COVID and EES1102 - 2022

We are doing everything we can to make this course as enjoyable and educational as possible despite the Covid uncertainties.

Due to the new Omicron restrictions we cannot offer the entire course in person as the TRACEs centre cannot handle the course enrolment.

Instead we will

1) **Offer the first 8 weeks online** (Jan-Feb). The goal here is to deliver all the course materials, learning objectives and complete all graded assignments.
2) **Offer the last 4 weeks in-person** (March). **TRACES Center EV215.** The goal is to give you hands-on experience. It is only possible if we are allowed back at full capacity. But as all the assignments have been completed, this should be a fun opportunity to get experience using all the instruments.
3) Should 2 not be possible, we will do all we can, outside of the official course offering, to schedule an "experience day" where you get to come back and use all the instruments first-hand for a full day in TRACES. We will offer this on a voluntary basis whenever we are allowed back without restrictions. This will not be officially part of the course so it will be optional for any students that would like to get some hands-on experience.

Please note that even for the online sessions, it is **highly interactive and based on experiential learning.**

These are a real-time labs.

We cannot record them, as you will be doing many of the components yourself. There are no lectures.

We have done everything we can to try and make the labs as enjoyable as possible given covid. Please attend and connect on time.

Please have your computer microphone and camera turned on. We will want you to interact, both with us and your other group members.

For the first week (Jan 12th) at 2pm please EVERYONE please join this link to go over the class logistics together
https://utoronto.zoom.us/j/84459656130

Analytical Chemistry for Environmental Scientists and Geochemists (EES 1102)
Location : Weeks 1-8 Online, Weeks 9-12 in TRACES Center EV215 (Env. Sci. and Chem. Building)
Course Time : Wed 2-6pm
Professor Andre Simpson
andre.simpson@utoronto.ca
Office Hours : Anytime by Appointment (E-mail for Zoom appointment)

COURSE DESCRIPTION

The course aims to expose environmental scientists and geochemists to cutting edge analytical chemical instrumentation in a hands-on laboratory. A wide range of instrumental techniques are covered that target organic contaminants, water, soils, crude oil, photochemistry and degradation. Techniques are presented in an accessible manner such that students without a strong chemical background can also participate.

COURSE OBJECTIVES

To expose students to modern chemical analysis as it pertains to environmental and geoscience in an accessible manner such that students without a strong chemical background can also participate.

SCHEDULE

Mon 12th Jan (2-6pm)
Mon 19th Jan (2-6pm)
Mon 26th Jan t (2-6pm)
Mon 2st Feb (2-6pm)
Mon 9th Feb (2-6pm)
Mon 16th Feb (2-6pm)
Mon 23rd Feb (Reading Week No Labs)
Mon 2nd Mar (2-6pm)
Mon 9th Mar (2-6pm)
Mon 16th Mar v (2-6pm)
Mon 23rd Mar (2-6pm)
Mon 30th Mar (2-6pm)
Mon 6th Apr (2-6pm)

EVALUATION

There will be no final exam for this course. Students will be assessed on the following criteria.

1) 3 x Lab reports. Lab reports are worth 33.3% each

You must wear safety specs and lab coat, turn up on time, keep a detail lab notebook, engage in discussion. Those not following the safety rules will be asked to leave the laboratory.

Evaluation will be carried out in accordance with the Graduate Grading and Evaluation Practices Policy (and how that policy is interpreted and applied in this Dept.) http://www.governingcouncil.utoronto.ca/Assets/Governing+Council+Digital+Assets/Policies/PDF/grading.pdf

EMERGENCY PLANNING

Students are advised to consult the university's preparedness site (http://www.preparedness.utoronto.ca) for information and regular updates regarding procedures relating to emergency planning.

