CHM 410H-1410H Analytical Environmental Chemistry
Course Syllabus: Fall 2020

Contact Information

Prof. Jessica D'eon, jessica.deon@utoronto.ca (Class content weeks 7-12)
Prof. Hui Peng, hui.peng@utoronto.ca (Class content weeks 1-6)

Classes: Tuesdays and Thursdays 4:00 – 5:00 PM EST
Online synchronous classes that will subsequently be posted online for asynchronous viewing

Laboratory: Friday 10:00 AM – 12:00 PM EST or Friday 1:00 – 3:00 PM EST
Details can be found in the laboratory section of the syllabus which begins on page 5.

Course Goals

This course seeks to produce analysts with a basic conceptual understanding of a broad range of modern analytical equipment relevant to trace environmental analysis. The lab component is designed to provide practical knowledge of sample collection and analysis, as well as data interpretation and visualization involved in environmental analysis.

Student Learning Outcomes

Upon successfully completing CHM 410H-1410H, students will be able to design an environmental analysis starting with a literature search through experimental design and data analysis.

To complete this task students must be able to:

1. Search the scientific literature for relevant background information and methodologies.
2. Make educated decisions related to analytical methodology and instrumentation.
3. Analyze, interpret, and effectively visualize analytical data.
4. Confidently ask for help or advice.

Grading Scheme

Laboratory Grade			70%
Labs 1-3 (Sept 25, Oct 2 and 9)		20%	
Lab 1 – Short report	4%		
Labs 2 and 3 – Full lab reports	15% (10% for the report with the highest grade)		
Participation and Preparation	1%		
Lab 4 – Field Trip and Analysis (Oct 16, 23, and 30)		20%	
Figure submission (Thurs Oct 29)	1%		
Report outline (Fri Nov 6)	4%		
Report (Fri Nov 20)	15%		
Lab 5 – Suspect Screening of MS Data (Nov 6, 20, and 27)		30%	
Top Down Worksheet (Fri Nov 6)	3%		
Bottom Up Worksheet (Fri Nov 20)	2%		
Presentation and defense (Fri Dec 4)	10%		
Report (Tues Dec 8)	15%		
Environmental Analysis Project			30%
Midterm Assignment (Oct 22)		10%	
Final Assignment and Oral Exam (final assessment period)		20%	

Discussion Topics

Unit 1: Sample Preparation and Quality Control These techniques ensure the concentrations we observe in the lab reflect the concentrations present in the environment.

Unit 2: Mass Spectrometry Instrumentation and Scan Types we will discuss the major types of mass spectrometers and how their various abilities to scan mass-to-charge ratios effects their applications to different environmentally-relevant chemical analyses.

Unit 3: Identification of Unknown Compounds Most of the semester is dedicated to quantifying concentrations of known analytes, however environmental issues are complex and sometimes it's not clear which compounds are most important. In this unit we will explore techniques researchers use to identify compounds without *a priori* knowledge.

Unit 4: Ionization for Mass Spectrometric Analysis We will discuss a variety of ways gas phase ions are produced for analysis by mass spectrometry and how these processes are optimized for environmental applications.

Unit 5: Chromatography Chromatography is relevant both as a separation technique to separate chemicals of interest from each other and possible interferences, as well as an effective means of delivering the compound of interest to the chosen detector.

Unit 6: Non-MS Analysis The majority of the class is focused on the analysis of organic contaminants through mass spectrometry hyphenated to a chromatographic separation. In this unit we will talk about spectroscopic detectors and analyzers and discuss the benefits and drawbacks to the two approaches.

