Supporting Information

A Project-Based Learning Experience That Uses Portable Air Sensors to Characterize Indoor and Outdoor Air Quality

Jessica C. D'eon‡*, Laura T. Stirchak‡, Abenen-Shepsu Brown¶, Yusra Saifuddin¶

‡Department of Chemistry, University of Toronto, Toronto, Canada

¶Visions of Science Network for Learning Inc., Toronto, Canada

*Email: Jessica.deon@utoronto.ca

This document includes:

Resources Related to the Chemistry of Air Quality

Building on the introductory atmospheric chemistry work done with the high school research students, YS and ASB, an analysis of ozone (O_3) and nitrogen dioxide (NO_2) data collected by the Canadian government has been added to our first-year lab curriculum. In doing so we produced a video explaining some aspects of the chemistry of air quality (https://play.library.utoronto.ca/1f19e6aa27d9c50e551ee8848292fe7c). The video describes the chemistry that produces tropospheric O_3 and its relationship with nitrogen dioxide NO_2, which is described by reactions [1] to [3] below.

$$NO_2 + \text{photon} \rightarrow NO + O \quad [1]$$

$$O + O_2 \rightarrow O_3 \quad [2]$$

$$O_3 + NO \rightarrow O_2 + NO_2 \quad [3]$$

Unfortunately, at this point there are no low-cost sensors for the analysis of NO_2, but this introductory discussion of the chemistry of air quality is useful for understanding the production of O_3 outdoors for this lab experiment.

Background information on the chemistry of air quality provided to the CHM410-1410 students can be found in the CHM410-1410 Lab Manual. Appendix 2 of the lab manual includes resources for accessing air quality data from the provincial and federal governments. Additional instructions for the TAs are also included here and additional background on the chemistry of air quality can be found in Appendix 2 of this document.

Resources Related to Data Analysis and Visualization

Many students come to CHM410-1410 with significant Excel skills; however, a surprising number are not confident using the spreadsheet software. For this reason, Appendix 3 of the lab manual includes Excel tips and tricks for making useful plots.

Writing Resources and Marking Scheme

At the outset of the semester students were provided with an annotated journal article to help them understand the structure and flow of the report expected. They were also provided with an incredibly detailed report marking scheme that the TAs used explicitly when grading the lab reports. The learning objectives of the lab are explicitly included in this scheme. In the Results & Discussion section there are 7 (out of 100) marks allocated to *"Presentation of data: Judicious use of tables & figures that summarize the important results"* and 5 marks to *"Referred to and used tables or figures when discussing results"*. These prompts are meant to ensure students include their visualizations in the report and understand their purpose in terms of illustrating the "story" of the report to the reader. There is also 5 marks allocated to *"Compared data to background literature"* so the role of scientific literature is the report is clear to students.

Yusra Saifuddin's Poster

The poster below was presented at the 2019 Visions of Science summer showcase and the University of Toronto Department of Chemistry summer research poster session.

Home Is Where the Air Is: *The Effects of Ventilation Indoors*

Yusra Saifuddin*, Laura Stirchak⌘, Jessica D'eon⌘
* Visions of Science Network for Learning, Toronto, ON
⌘ Department of Chemistry, University of Toronto, Toronto, ON

Introduction

Chemistry in the indoor environment is not as well understood as the outdoor environment. It is influenced by factors such as lighting conditions, building design, use of the room and, importantly, ventilation. In this study we explored concentrations of carbon dioxide, ozone, and particles as markers of air quality both indoor and outdoor environments to better understand factors affecting indoor air quality in a home in the City of Toronto.

Instruments

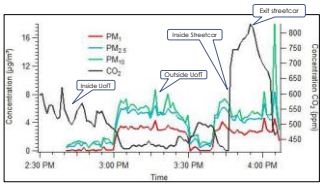
CO_2 Monitor
- Non-dispersive infrared (NDIR) sensor
- 0-5000 ppm

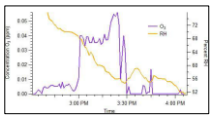
Ozone Monitor
- Gas sensitive semiconductor (GSS) sensor
- 0-0.15 ppm

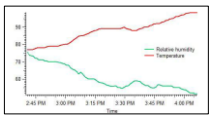
AirBeam
- LED light scattering
- PM measured in Micrograms per Cubic Meter (μg/m³)

Results and Discussion

Walking In/Out of Buildings

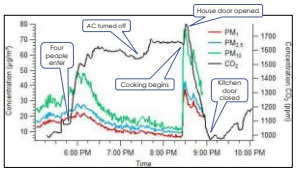


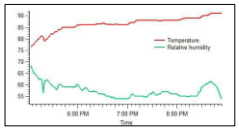




- CO_2 concentration in an outdoor environment is significantly lower than the indoor environment
- More ozone and particles are present outdoors in comparison to indoors

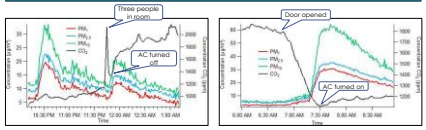
Human Activity

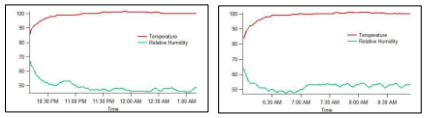




- Greater occupancy of a room increases CO_2 concentration
- Human activity such as cooking cause various shifts in the amount and type of particles present
- No ozone detected indoors

Sleeping





- Air conditioning decreased the amount of CO_2 in the room, likely because of increased ventilation
- Sleeping in an occupied enclosed space resulted in an increasing concentration of CO_2
- Opening a door increased the concentration of particulate matter while simultaneously decreasing the concentration of CO_2
- No ozone detected indoors

Conclusion

- Increased ventilation increased the concentration of particulate matter, suggesting that in the summer outdoor air is a source of particles to this indoor environment
- The concentration of CO_2 increased with occupancy and decreased with increasing ventilation, confirming it is a useful marker of these two parameters
- Different types of human activity have a large impact on the concentration of particles and CO_2

Acknowledgements

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Lab 2: Measuring Markers of Polluted Air

Introduction

In 2015, the world health organization (WHO) passed a resolution addressing the health impacts of air pollution (both outdoor and indoor). According to the WHO resolution, 4.3 million deaths occur each year due to indoor air pollution and 3.7 million deaths can be attributed to outdoor air pollution (www.who.int). People living in the developing world bear the brunt of this difficult situation, however understanding air quality is relevant to everyone and concentrations present in the indoor environment remain particularly poorly understood. In this lab you will use two types of air samplers to investigate the atmospheric concentrations of three classes of chemical markers of anthropogenic contamination: CO_2, ozone (O_3), and fine particulate matter known as $PM_{2.5}$.