ACCESSIBILITY NEEDS

The University of Toronto is committed to accessibility. If you require accommodations for a disability, or have any accessibility concerns about the course, the classroom or course materials, please contact The UTSC Accessibility Services as soon as possible:
http://www.utsc.utoronto.ca/~ability/
We also suggest you also refer to the following University of Toronto Scarborough Library link:
http://utsc.library.utoronto.ca/services-persons-disabilities

PLAGIARISM

University of Toronto code of Behaviour on Academic Matters states that "it shall be an offense for a student knowingly: to represent as one's own any idea or expression of an idea or work of another in any academic examination or term test or in connection with any other form of academic work, i.e., to commit plagiarism."

For accepted methods of standard documentation formats, including electronic citation of internet sources please see the UofT writing website at: http://advice.writing.utoronto.ca/using-sources/documentation.

The full Code of Behaviour regulations could be found from consulting
http://www.sgs.utoronto.ca/facultyandstaff/Pages/Academic-Integrity.aspx

WRITING AND ENGLISH LANGUAGE

As well as the faculty writing support, please see English Language and writing support at University of Toronto:
http://www.sgs.utoronto.ca/currentstudents/Pages/English-Language-and-Writing-Support.aspx
Students have commented that they found the latter address extremely helpful for writing term papers.

The following are also useful:

Sylvan Barnett, *A Short Guide to Writing About Art*. 5-7th edition (New York: Harper-Collins, 1997)
William Strunk Jr., E.B. White. The Elements of Style (New York: MacMillan Publishing)

LATE WORK

Late work with not be accepted unless accompanied by a Dr.'s note.

READINGS

All course materials will be provided.

FINAL EXAM DATE (IF APPLICABLE)

NA

EES1102 – Analytical Chemistry for Environmental Scientists and Geochemists

The course will be split into 4 main sections that will run concurrently. You will spend 3 weeks working on each project. (2 online and hopefully 1 in person should covid restrictions allow)

The 4 sections will take the form of a specific environmentally relevant "mini projects" that introduce you to key modern instrumentation giving you hands on experience in sampling, data acquisition, data analysis and interpretation. You must never be in the lab unaccompanied; you should not use any of instrumentation without supervision.

Unless stated otherwise we will always meet in S141 beside the TRACEs Center

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Assessment

There will be ***no*** final exam for this course. Students will be assessed on the following criteria.

1) 3 x Lab reports. Lab reports are worth 33.3% each
This year the metals lab (Tony) will not be marked. You do not have to hand in a report for this section.

2) **Prelab:** At the start of each lab there is a small summary of the techniques and instrumentation you will be using. At the end of this section there are a few questions you must answer briefly and present to your TA/instructor on the first week of a new rotation (i.e. before you start work on a new instrument). These questions are not marked specifically but if you do not attempt them then your Ability and Performance mark will be penalized -5%. The questions are simply to ensure you read ahead and understand the very basics of the instruments you will be using and in turn get as much from the lab experience as possible.

Lab reports are to be written individually and each student will be expected to attach their own copies of the relevant chromatograms, spectra etc. with their reports. Plagiarized reports will not be accepted.

Late lab reports cannot be accepted. A late report will automatically be assigned a zero unless a Dr's note is provided.

The Projects are Summarized as :

Project 1 : Lead and Cadmium from Vehicle Exhaust ?

You will be measuring cadmium and lead concentrations in plant, soils, and water samples at different distances from major roadways. You will compare the major technologies used for metals analysis in environmental science. The lab is designed to give you a background and exposure to all aspects of metals analysis as it relates to environmental science.

Topics Taught

1) **How to collect samples for metals analysis**
2) **How to measure metals in complex environmental samples**
3) **How to use total reflection X-ray fluorescence spectroscopy (TXRF)**
4) **How to use X-ray fluorescence spectroscopy (XRF) in the Lab**
5) **How to use Portable X-ray fluorescence spectroscopy (XRF) in the Field**
6) **How to used Atomic Adsorption Instrumentation**
7) **How to contrast and compare different analytical approaches and assess their advantages and disadvantages**

Warning : It is against Canadian Law to operate X-Ray equipment if not in the presence of a trained X-ray officer.