Class Schedule

September	10 R	Class Introduction	D'eon / Peng
	15 T	Lab Format and Discussion	D'eon
	17 R	U1: Chemical Partitioning	Peng
	22 T	U1: Sample Extraction and Cleanup	Peng
	24 R	U1: Quality Control	Peng
	29 T	U2: Mass Spectrometry Instrumentation I	Peng
October	1 R	U2: Mass Spectrometry Instrumentation II	Peng
	6 T	U2: Mass Spectrometry Instrumentation III	Peng
	8 R	U2: Mass Spectrometry Scan Types and Applications I	Peng
	13 T	U2: Mass Spectrometry Scan Types and Applications II	Peng
	15 R	U3: Introduction to Nontargeted Chemical Analysis	Peng
	20 T	U3: Isotopes and Fragmentation Patterns	Peng
	22 R	U3: Computation Algorithms	Peng
	27 T	U4: Mass Spectrometer and Ionization I	D'eon
	29 R	U4: Mass Spectrometer and Ionization II	D'eon
November	3 T	U4: GC-MS Ionization Interfaces	D'eon
	5 R	U4: LC-MS Ionization Interfaces	D'eon
	10 T	Study Break	
	12 R	Study Break	
	17 T	U4: EI Fragmentation Schemes	D'eon
	19 R	U5: Introduction to Chromatography	D'eon
	24 T	U5: Gas Chromatography	D'eon
	26 R	U5: Liquid Chromatography	D'eon
December	1 T	U6: Spectroscopy (UV and fluorescence)	D'eon
	3 R	U6: Spectroscopy (Real-time Gas Phase Analysis)	D'eon
December	8 T	Review/Discussion	D'eon

Environmental Analysis Project

This year CHM410H-1410H will not include any tests or exams. Instead the class will include a project where each student receives a unique environmental pollutant and through a midterm and final assignment builds an appropriate analysis for their pollutant and then discusses and defends their plan in a 20-minute oral exam. Additional details on these assessments will be provided on Quercus.

Website and Online Interfaces

All material for both class and lab will be provided through Quercus. You are responsible for checking this site regularly. Synchronous classes and labs will be conducted over Zoom. Specific details for each meeting will be provided on Quercus.

Class Recording and Copyright

All aspects of the synchronous classes and labs in this course, including your participation, will be recorded on video and will be available to students in the course for viewing remotely and after each session. Course videos and materials belong to the instructors and TAs and are protected by copyright. In this course, you are permitted to download session videos and materials for your own academic use, but you should not copy, share, or use them for any other purpose without the explicit permission of the specific instructor. For questions about recording and use of videos in which you appear please contact Prof. D'eon.

Student Hours

Prof. Peng and Prof. D'eon enjoy student hours tremendously. We want you to know that this is time we have set aside to answer your questions or just chat with you about the class or environmental analysis in general. With this in mind we want to be clear that we are looking forward to speaking with you, so please attend! Helping you be successful in this class is our job! Student hours will be scheduled using student feedback after the start of class.

Technological Requirements

This course requires the use of computers, and of course sometimes things can go wrong when using them. You are responsible for ensuring that you maintain regular backup copies of your files, use antivirus software (if using your own computer), and schedule enough time when completing an assignment to allow for delays due to technical difficulties. Computer viruses crashed hard drives, broken printers, lost or corrupted files, incompatible file formats, and similar mishaps are common issues when using technology, and are not acceptable grounds for a deadline extension.

Specific guidance from the U of T Vice-Provost, Students regarding student technology requirements is available here: https://www.viceprovoststudents.utoronto.ca/covid-19/tech-requirements-online-learning/

Advice for students more broadly regarding online learning is available here: https://onlinelearning.utoronto.ca/getting-ready-for-online/

Online Etiquette

The University of Toronto is committed to equity, human rights and respect for diversity. All members of the learning environment in this course should strive to create an atmosphere of mutual respect where all members of our community can express themselves, engage with each other, and respect one another's differences. U of T does not condone discrimination or harassment against any persons or communities.

Textbook or Readings

There is no textbook requirement for CHM 410H-1410H. As this course aims to present current topics in environmental analytical chemistry, primary scientific literature resources are provided when appropriate and can be accessed via Quercus. Students are encouraged to read the book *Mass Spectrometry* by Jürgen H.

Gross which is available online through the U of T libraries using the following link: http://go.utlib.ca/cat/8187279. Additional resources may be provided for specific classes or topics.

Email Policy

Prof. D'eon and Prof. Peng look forward to communicating with you and welcome your emails. We will try our best to respond to your emails within 24 hours on weekdays.

Late Policy

Anything handed in late, in the lab or the class, will be docked 10% per day including the weekend. If you require an extension on course work contact Prof. D'eon by email as the CHM 410H-1410H course coordinator.