In an outdoor environment with significant anthropogenic emissions, such as a city, concentrations of these pollutants are determined by the sources present (e.g. emissions from vehicles, furnaces, power generation…) as well as time of day as many atmospheric processes are driven by photolysis. Pollutants emitted directly into the atmosphere are called 'primary pollutants' and those resulting from photochemical reactions are called 'secondary pollutants'. The situation is a little different in the indoor environment as the primary pollutants from the off-gassing of compounds present in furniture, paints, carpets, etc. are different than those from vehicles and typical outdoor sources and the lack of high energy radiation from the sun limits photochemical processing. As part of the lab you will have to develop a hypothesis related to air pollution (either indoor, outdoor, or both) and test it by sampling in relevant environments.

You will be using two different types of air samplers during this experiment. The first type of air samplers measure O_3 and CO_2 separately. The O_3 sensor is a gas sensitive semiconductor that uses changes in resistance to calculate the concentration of O_3 down to 0.001ppm. The CO_2 sensor is a non-dispersive infrared sensor (NDIR), which uses infra-red light, a narrow band-pass filter and a photodiode to measure CO_2 concentration via light absorption. The band-pass filter used in this NDIR sensors is specific to CO_2 and has a resolution of 1ppm. Both the CO_2 and O_3 sensors collect data with a resolution of one minute.

The other personal air samplers you will be using are called AirBeams; they determine the real-time concentration of $PM_{2.5}$ by measuring the amount of scattered LED light. The AirBeam can also sample relative humidity, temperature and noise. Relative humidity and temperature can provide supporting information to help explain the chemistry of the environment, especially if a person is studying the formation of secondary chemicals and their transport. The AirBeams record data with a resolution of one second.

Background Information on Fine Particulate Matter ($PM_{2.5}$)

Fine particulate matter is a complicated marker of air pollution as it can have multiple components and is often a mixture of organic and inorganic substances. The AirBeams measure $PM_{2.5,}$ which are fine particles with a diameter of 2.5µm or less. These small particles are of particular interest as they can penetrate

deep into the lung and have serious implications for respiratory health[1]. $PM_{2.5}$ can be formed via primary pathways (incomplete combustion, cooking etc.) or via secondary pathways, which consist of particle nucleation via the condensation of low volatility compounds such as oxidized organics or the reaction of gas phase acids and bases[2–4]. These small particles are typically lost from the atmosphere via wet or dry deposition.

Background Information on Ozone (O_3)

Ozone is formed in the troposphere via the reaction of an oxygen atom with molecular oxygen (reaction R2). The oxygen atom is typically formed from the photolysis of nitrogen dioxide (NO_2) (reaction R1). NO_2 is produced from the oxidation of volatile organics (VOCs) in the presence of NO, both of which are emitted in vehicle exhaust. It is important to understand tropospheric ozone concentrations a it is one of the main contributors to the negative health effects associated with air pollution and photochemical smog.

$$NO_2 + h\nu\ (\lambda < 550\ nm) \rightarrow NO + O \qquad [R1]$$

$$O_2 + O \rightarrow O_3 \qquad [R2]$$

The main source of ozone indoors is thought to be transport of outdoor O_3 inside. Other potential, smaller sources include different cleaners, office equipment etc.[1,5–7]

Background Information on Carbon Dioxide (CO_2)

Carbon dioxide (CO_2) is a product of fossil fuel combustion as well as cellular respiration. As it is not chemically reactive it can be used as a chemical marker for human occupation and as a tracer for indoor ventilation[8,9]. Outdoor concentrations of CO_2 are typically between 350 and 450ppm, while indoor environments which have good air exchange can range between 350 and 1000ppm. Higher concentrations of CO_2 can lead to "stuffy" air and different health problems.

An example of how CO_2 can be used to calculate indoor ventilation can be found in the 2014 paper by Turanjanin *et al.*[9] where they studied air quality in Serbian schools. Observed fluctuations in CO_2 concentrations over time (dC/dt) (Eqn 1) were described by the inflow of air ($Q*C_o$), defined as the air flow (Q) times the outside concentration (C_o), the outflow of air ($Q*C(t)$), defined as the air flow (Q) times the indoor concentration at time t ($C(t)$), indoor emission sources (S), and chemical degradation $k*C(t)$.

$$V\frac{dC}{dt} = Q * C_o - Q * C(t) + S - k * C(t) \qquad \text{Eqn 1}$$

Equation 1 was then rearranged to calculate the Air Exchange Rate (AER), or the air flow (Q) over the volume of the classroom (V) (Eqn 2). This can be done by removing chemical degradation because CO_2 is chemically inert and by removing sources of CO_2 by sampling when humans are not present.

$$AER = \frac{Q}{V} = \frac{1}{t} ln \frac{C(0)-C_o}{C(t)-C_o} \qquad \text{Eqn 2}$$

The authors then measured CO_2 concentrations inside and outside the school. The classrooms were spiked with CO_2 and the CO_2 concentrations were measured overnight. These concentrations were then entered into Eqn 2 and the air exchange rates in each classroom were calculated.

Pre-lab Hypothesis Development and Sample Collection

In this lab, you will measure the concentrations of three chemical markers that are known to be indicators for polluted air. You will have to develop a hypothesis that you will be able to test during the experiment. It is best if you come up with potential hypotheses before you meet with the TA. For example, you could hypothesize that the concentrations of $PM_{2.5}$, CO_2 and O_3 will be higher in certain rooms of a house, based upon the sources and sinks in each room, or test changes in concentrations with changes to the indoor environment such as cooking or changes in ventilation by opening or closing certain doors. You can also test changes in the concentrations of these chemical species as you move through your day or on your commute. You can be as creative as you wish with these hypotheses. The only requirement is that **your hypothesis must include** all three chemical markers.