Project 2 : The Distribution Coefficient of Pesticides in soil ?

You will be sampling soil and performing batch sorption experiments with pesticide mixtures. Using Liquid Chromatography and various detectors (MS/DAD) you will measure the concentrations that remain in solution. You will perform elemental analysis to obtain for the carbon content for your soil. Using the data you will calculate the K_{oc} distribution coefficient itself essential for understanding and predicting how chemicals move in the environment.

Topics Taught

1) **How to measure the distribution coefficient of a pesticide/herbicide in soil. In turn this coefficient is key to understanding the transport of chemicals in the environment**
2) **How to prepare and extract environmental samples.**
3) **How to measure carbon content of samples using combustion elemental analysis**
4) **How to use High Performance Liquid Chromatography Apparatus**
5) **How to use a Mass Spectrometer (MS)**
6) **How to use Diode Array Detector (DAD) i.e. UV-VIS detector**
7) **How to contrast and compare different analytical approaches and assess their advantages and disadvantages**

Project 3 : Environmental Fingerprinting of Gasoline ?

You will learn all the capabilities of GC with both MS and flame ionization detection. You will use NIST mass spectrometry libraries to detect and identify unknowns in gasoline. You will compare gasoline from different manufacturers and learn how GC-MS can be used a fingerprinting tool to help identify the source of a spill. You will compare different remediation techniques and monitor the composition of BTEX residues left over after remediation.

Topics Taught

1) **The basics of GC and method optimization for a complex mixture (gasoline).**
2) **Use both manual and automatic injectors.**
3) **How to use an FID detector.**
4) **How to use an MS detector .**
5) **How to identify components from gasoline using NIST libraries.**
6) **How to use the overall spectral profile for fingerprinting.**
7) **Test how environmental aging and degradation changes gasoline composition.**
8) **Use some basic chemical and material sorbents and soak up gasoline and analyse the remaining BTEX resides.**

Project 4 Oil Spills: More than just a surface problem?

Oil spills have a high public profile. The oil will remain on the surface of water for extended periods of time, coating wildlife and beaches. Clean up often involves the use of surfactants to break up the oil and once it is no longer visible, at least in the "public eye" the problem dissipates. However, what happens at the molecular level ? Crude Oil and gasoline contain a wide range of toxic chemicals especially components known as BTEX. BTEX is an acronym that stands for benzene, toluene, ethylbenzene, and xylenes. Toluene, ethylbenzene, benzene and xylenes all have known toxic effects. BTEX compounds are highly volatile and are found to as contaminants in soil and water around the world. Do these and other chemicals from the oil or gasoline transfer into the aqueous phase? Is there a lot more to an oil spill than "meets the eye"? Could the use of surfactants potentially disperse more toxic chemicals into the water phase? Do we have any analytical technique that can study a complex process such as an oil spill in real time and with molecular resolution?

Later in this lab you will create a mini oil spill inside an NMR tube. The oil will be position above the detection coil and we will watch the transfer of components from the organic layer into the water layer. We will use NMR to help us identify and quantify the transfer of components between the layers. We will also use simple treatments such as shaking, and the use of a surfactants to see how it influences the process. You will learn how NMR is a powerful non-invasive tool that can provide a complete qualitative and quantitative molecular analysis for environmental matrices.

NMR Spectroscopy is the most powerful tool in modern science for determining organic structures and their interactions. However, the technique is under-utilized in environmental

research in large part due to thinking that NMR is not accessible to the non-expert. This does not have to be the case and this lab will introduce NMR in an easy to understand fashion.

What you will learn ?