Academic Integrity

As a teaching team we want you to feel supported in your learning and so you are welcome you to seek guidance from the TAs and instructors. You are also welcome to work constructively with your peers on the general content and understanding of the material. However, **all reports and assignments submitted in this class MUST represent your own independent work and comprehension**. Academic integrity is essential to the pursuit of learning and scholarship in a university, and to ensuring that a degree from the University of Toronto is a strong signal of each student's individual academic achievement. As a result, the University treats cases of cheating and plagiarism very seriously. The University of Toronto's Code of Behaviour on Academic Matters (https://governingcouncil.utoronto.ca/secretariat/policies/code-behaviour-academic-matters-july-1-2019) outlines the behaviours that constitute academic dishonesty and the processes for addressing academic offences. Potential offences include, but are not limited to:

In papers and assignments: Using someone else's ideas or words without appropriate acknowledgement; Submitting your own work in more than one course without the permission of the instructor; Making up sources or facts; Obtaining or providing unauthorized assistance on any assignment.

On tests and exams: Using or possessing unauthorized aids; Looking at someone else's answers during an exam or test; Misrepresenting your identity.

In academic work: Falsifying institutional documents or grades; Falsifying or altering any documentation required by the University.

All suspected cases of academic dishonesty will be investigated following procedures outlined in the Code of Behaviour on Academic Matters. If you have questions or concerns about what constitutes appropriate academic behaviour or appropriate research and citation methods, you are expected to seek out additional information on academic integrity from your instructor or from other institutional resources (see https://www.academicintegrity.utoronto.ca/).

Accessibility

Students with diverse learning styles and needs are welcome in this course. The University of Toronto is committed to accessibility: if you require accommodations for a disability, or have any other accessibility concerns about the course, please contact Accessibility Services as soon as possible.

Additional Services and Support

The following are some important links to help you with academic and/or technical service and support: General student services and resources at Student Life; Full library service through University of Toronto Libraries; Resources on conducting online research through University Libraries Research; Resources on academic support from the Academic Success Centre; Learner support at the Writing Centre ; Information for Technical Support/Quercus Support

CHM 410H-1410H Virtual Laboratory
Fall 2020

Laboratory Coordinator

Prof. Jessica D'eon, jessica.deon@utoronto.ca

Hello! I am the lab coordinator for CHM 410H-1410H and I am so excited to work with you on the practical aspects of the course.

Laboratory: Friday 10:00 AM – 12:00 PM EST or Friday 1:00 – 3:00 PM EST

The Fall 2020 CHM 410H-1410H laboratory session begins on Friday September 18 and runs for 10 weeks excluding the Friday of the Fall study break (November 13). Each Friday the lab includes two distinct sessions; one on Friday mornings with a synchronous meeting with a lab TA from 10-12 and the other on Friday afternoons with a synchronous meeting with a lab TA from 1-3. Undergraduate students chose one of these sessions during enrolment and the laboratory coordinator will enroll graduate students in one of the sessions according to their availability.

Laboratory Groups

Each session will be divided into three lab groups (morning – Groups A, B, C and afternoon – Groups D, E, F), each with a maximum of six students. When the laboratory was offered in-person, the students in each lab group worked together to complete the physical work of each lab. In the online environment the lab groups will be used in much the same way. You will complete lab together with your group mates and you are encouraged to work together and form a cohort who moves together through the class. You will sign up for a lab group during the first week of classes.

Laboratory Objective

The CHM 410H-1410H laboratory provides students with practical experience in the analysis of environmental contaminants. When the labs are presented in person, mastery of the lab skills necessary to perform these high-level analyses is a clear learning objective of the lab. However, this has only ever been a minor objective of the laboratory. The major objective is to solidify the in-class learning by handling, manipulating and visualizing data (third learning objective of the class) and this learning objective is just as relevant online as it was in person.

Laboratory Teaching Assistants

We have a fantastic teaching team in CHM 410H-1410H that includes five amazing graduate student teaching assistants. All of the TAs are graduate students in our environmental chemistry program and have either taken the class or TAed it (or both) in the past, and they are looking forward to working with you. This being said, the TAs work on contract with very specific hour allocations for contact with the CHM 410H-1410H students and if you require assistance outside the lab meeting time it is best practice to attend lab student hours or send an email to the lab coordinator, Prof. D'eon.

Laboratory Student Hours

As the laboratory coordinator, Prof. D'eon I will be holding lab-specific student hours. I want you to know that I have set aside this time to answer your questions or just chat with you about the lab experience. With this in mind I want to be clear that I am looking forward to speaking with you, so please attend! I don't ever want to hear "I didn't want to bother you…" as a reason you didn't seek help. You are NOT bothering me!! Helping you be successful in this class is my job! Student hours will be scheduled using student feedback after the start of class.