Four days before you complete the lab a TA will come to class and meet with the two demo groups performing Lab 2 that week to distribute the AirBeams, CO_2 monitor and the O_3 monitor. The TA will describe how to operate the different air monitors and answer any questions you may have about the lab. They will also discuss possible hypotheses with you, and help you iron out the details of your sampling plan. The suggested sampling time for each monitor is at least 1-2 hours. The AirBeams record data every second while the CO_2 and O_3 monitors record data every minute. Each monitor has a warm up time, with the AirBeams and CO_2 monitor requiring approximately 15 minutes to warm up, while the O_3 monitor requires approximately 1 hour.

You are responsible for deciding on the best location and time of day for obtaining samples that will help test your hypothesis, although you can certainly ask for the TA's opinion. As you sample with the different monitors please note of the time you began sampling, when you finished sampling, and the location(s) at which you sampled. You should record in your notebook if anything relevant occurred during sampling (e.g. cooking, cleaning, changes in ventilation like opening or closing doors or windows, walking by construction sites or food trucks). You should also record in your notebook the name you gave to each of your AirBeam sessions. For detailed instructions on how to use the different monitors, please see Appendix I.

Pre-lab Assignment

1. Read all lab materials before meeting with your TA prior to the lab period so you are prepared to discuss relevant hypotheses.
2. Come to lab with relevant sampling details (described above) recorded in your notebook. If you were not present for sample collection be sure to obtain these details before coming to lab.
3. Generate a hypothesis regarding the sources and sinks of CO_2, O_3, and $PM_{2.5}$ for your chosen study area(s). Use this hypothesis to predict the results of your sampling campaign. (e.g. what trends do you expect to see with your data?)

4. All three samplers will be calibrated before they are given to you. Is there a test you might be able to do to prove to yourself that the monitors are providing accurate concentrations of the different chemical markers?

Making Figures/Displaying your Data

During the lab period, you will be asked to analyze your data and begin to decide how to best present your data. At least one of your figures should compare two of your data sets. You will have to decide which combination will make the best "story". During the lab period, everyone will display a figure they made, and your group will talk about what they liked/disliked about each figure and what could be improved. Your TA will help you make the figure in Excel, and there are instructions on how to put a secondary axis on a graph in Appendix 3.

Report Questions

1. Include at least one figure that provides the reader with a visual representation of your experiment and resulting conclusions.
2. Within your report, comment on how the sampling rates of the various air monitors affected the conclusions that could be drawn.
3. Include a "Future Directions" section in your lab report and be sure to answer the following questions.
    a. Is there another measurement that would have been helpful in interpreting your results?
    b. If you were able to run this experiment again, would there be anything you would change about your sampling technique and or/hypothesis?

Background References

http://www.who.int/mediacentre/news/releases/2015/wha-26-may-2015/en/

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Appendix 1: How to Use the Air Samplers

The AirBeams

The AirBeams connect only to Android devices using an app called AirCasting. CHM410 has two Android phones to use with the AirBeams, and these phones have been set-up to work with the AirBeams right away. You may choose to use your own Android device, but that will require additional set-up steps.

How to use the BLU phone

1. The power button on the phone is on the right-hand side of the phone and is the lowest button of the three buttons. The other two are the volume controls for the phone.
2. There will be three buttons at the bottom of the screen when the phone is on. These are:
    a. A triangle pointing to the left. This is the go back button.
    b. A circle. This is the go back to the home screen of the phone button.
    c. A square. This will let you see all the apps that you have opened, and by swiping left on those apps you can close them out.
3. The button in the middle above the triangle, circle and square will let you see all the apps that are installed on the phone.
4. The AirCasting app is on the home screen of the phone.
5. The Bluetooth and GPS should be on as soon as you turn the phone on, but in the off-chance that they aren't, they can be activated by "pulling down" from the top of the screen. This should cause about 5 settings options to appear, and if you press on the down arrow at the right of those 5 setting options, more will open. At the bottom of this longer list are the Bluetooth and location buttons.
6. The phone and the AirBeam should have already been "paired." But on the off-chance that they aren't, go to the Bluetooth page in the settings menu (click on the gear after you have "pulled down" twice. This will open the settings menu, and from there click "Bluetooth". The phone at this point should start to search for available devices to pair with. Turn the AirBeam on, and the red light should start flashing. The phone should detect the AirBeam within a few minutes. Click "pair" and say yes when the phone asks your permission to pair the two devices. After that, you should never have to pair the devices on the Bluetooth page again.

Using the AirBeam

1. Open the AirCasting App and click the "connect external device" option in the lower right corner. Click "connect" to connect the device to the AirBeam. If you click the "pair new device" option, this will take you to the Bluetooth settings page, where you can pair with a new device (this is a nice shortcut).
2. Once you have been paired, the dashboard will now be ready to take data. You will see that the session name (right under the Dashboard heading) will be called "unnamed", and below that you will see different sections titled "AirBeam-F", "AirBeam-PM" and

"AirBeam-RH". These are the temperature, particulate matter and relative humidity data sections, respectively. All of these should be grey.

3. Before you start collecting data, you may want to contribute your data to the crowd map. To ensure that this option is activated, click on the three lines next to the Dashboard, and then click settings. The first option will be "contribute to CrowdMap". Make sure the box next to it is blue with a white checkmark.
4. If you scroll down, you will be able to see other options that you may wish to use during your sampling.
5. Click the back button to go to the Dashboard screen. Click the recording button up in the top right corner (should look like a small blue circle inside a larger white circle. Once you click that button, you will be asked to fill in session details. You should title your session, but you don't have to include tags if you do not wish to.
6. Now press the start button. You will find that the three sections now have coloured circles (on the right-hand side of the screen). These circles will change color, depending upon how high the measurement is (I'm pretty certain this is somewhat arbitrary).
7. During sampling, you can make notes to yourself at various time points. To do this on the app, click the button that looks like a pencil in a comment bubble. You should probably record notes in your lab notebook and on the app, but this is up to you.
8. The AirCasting app will now give you 1-minute averages to the left of the last second circles. I do not find this to be useful as it gets rid of a lot of the finer details. If you want to look at one of the three types of data collected in real time. Simply tap somewhere in that box, and box titled "Stream View" should pop up. You can then choose whether you want to see your data in a graph or overlaid on a map (if you are not CrowdMapping your data, this option may not be available). You can only see one type of data collected at a time.
9. Once you are done sampling, click the stop recording button (small blue circle in a white box). Everything should go back to grey.