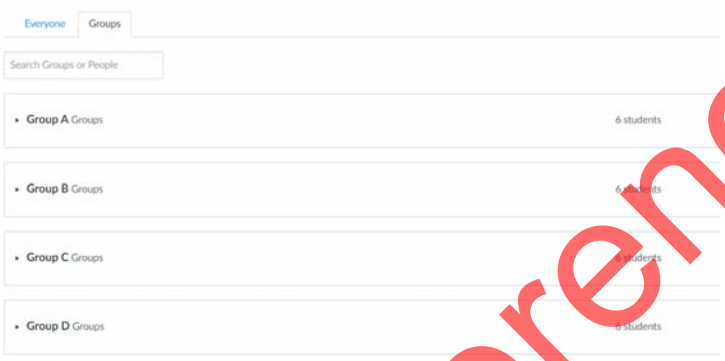
1) The basics of nuclear magnetic resonance (NMR) spectroscopy
2) How to acquire, process and interpret NMR data
3) How to perform water suppression in NMR
4) How to monitor a complex dynamic process by NMR
5) Using simulations to generate the NMR Spectrum for unknowns
6) How to combine various NMR methods to make unambiguous spectral assignments.
7) The potential of NMR spectroscopy to understand a complex process in real-time.
8) Identification of benzene, ethylbenzene, toluene and xylene (BTEX) components in complex matrices such as crude oil
9) Analysis of structural isomers
10) Use of standard addition to confirm NMR peak assignments
11) How to use Electronic REference To access In vivo Concentrations (ERETIC) as a simple and powerful quantification tool
12) How to quantify separate components of a complex mixture
13) Appreciation of detection and quantification limits in NMR
14) How NMR is an important “discovery tool” and, when used in combination with more widely-applied approaches such as GC-MS and LC-MS, is a powerful and complementary tool for environmental research
15) Formation of micelles, partitioning and chemical equilibrium
16) Standard addition and serial dilution techniques

Logistics

The course will be split into 4 main sections :

Section 1. NMR (oil spill)
Section 2. HPLC and HPLC-MS (soil)
Section 3. GC and GC-MS (gasoline)
Section 4. RAMAN, TRXRF, CE (metals)

On the Quercus page, under people, you can find out what group you are in.



The groups are labelled A-D. Just join the session that you will be doing for that week, based on the table on the next page.

Use the following zoom links per section

Section 1. RAMAN, TRXRF, CE (METALS)
https://utoronto.zoom.us/j/81869135396

Section 2. NMR (OIL)
https://utoronto.zoom.us/j/84459656130

Section 3. GC and GC-MS (GASOLINE)
https://utoronto.zoom.us/j/83086048704

Section 4. HPLC and HPLC-MS (SOILS)
https://utoronto.zoom.us/j/86176690892

Lab Session by Group. Note Yellow is online and Green in-person (covid restrictions permitting).

In Person will occur if Covid Restrictions are Lifted

Date	Oil Spill	Soil	Gasoline	Metals	Comment
Wed 12th Jan	**A+B**	**-**	**-**	**C+D**	Online
Wed 19th Jan	***A+B***	**-**	**-**	**C+D**	**Online**
Wed 26th Jan	***C+D***	**-**	**-**	**A+B**	Online
Wed 2nd Feb	**C+D**	**-**	**-**	**A+B**	Online
Wed 9th Feb	**-**	**A+B**	**C+D**	**-**	Online
Wed 16th Feb	**-**	**A+B**	**C+D**	**-**	Online
Wed 23rd Feb	**----------Reading Week No Class ----------**				
Wed 2nd Mar	**-**	**C+D**	**A+B**	**-**	Online
Wed 9th Mar	**-**	**C+D**	**A+B**	**-**	**Online**
Wed 16th Mar	**A**	**B**	**C**	**D**	In-Person
Wed 23rd Mar	**B**	**C**	**D**	**A**	In-Person
Wed 30th Mar	**C**	**D**	**A**	**B**	In-Person
Wed 6th Apr	**D**	**A**	**B**	**C**	In-Person

Contacts and Office Hrs

Office Hrs. If you need to meet with me during the course feel free to e-mail me andre.simpson@utoronto.ca. I will send you a zoom link and we can chat online.