Laboratory Content

The CHM 410H-1410H laboratory is divided into three sections; Labs 1-3, Lab 4 and Lab 5.

Labs 1-3 are introductory in the sense that they have been designed to expose students to the analysis of a variety of matrices (gas, liquid and solid) and the use of different instrumentation (NMR, real-time sensors, and LC-MS/MS). Lab groups will rotate through these activities using the following schedule.

Date	Lab 1		Lab 2		Lab 3	
	10-12	1-3	10-12	1-3	10-12	1-3
Sept 25	A	D	B	E	C	F
Oct 2	C	F	A	D	B	E
Oct 9	B	E	C	F	A	D

Lab 1: NMR as a Tool for Quality Control in the Food Industry

TA: Jeremy Gauthier, jeremy.gauthier@mail.utoronto.ca

Lab 1 involves the analysis of honey using nuclear magnetic resonance spectrometry. Using your generated spectra, you will identify and quantify the sugars present and then compare your entire spectra to previous samples using principle component analysis (PCA) to try to identify honey from different regions or samples that may be adulterated.

Lab 2: Markers of Polluted Air

TA: Mark Panas, mark.panas@mail.utoronto.ca

Lab 2 involves the use of portable air monitors for the analysis of fine particles, ozone and carbon dioxide to investigate the quality of the indoor or outdoor air in the City of Toronto. The focus of this lab is using data visualization to identify and understand trends between analytes.

Lab 3: Analysis of Organophosphate Flame Retardants in Dust

TA: Andrew Folkerson, andrew.folkerson@mail.utoronto.ca

Lab 3 involves the extraction and analysis of dust samples that students bring to the lab for a suite of six organophosphate flame retardants. This lab provides students with extensive experience in the quality control protocols that are required to ensure data quality and how to present and discuss this type of analytical data.

Lab 4: Analysis of Perfluoroalkyl Acids in Lake Niapenco

Holly Barrett, holly.barrett@mail.utoronto.ca

Lab 4 involves a field trip for the collection of water, sediment and biological (fish, shrimp, snails, bugs…) samples, with subsequent matrix-specific extraction and analysis for four perfluoroalkyl acids (PFAAs). Outside of the practical aspects, this lab provides students with an opportunity to synthesize data from a range of PFAAs in a wide range of sample matrices within the same ecosystem.

Lab 5: Suspect Screening of in High-Resolution Mass Spectral Data

Steven Kutarna, steven.kutarna@mail.utoronto.ca

Lab 5 will walk you through the identification of chemicals in high-resolution mass spectral data from an extracted dust sample. Following this exercise, lab groups will be assigned chemical classes and a set of samples for analysis.

Lab Preparation
Similar to an in-person lab, you are required to come to each synchronous lab session prepared to discuss the relevant topic. Specific preparation for each lab will be outlined on Quercus, any questions should be directed to the lab coordinator, Prof. D'eon.

Lab Participation
Introductory labs 1-3 all include a preparation grade (completion of the pre-lab assignment on Quercus by noon on Thursday on the day prior to your meeting with the TA), and a participation grade (for reasonable participation during the synchronous session). If for any reason you are unable to attend the synchronous session the participation grade will be determined by a 20-minute discussion with the lab coordinator.

Lab Reports
Reports for labs 1-3 are due at the beginning of the subsequent Friday synchronous session with the lab TA. Lab 4 includes a report outline due before class on Tuesday November 3 and the final report on Friday November 20 prior to your scheduled synchronous lab session. Lab 5 includes an initial report on organophosphate flame retardants on Friday November 6, followed by a presentation of the group dataset during the typical lab periods on Friday November 27 and the final report is due on Tuesday December 8 before class. Marking schemes for each report will be provided in advance on Quercus.

Turnitin
Students will normally be required to submit their lab reports to Turnitin.com for a review of textual similarity and detection of possible plagiarism. In doing so, students will allow their lab reports to be included as source documents in the Turnitin.com reference database, where they will be used solely for the purpose of detecting plagiarism. The terms that apply to the University's use of the Turnitin.com service are described on the Turnitin.com web site.