Note: You can choose to disable your devices microphone so that the AirBeam does not record decibel levels while you are sampling. This is done by going to the setting menu and clicking the option that reads "Disable phone microphone." You cannot disable any of the other sampling options.

Saving the Data

1. To export your data to your computer, click the three lines next to the Dashboard and click the "Sessions" option.
2. Click on the session you want to export, and box entitled "Sessions Options" should pop up. To share your data, click the "Share" option. You will be asked if you want to "share link" or "share file". The share link option only means that you will be able to see your data on the website. To be able to work with your data, click the share file option. You will have a choice of "save to Google Drive", "Bluetooth" or "Gmail". As more apps are added to the phone, new options will become available.

3. If you choose the email option, you will be sending yourself an email using the CHM410 email. Your data will be attached as CSV inside a zip file.

Looking at Old Sessions

1. If you want to look at older sessions on the AirCasting app, go to the sessions page, using the instructions above and click on the session.
2. In the "Sessions Options" box, click the "Add to Dashboard" option and then go back to the Dashboard page.
3. There you should see your data (everything will be in color). If you want to look at things graphed, rather than in the 1-minute average format, you may do so.
4. You can have multiple old sessions available on the Dashboard if you want an easy comparison.

Using the CO_2 and Ozone Air Monitors

Turning on the Monitors/Beginning Screens

1. Press the power button on the left-hand side of the monitor for approximately 2 seconds (or until the screen activates). The monitor should beep, and the opening screen should say Aeroqual at the top with Monitor S500 V6.4 Lithium Battery.
2. This screen should be up for a few seconds, and then should change to a screen that tells you what sensor is connected (CO_2 5K or O_3 VLOW). Below the sensor identity should be the words "warming up" followed by an amount of time remaining in the warming up period.
    a. The two sensors take approximately 3 minutes each to warm up. No measurements will be taken during this time.
3. There will be a small "M" and "L" below the bigger words. This is the monitor identity and location identity.
    a. Monitor 1 is currently connected to the CO_2 sensor.
    b. Monitor 2 is currently connected to the O_3 sensor
4. After the 3-minute warming up period, the instrument will move into the "stabilizing period", which lasts for 7 minutes. During this time, the instrument will flash the measurement. Once the number stops flashing, the instrument has been stabilized.
5. NOTE: When the monitor is on DO NOT remove the sensor. This will cause the monitor to shut down as this may damage the unit.

Taking Measurements

1. To take measurements, click the "enter" button (shown as an arrow) on the top right-hand side of the monitor screen.
2. Scroll down to "Max Min Avg" and click the enter button. This should make the option "Start" show up on the right-hand side of the now highlighted "Max Min Avg". Do not press the enter button (this will turn that option off).
3. Now use the down arrow key to select "Logging Setup". Click the enter key to select
    a. The first option will be "Log Freq" you can choose whatever frequency you want, but the lowest/fastest option is 1 minute (this is what the monitor is set to). Use the arrow buttons if you want to choose a different frequency and click the enter button
    b. You will now be at the option "clear log". You do not have to use this option (use the arrow buttons to choose between yes or no). The logging memory will at some point be used up. You will then have to clear the log at that time. Click the enter button once you have made your selection.
    c. You will then come to option "Logging". To turn the logging function on, choose "yes" (this may involve using the arrow keys). Then press enter. This will bring you back to the main menu. Choose the "exit" option to back to the main screen. The screen should now show the real time data, the max, min and average concentrations. The data is collected every minute.
4. To turn off the logging function, especially at the end of your sampling time, simply repeat steps 3a-3c, this time choosing "Logging off".
5. NOTE: If using sensors with a gas/your breath, place the sensor head **perpendicular** to the air flow to avoid sensor damage.

Retrieving Logged Data

1. Download the free software from https://www.aeroqual.com/support/product-software. Choose the option "Series 500 monitor PC software and follow the instructions to install the software on your computer. The company will ask you to register yourself, use the University of Toronto as your company name.
2. Connect the USB to monitor cable and ensure that your computer has downloaded the necessary hardware (your computer should do this automatically).
3. Now open the software (entitled Aeroqual Series S500 Monitor Software V6.5), and then click on the "File" button. Choose the first option "Search for connected monitor). NOTE: the monitor in question must be turned on for this connection to be made.
4. A screen titled "Monitor Info" will pop up. Click "okay".
5. Now go back to the "File" menu and click "Download Logged Data". The data will automatically begin to download. The USB connector will start to flash green and red.

6. Once the data is downloaded, click the “File” menu and click “Export Logged Data”.
    a. A window will pop up that asks you to choose what portion of the data you want to export (includes date and time) so that you only need to choose the times of certain sessions if you want to. Click “Export” when done. The data will be saved as a CSV file (same as the AirBeams).
    b. The data in the CSV file will consist of 4 columns (date time, monitor identity, location identity and sensor readings). The location identity will only matter if you want to keep track of where you sampled (for example if you were looking at CO_2 in different rooms). Otherwise, you can delete those columns.

Turning the Monitor off

1. To turn the monitor off, press down on the power button for about 2 seconds. The monitor will beep, and the screen will go blank.
2. There is also a standby mode, which can be used if you need to conserve power for a short period of time between samplings. It basically reduces the warm up time needed when you turn the monitor on again. To enter this mode, press the power button once. There will be a special symbol in the top right-hand corner, which will only appear when the monitor is in the standby mode.