Lab Books, Cleaning Up, and Leaving

Before Leaving

Make sure all chemicals have been returned and that all apparatus, has been cleaned an returned to its correct location. YOU WILL LOOSE MARKS IF YOU LEAVE A MESS. LOTS OF THE EQUIPMENT YOU WILL BE USING IS VERY EXPENSIVE RESEARCH EQUIPMENT, TREAT IT WITH RESPECT !!

Lab Manuals :

Lab Manuals are to be kept throughout the course. ***You must get these initialed by the instructor or demonstrator at the end of each session*** after you have cleaned up and shut down all the instrumentation properly. Lab manuals **must be handed in along** with the last lab report. **It is your responsibility to get you lab book signed each week. IF SIGNATURES OR LAB BOOKS ARE MISSING AT THE END OF THE COURSE THEN YOU WILL LOSE MARKS.**

All students are required to make their own notes and observations in the lab books as they feel appropriate

IN TERMS OF THE REPORTS THE MARKING SCHEME IS GIVEN AFTER EACH OF THE QUESTIONS. MAKE SURE YOU ANSWER THEM ALL. YOU WILL ONLY BE ASSIGNED MARKS FOR ANSWERING THE QUESTIONS.

Example Lab Report + Schedule

Overall Title (i.e. Gas Chromatography)

Name : Student Number Date :

Names of Other Student in the same practical group

Subtitle (i.e. Week 1 : Determination of Optimal Flow Rate in Gas Chromatography)

Make a note here of any special circumstances. For example : *"As is was the first week of class only 4 of the 6 compounds were available"*

Treatment of Data and Results

Here you will be expected to work chronologically through the practical write up. You are expected to carry out all the instructions in the "Treatment of Data Sections" throughout the text. You will be expected to clearly label and hand in all spectra or data collected during the practical. Each individual will be responsible to obtaining his own individual copy of any relevant data. Any appropriate experimental conditions should be clearly marked. In this section discuss any relevant finding or observations that you made during the practical.

Questions

Answer all questions throughout the text as fully as possible.

Conclusions

In this section summarize your major findings, and what you think you learnt from the practical session. Address any problems encountered. Suggest improvements that could be made to improve the results.

Repeat Format for week 2 and hand in complete report.

The practical report should be submitted in full the week following the last practical session on a particular type of instrumentation. Exact dates for handing in each assignment are given on the next page.

Dates Reports are Due !!!!

Note if classes are changed (weather etc.) – REPORTS ARE ALWAYS DUE ONE WEEK AFTER THE LAST CLASS ON THAT SPECIFIC INSTURMENT

Date	Oil Spill	Soil	Gasoline	Metals	Comment
Wed 12th Jan	-	-	-	-	
Wed 19th Jan	-	-	-	-	
Wed 26th Jan	**A+B**	-	-	-	**1st Lab Report Due**
Wed 2nd Feb	-	-	-	-	
Wed 9th Feb	**C+D**	-	-	-	**2nd Lab Report Due**
Wed 16th Feb	-	-	-	-	
Wed 23rd Feb	**----------Reading Week No Class ----------**				
Wed 2nd Mar	-	**A+B**	**C+D**	-	**3nd Lab Report Due**
Wed 9th Mar	-	-	-	-	
Wed 16th Mar	-	**C+D**	**A+B**	-	**4th Lab Report Due**
Wed 23rd Mar	-	-	-	-	
Wed 30th Mar	-	-	-	-	
Wed 6th Apr	-	-	-	-	

WE MUST RECEIVE YOUR REPORT BY 2PM ON THE DATE INDICATED IN THE TABLE ABOVE.

Late Reports will have 5% removed for each hour they are late unless you have a Dr's note

The submission time in Quercus will be used to determine this. Reports are due by 2pm