn something about your topic by reading your paper.

References should be given in the style of an ACS journal. You are expected to cite sources for any ideas presented in your paper. If you have doubts about how to cite sources appropriately, please talk to me. Failure to appropriately cite sources can lead to charges of plagiarism.

Your paper will be submitted through `turnitin.com`. Instructions on the use of this service will be provided later in the term. `Turnitin.com` provides, among other things, a plagiarism detection system. Our class will be set up in `turnitin` so that (a) your papers will be saved in `turnitin`'s database, preventing future students from plagiarizing your work, and (b) you can view your own originality reports prior to the submission deadline.

If you object to the storage of your paper in `turnitin`'s database, then please talk to me as soon as possible. My view is that this protects your paper from being stolen by some future student, but I know that views differ on this point.

An originality report is generated by matching your paper to the documents in `turnitin`'s database, which consist of past student papers, peer-reviewed journal articles, books and web pages. Any similar passages are flagged, and the original sources can typically be viewed (with some exceptions; in particular student papers can't be viewed without requesting permission from the instructor of the course to which the paper was originally submitted). To me, the best and most important feature of `turnitin` is that students can generate their own originality reports as they are working. This should, at least in principle, avoid the most obvious kinds of plagiarism since you can catch yourself before you submit anything. I **strongly** encourage you to submit a draft of your paper to `turnitin` well before the submission deadline. If you have any questions about your originality report, you can then talk to me. I will not look at materials submitted to `turnitin` before the deadline except on student request.

If you make some corrections to your paper and resubmit it to `turnitin`, a new originality report will be generated promptly (usually within a few minutes) the first three times you resubmit. After that, there will be a delay of 24 hours before a new originality report is generated. You shouldn't be trying to iteratively tweak your wording to "pass" a `turnitin` scan. If you identify a significant plagiarism issue in your own work, take the time to fix it properly by deleting the offending section and rewriting it "cold", i.e. without looking at the problematic text.

Advice on avoiding plagiarism

The emphasis on plagiarism in this document and, indeed, in Western universities in general, has a philosophical origin: Western university culture values individuality and originality. Accordingly, when you write a paper, I want to see **your** ideas expressed in **your** words. The problem is that modern tools make it easy for you to deviate from this ideal without meaning to: It is far too easy to cut-and-paste from various sources into your working document, thinking that you will rewrite the passage in your own words later. However, it is very hard to rewrite something in your own words if you are staring at a perfectly well-written sentence that says something you want to say. Worse, once you start doing this, you might find yourself grabbing a whole paragraph, or even two, and now you have definitely crossed a line you ought not to have crossed. In any event, cutting-and-pasting from sources defeats the purpose of finding out what **you** have to say about an issue.

My first piece of advice on avoiding plagiarism is to work with your sources using old-fashioned methods: Get out a pad of paper and a pen, and write notes about particularly important points as you read your sources, with a precise reference back to the document in case you want to look it up again later. You can also annotate the document itself, either in writing if you have a printout or electronically if the document is a pdf file, but your primary research tool should be a pad of paper. Just jot down key ideas in a few words as you go, and resist the urge to copy full sentences unless someone has said something so well that you intend to quote them directly. Note however that direct quotation is rare in scientific writing.

When the time comes to write your outline, look at your notes. They should contain enough details to jog your memory about most of the key points you want to make. Go back to the primary sources only if something still isn't clear.

While writing your outline, start by asking yourself what major point(s) you want to make. What background do you need to present in order for the story to make sense? What points do you need to make in support of your major point(s)? In what order would it make most sense (to you) to present the material? Answering these questions will lead to an outline that is your own work, which is what I want to see. Use your notes to remind yourself of things you read as you work through this process.

When you start writing your paper, just fill in the points suggested by your outline in your own words. Go back to your sources to check on technical points, but **don't write while you're looking directly at your source material**. If you do, you will end up writing sentences that look like those in your source, and again you might run into trouble with plagiarism.

Writing with confidence

Many, many cases of plagiarism originate in a lack of confidence of the writer, either in their understanding of the material or in their ability to write correct, grammatical English. The point of university term papers is to teach you to write and, hopefully, eventually to get you to the point where you can write competently, and have some confidence that you can do so. Plagiarizing someone else's work does not contribute to this objective.

Quite apart from the possibility of penalties and the self-defeating nature of plagiarism, you should tell yourself that there are support systems in place to enable you to succeed in your writing tasks. If you really don't know how to write a term paper, look for on-campus workshops on this topic, or get in touch with the Writing Centre.

More likely, you sort of know how to go about this task, and you just need to convince yourself that you are smart enough to read up about your topic, understand it, and convey that understanding to others. You may need help understanding some parts of your readings. If so, drop in during office hours after giving me some forewarning of what you need help with.

With respect to spelling and grammar, turn on any spell-checking or grammar-checking features of your word processor or text editor. Don't ignore warnings. If you're not sure what a warning means, ask someone. Be aware that grammatical warnings, in particular, don't always give correct advice on correcting a sentence. For example, Microsoft Word routinely warns that the word "which" should be preceded by a comma. Often however the required correction is actually to replace "which" by "that" rather than inserting a comma. Tell yourself that the grammar checker has highlighted a part of the sentence you need to look at, but that it's up to you (possibly with some help) to figure out exactly what is wrong.

You can also help yourself a great deal by writing in plain English. There is some excellent scientific writing out there. There is also some scientific writing that is much more complicated than it needs to be, to the point of being unclear. Don't think that because you have seen others write very complicated sentences, you have to do the same. Concentrate on writing clear, direct sentences. There are no points in my grading scheme for sentence complexity or for using obscure vocabulary.