NOTE: DO NOT REMOVE THE SENSORS HEADS

Appendix 2: Additional Data Resources

If you collected samples outdoors it may be useful to use archived meteorological data to obtain additional information that can assist you in your data interpretation.

OMECC Air Quality Ontario

The Ontario Ministry of the Environment and Climate Change (OMECC) has a website that reports real-time and archived ozone measurements (www.airqualityontario.com). The website has information on the Air Quality Health Index (AQHI) as well as provides hourly ozone (O_3), $PM_{2.5}$ and NO_2 data measured at 39 different stations across Ontario (click on "Pollutant Concentrations" on the menu on the left of the screen). You can locate the station closest to your sampling location and compare your results to those reported by the OMECC. For example, high levels of ozone may correspond to high aldehyde levels since they are both formed as products of photochemical reactions that produce smog. Therefore, if there are high levels of ozone at night, this may explain your observations of high aldehyde concentrations even though you hypothesized otherwise. Again, you must determine if the information from this website is appropriate for analyzing your results.

AirCasting Website

The makers of the AirBeams have a website (http://aircasting.org) which includes an interactive map. At the top left of the page, click on "map". There are three types of maps available for you to look at: Fixed, Mobile and CrowdMap. To look at your data, go to the Mobile map (at the top right of the screen, click the Mobile tab), and then choose what sensor data you want to look at. To find your data, write "CHM410" under profile names, and then look at the left-hand screen in the box labeled "sessions". Click on your desired session, and what sensor you wish to have displayed. The only way to get this picture/map will be to do a screen shot and save it as a photo. You may find this option helpful as it lays out concentrations as a function of your movements.

Appendix 3: Excel Tips

Making a Secondary Axis

1. Make your graph with the two data series and add your second data series to that graph using the original axis.
2. Right click on the data series that you want to put on the secondary axis and click 'format data series' at the bottom of the resulting menu that pops up.
    a. NOTE: whichever data series you select as your primary "y" axis dictates your x-axis. This becomes important if you are plotting $Pm_{2.5}$ vs either CO_2 or O_3 because of the variation in time steps.
3. In the gray box on the right-hand side of the excel window, there should be the option to 'Plot Series On' 'Primary Axis' or 'Secondary Axis'. Choose Secondary Axis and the graph should automatically change for you.

Making Time Stamps

1. Click on a column and in the 'Number' section on the 'Home' menu, click on the arrow next to 'General' and select 'Time'.
2. Write your initial time in a cell of that column and press enter (pretend it is B2).
3. In the next cell down, use the TIME function (=TIME) to add one minute or one second to the time in "B2".
    a. write '=B2+TIME(hr,min,sec) as '=B2+TIME(0,1,0) if you want to add one minute or '=B2+TIME(0,0,1) if you want to add one second.
4. Then double click the right corner if you see the '+' sign and the column will fill with your time increasing in minutes or seconds.

Formatting Fractional Time

If you are plotting O3 or CO2 and PM2.5 on the same graph, you cannot use the same time stamps as PM2.5 has data every second and CO2/O3 have data every minute. Therefore, you will have to use 'fractional' time for one of your data series (HINT: it should be the series you choose to plot on your secondary axis). You can do this one of two ways.

1. Using the steps outlined in the section above, format your time series with the column formatted as 'Time' and then revert that column to 'General' (or copy and paste to a new column). The time should go to 'fractional time' (ie in decimals).
2. You can use the following equation to format your own time.
    a. $\frac{hour+{}^{min}/_{60}}{24}$

Lab 2: Measuring Markers of Polluted Air

TA Information

Overall Concepts

- To learn how to organize and execute an experimental plan in the context of a field study (i.e., developing a reasonable hypothesis, testing the hypothesis by sampling in appropriate environments, etc.).
- To learn how to analyze and manipulate large data sets
- To learn how to visually present data so that your figure tells a story

Practical Notes

Part I: Getting Ready Before the Labs Begin

Before the semester begins, you are responsible for locating and charging the following equipment:

- 2 CO_2 monitors
- 2 O_3 monitors
- At least 2 AirBeams: measure PM_{10}, $PM_{2.5}$, PM_1, RH and T
- 2 Phones

The CO_2 and O_3 monitors take approximately 3 hours to charge, while the AirBeams and phones take approximately 2 hours. The CO_2 and O_3 monitors also need to be run for ~48 hours after you charge them (or during) to burn off any contaminants that may have built up on the sensors since the monitors were last used.

Part II: Pre-Lab Talk

Actual field sampling time is to be done by students outside laboratory time. TAs generally distribute the air monitors (1 AirBeam, 1 CO_2 and 1 O_3) to each group in a brief meeting after class around four days before the lab period. During this meeting, the two groups that meet with you (e.g. Groups B + E) will each develop a hypothesis and decide how to test it. They **are not allowed to leave** the talk without running their plan past you.

Developing a Hypothesis

The hypothesis that each group develops can be about outdoor and/or indoor air quality. If the groups have difficulty deciding upon a hypothesis they would like to test, you may suggest some ideas to the students. Some ideas include: the effects of cooking and/or cleaning on the production/concentration of chemical markers, looking at the pollution of their respective commutes to school, etc. The only requirement of their hypothesis is that it **must include all five chemical markers**, although it is suggested that students do either a combination of indoor and outdoor sampling, or indoors alone. Many students will try to make their hypotheses too complicated, so try to suggest ways to simplify their ideas. If you would like some sample hypotheses, below are two examples:

Hypothesis 1:

Different buildings will have different ventilation rates which will affect the concentrations of CO_2, O_3 and PM by altering sources and sinks.

Hypothesis 2:

Different types of cooking produce different concentrations of the CO_2, O_3 and PM.

Field Sampling

Students are encouraged to design their own sampling strategy that they feel will test their hypothesis. They must determine where they will sample, how they would like to sample, and the duration of sampling. All chemical markers must be sampled more than **1 hour** during each sampling period and all monitors must be run at the same time. If students are planning on perturbating the system, they must sample before they perturbate the system to get the background level concentrations. The students should note down **all** these details in their lab notebooks (they are told this in the lab manual). We encourage students to sample for at least 4 hours (with each monitor) so that they get adequate data.

The students have been given directions on how to use the AirBeams and CO_2/O_3 monitors, which are all relatively easy to use in the field. You have most of these instructions in Appendix 1 (and in a separate document). The only responsibility of the students after sampling is to ensure that they share the data files from the AirBeams with you and their group members. They can do this via email (preferably using the CHM410 Gmail) or on the CHM410 Google Drive. Students may use the phones that were purchased to be used with the AirBeams, or they can use their own Android devices. If they use their own devices, they must sign into the CHM410 AirCasting profile (see Appendix 1 for details).

Part III: During the Lab Period

Downloading/Sharing Data

The students must download the data off the CO_2 and O_3 monitors in lab using the Aeroqual software and correct USB cords (found in the box with the monitors). The instructions for downloading the data can be found in Appendix 1. This data should be shared with you and all the group members, along with the AirBeam data. The student(s) that did the sampling must share all pertinent information with their group mates (see lab manual for suggestions).

Interpreting and Displaying Results

Once the data has been passed around, you (the TA) can help the students with the manipulation of the data and the interpretation of their results. The students are required to make one figure during the lab period that displays the $PM_{1/2.5/10}$ and O_3 or CO_2 data series. Students can use the T and/or RH data if they would like, but there are limitations to this data. You should then look at each student's figure as a group and discussed what you liked about the figure, and what could be improved. Also during this discussion, you should cover topics such as: how they want/should present their data, how to form a story from their data and general data analysis. Many of the students will probably have never worked with large data sets, so you will have to help them with that.

Formation of O_3 and PM Indoors versus Outdoors

You should walk the students through a simple diagram of how O_3 is formed in the troposphere and its sources indoors. You should do the same for PM, touching on the fact that it can be a secondary and primary pollutant in both environments. A sample diagram can be found in the PowerPoint.

Demonstration of OMECC and AirCasting Maps Websites

The purpose of this part of your talk should be to introduce students to the two websites and how they might use that information in their lab reports to strengthen their story. The students do not have to use the data from these websites, but they should be encouraged to do so if it is suitable for their hypothesis.

Air Quality Learning Objectives

- What is the difference between a primary and a secondary pollutant? What is O_3? NO_x? $PM_{2.5}$? Are their classifications different in the indoor versus outdoor environment?

  A primary pollutant is directly emitted into the atmosphere whereas a secondary pollutant is formed in the atmosphere by photochemical reactions. Examples of primary pollutants are NO, SO_2, CO. Examples of secondary pollutants are O_3, NO_2, aldehydes, HNO_3, NH_3. Aldehydes are complicated as they can also be released directly into the atmosphere, making them also primary pollutants. Ozone is the most important secondary pollutant. Indoors, aldehydes are the primary pollutants, while NO_2 are the secondary pollutants. $PM_{2.5}$ in both environments can be primary or secondary pollutants.

- What are some sources of these pollutants?

Sources of NO_2 are:

- *Transportation*
- *Fuel combustion*
- *Industrial sources*
- *Electric utilities*
- *Conversion from NO that has been transported indoors*

Sources of O_3 are:

- *Photolysis of NO_2*
- *Air Purifiers*
- *Cleaning*
- *Cooking*

Sources of $PM_{2.5}$:

- *Smoking*
- *Vehicular gas*
- *Incomplete combustion of fireplaces and woodstoves can include*
- *Cooking*
- *Particle nucleation*
- *Potentially from cleaning supplies*

Appendix 1: How to Use the Air Samplers

Using the AirBeam

1. Turn on the AirBeam by clicking the white button on the bottom of the AirBeam. A light should start blinking when the device is on and searching for a connection. The light will turn green after a few seconds.
2. Once the light is green, open the AirCasting App and click the "Configure AirBeam2" option in the middle of the screen. Click "connect" to connect the device to the AirBeam. If you click the "pair new device" option, this will take you to the Bluetooth settings page, where you can pair the app with a new device (this is a nice shortcut).
3. Once you have connected the phone and the AirBeam, the app will ask if you want to do a "Mobile" or "Fixed" measurement session. Click "Mobile".
4. The dashboard will now be ready to take data. You will see that the session name (right under the Dashboard heading) will be called "unnamed", and below that you will see different sections titled "AirBeam-F", "AirBeam-PM1", "AirBeam-PM2.5", "AirBeam-PM10", and "AirBeam-RH". These are the temperature, particulate matter and relative humidity data sections, respectively. All of these should be grey. NOTE: at this point you can skip to Step 6.
5. Before you start collecting data, you may want to contribute your data to the crowd map. To ensure that this option is activated, click on the three lines next to the Dashboard, and then click settings. The first option will be "contribute to CrowdMap". Make sure the box next to it is blue with a white checkmark. If you scroll down, you will be able to see other options that you may wish to use during your sampling.
6. Click the back button to go to the Dashboard screen. Click the recording button up in the top right corner (should look like a small blue circle inside a larger white circle. Once you click that button, you will be asked to fill in session details. You should title your session, but you don't have to include tags if you do not wish to. Press "Start Session". Note: Make sure you know what you entitled your session.
7. Now press the start button. You will find that the three sections now have colored circles (on the right-hand side of the screen). These circles will change color, depending upon how high the measurement is.
8. During sampling, you can make notes to yourself at various time points. To do this on the app, click the button that looks like a pencil in a comment bubble. You should probably record notes in your lab notebook and on the app, but this is up to you.
9. The AirCasting app will now give you 1-minute averages to the left of the last second circles. I do not find this to be useful as it gets rid of a lot of the finer details. If you want to look at one of the three types of data collected in real time. Simply tap somewhere in that box, and box titled "Stream View" should pop up. You can then choose whether you want to see your data in a graph or overlaid on a map (if you are not CrowdMapping your data, this option may not be available). You can only see one type of data collected at a time.
10. Once you are done sampling, click the stop recording button (small blue circle in a white box). Everything should go back to grey.

Saving the Data

1. To export your data to your computer, click the three lines next to the Dashboard and click the "Sessions" option.
2. Click on the session you want to export, and box entitled "Sessions Options" should pop up. To share your data, click the "Share" option. You will be asked if you want to "share link" or "share file". The share link option only means that you will be able to see your data on the website. To be able to work with your data, click the share file option. You will have a choice of "save to Google Drive", "Bluetooth" or "Gmail". As more apps are added to the phone, new options will become available.
3. If you choose the email option, you will be sending yourself an email using the CHM410 email. Your data will be attached as CSV inside a zip file.

Looking at Old Sessions

1. If you want to look at older sessions on the AirCasting app, go to the sessions page, using the instructions above and click on the session.
2. In the "Sessions Options" box, click the "Add to Dashboard" option and then go back to the Dashboard page.
3. There you should see your data (everything will be in color). If you want to look at things graphed, rather than in the 1-minute average format, you may do so.
4. You can have multiple old sessions available on the Dashboard if you want an easy comparison.

Using the CO_2 and Ozone Air Monitors

Turning on the Monitors/Beginning Screens

1. Press the power button on the left-hand side of the monitor for approximately 2 seconds (or until the screen activates). The monitor should beep, and the opening screen should say Aeroqual at the top with Monitor S500 V6.4 Lithium Battery.
2. This screen should be up for a few seconds, and then should change to a screen that tells you what sensor is connected (CO2 5K or O_3 VLOW). Below the sensor identity should be the words "warming up" followed by an amount of time remaining in the warming up period.
    a. The two sensors take approximately 3 minutes each to warm up. No measurements will be taken during this time.
3. There will be a small "M" and "L" below the bigger words. This is the monitor identity and location identity.
    a. Monitors 1 and 3 are currently connected to the CO_2 sensors.
    b. Monitors 2 and 4 are currently connected to the O_3 sensors.
4. After the 3-minute warming up period, the instrument will move into the "stabilizing period", which lasts for 7 minutes. During this time, the instrument will flash the measurement. Once the number stops flashing, the instrument has been stabilized.

5. NOTE: When the monitor is on DO NOT remove the sensor. This will cause the monitor to shut down as this may damage the unit.

Taking Measurements

1. Before you begin measurements, you should check that the clock and date on the monitors are correct. To do this:
    a. Press the "enter" button at the top right of the monitor and use the arrows keys and scroll down to "Monitor Setup". Press the enter button again.
    b. Now scroll down to the option "Clock Setup".
    c. If the time is not correct, use the arrows to change the hour. Then press "enter". Do this for the minutes and seconds settings. You can also change the date using the same technique.
    d. To finish up, press the enter button until you are back to the "Monitor Setup" screen (and press "exit" until you are back at the home screen).
    e. NOTE: if you do not check the time, you cannot be sure that the monitor is correctly setup, and this will affect when your data was "logged".
2. To take measurements, click the "enter" button (shown as an arrow) on the top right-hand side of the monitor screen.
3. Now use the down arrow key to select "Logging Setup". Click the enter key to select which option you want.
    a. The first option will be "Log Freq" you can choose whatever frequency you want, but the lowest/fastest option is 1 minute (this is what the monitor is set to). Use the arrow buttons if you want to choose a different frequency and click the enter button.
    b. You will now be at the option "clear log". You do not have to use this option (use the arrow buttons to choose between yes or no). The logging memory will at some point be used up. You will then have to clear the log at that time. Click the enter button once you have made your selection.
    c. You will then come to option "Logging". To turn the logging function on, choose "yes" (this may involve using the arrow keys). Then press enter. This will bring you back to the main menu. Choose the "exit" option to back to the main screen. The screen should now show the real time data, the max, min and average concentrations. The data is collected every minute.
4. To turn off the logging function, especially at the end of your sampling time, simply repeat steps 3a-3c, this time choosing "Logging off".
5. NOTE: If using sensors with a gas, place the sensor head perpendicular to the air flow to avoid sensor damage.

Retrieving Logged Data

1. Download the free software from https://www.aeroqual.com/support/product-software. Choose the option "Series 500 monitor PC software and follow the instructions to install the software on your computer. The company will ask you to register yourself, use the University of Toronto as your company name.
2. Connect the USB to monitor cable and ensure that your computer has downloaded the necessary hardware (your computer should do this automatically).
3. Now open the software (entitled Aeroqual Series S500 Monitor Software V6.5), and then click on the "File" button. Choose the first option "Search for connected monitor). NOTE: the monitor in question must be turned on for this connection to be made.
4. A screen titled "Monitor Info" will pop up. Click "okay".
5. Now go back to the "File" menu and click "Download Logged Data". The data will automatically begin to download. The USB connector will start to flash green and red.
6. Once the data is downloaded, click the "File" menu and click "Export Logged Data".
    a. A window will pop up that asks you to choose what portion of the data you want to export (includes date and time) so that you only need to choose the times of certain sessions if you want to. Click "Export" when done. The data will be saved as a CSV file (same as the AirBeams).
    b. The data in the CSV file will consist of 4 columns (date time, monitor identity, location identity and sensor readings). The location identity will only matter if you want to keep track of where you sampled (for example if you were looking at CO_2 in different rooms). Otherwise, you can delete those columns.

Turning the Monitor off

1. To turn the monitor off, press down on the power button for about 2 seconds. The monitor will beep, and the screen will go blank.
2. There is also a standby mode, which can be used if you need to conserve power for a short period of time between samplings. It basically reduces the warmup time needed when you turn the monitor on again. To enter this mode, press the power button once. There will be a special symbol in the top right-hand corner, which will only appear when the monitor is in the standby mode.

NOTE: DO NOT REMOVE THE SENSORS HEADS

Appendix 2: Basic Atmospheric Chemistry Reactions
Tropospheric production of ozone and aldehydes

Production of ozone

$NO_2 + h\nu \rightarrow NO + O$

$O + O_2 \rightarrow O_3$

Note: NO_2 is a primary pollutant and O_3 is a secondary pollutant.

Formation of aldehydes

Step 1: Forming the hydroxyl radical

$O_3 + h\nu \rightarrow O_2 + O(^1D)$

$O(^1D) + M \rightarrow O(^3P) + M$

$O(^1D) + H_2O \rightarrow 2\ OH$

Step 2: Reaction of the hydroxyl radical with hydrocarbons

$OH + RH \rightarrow RO_2 + H_2O$

$RO_2 + NO \rightarrow RO + NO_2$

Note: The hydrocarbons are either alkanes or alkenes.

Step 3: Formation of the aldehyde

$RO + O_2 \rightarrow RCHO + HO_2$

$HO_2 + NO \rightarrow HO + NO_2$

Annotated Paper from Environmental Science and Technology

Environ. Sci. Technol. 2001, 35, 1339−1342

Descriptive, concise title

Global Distribution of Perfluorooctane Sulfonate in Wildlife

JOHN P. GIESY* AND KURUNTHACHALAM KANNAN

Department of Zoology, National Food Safety and Toxicology Center, Institute for Environmental Toxicology, Michigan State University, East Lansing, Michigan 48824

Your abstract must include the following information: purpose, what you did (samples… I would also include the analytical instrument used), results, implication of results and how it fits in with the current literature

Here we report, for the first time, on the global distribution of perfluorooctanesulfonate (PFOS), a fluorinated organic contaminant. PFOS was measured in the tissues of wildlife, including, fish, birds, and marine mammals. Some of the species studied include bald eagles, polar bears, albatrosses, and various species of seals. Samples were collected from urbanized areas in North America, especially the Great Lakes region and coastal marine areas and rivers, and Europe. Samples were also collected from a number of more remote, less urbanized locations such as the Arctic and the North Pacific Oceans. The results demonstrated that PFOS is widespread in the environment. Concentrations of PFOS in animals from relatively more populated and industrialized regions, such as the North American Great Lakes, Baltic Sea, and Mediterranean Sea, were greater than those in animals from remote marine locations. Fish-eating, predatory animals such as mink and bald eagles contained concentrations of PFOS that were greater than the concentrations in their diets. This suggests that PFOS can bioaccumulate to higher trophic levels of the food chain. Currently available data indicate that the concentrations of PFOS in wildlife are less than those required to cause adverse effects in laboratory animals.

Here, the authors provide background information on their analytes and the analytical methods they are going to use, including analytical challenges in measuring these specific compounds

Introduction

Research investigating the environmental fate of halogenated compounds has focused largely on chlorinated and brominated compounds. Fluorinated organic compounds (FOCs) have received less attention because their measurement is more difficult. Because they have surface-active properties, FOCs are more difficult to separate from tissues than the more classical neutral residues that have been studied. Also, because they are nonvolatile and have relatively high molecular weights, they require specialized liquid chromatography/mass spectrometry methods for analysis. Because much of the FOCs were incorporated into polymers, they are perceived as more biologically inert and therefore, less likely to have an impact on human health or the environment.

FOCs have been manufactured for over 50 years. FOCs are used as refrigerants, surfactants, and polymers, and as components of pharmaceuticals, fire retardants, lubricants, adhesives, cosmetics, paper coatings, and insecticides (*1*). Because of their many useful properties, since the 1970s there has been a steady increase in the use of FOCs for a variety of industrial applications.

Although partially fluorinated hydrocarbons may undergo chemical breakdown at functional group bonds (*2*), given

* Corresponding author phone: (517) 353-2000; fax: (517) 432-2310; e-mail: jgiesy@aol.com.

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PFOS (Perfluorooctane sulfonate) $C_8F_{17}SO_3^-$

PFHS (Perfluorohexane sulfonate) $C_6F_{13}SO_3^-$

PFOSA (Perfluorooctanesulfonylamide) $C_8F_{17}SO_2NH_2$

PFOA (Perfluorooctanoic acid) $C_7F_{15}COOH$

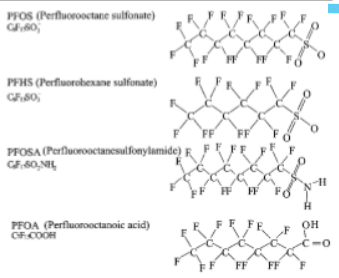

FIGURE 1. Structures of target fluorinated organic compounds.

Structures of analytes with names and abbreviations. If you have a lot of analytes, some of this can be moved into your SI and you can provide general structures in the main text

the high energy of the carbon−fluorine bond (known to be the strongest of covalent bonds), some perfluorinated compounds are very stable in the environment (*3*). Even though FOCs could be persistent, the magnitude and extent of distribution of FOCs in the environment was unknown. However, the occurrence of FOCs in human blood sera was reported as early as 1968 (*4*). Further reports of FOCs in human sera from various locations in the U.S., South America, and Japan appeared over the next several decades (*5*−*8*). These reports would indicate a relatively widespread distribution of these materials in human sera and would suggest the potential for distribution in the environment. However, no compound-specific information on the extent of the distribution of FOCs in the environment or in wildlife was available. This was due, in part, to the lack of a practical compound-specific method of analysis that could be applied to a wide range of sample types with sufficient sensitivity to measure ecologically relevant concentrations of specific compounds. Recent development of a compound-specific method for the analysis of some FOCs using high-performance liquid chromatography−negative ion electrospray tandem mass spectrometry (*9*) permitted the survey of four FOCs in liver and blood plasma of wildlife on a global scale.

The number of synthetic FOCs has increased over the past few years. Among them, sulfonyl-based fluorochemicals have been produced and used for over 40 years. Perfluorooctanesulfonyl fluoride (POSF) is the basic building block of a series of perfluorinated alkyl sulfonates that are used as surface protectors in carpets, leather, paper and packaging, fabric, and upholstery. It has been hypothesized that, during their life cycles, POSF and some POSF-based products could ultimately degrade to other fluorochemicals including perfluorooctane sulfonate (*10*) (PFOS; Figure 1).

The studies on which we report here are part of a larger, ongoing, comprehensive program of investigation of global distribution and fate of PFOS in the environment. The objectives of this study were to elucidate the current environmental distribution of PFOS by use of biomonitoring and to evaluate bioaccumulation and biomagnification potential in aquatic and terrestrial food webs. Tissues of a variety of wildlife species, living near urban areas and in more remote areas, including the Arctic and the Antarctic, were studied to monitor for the presence of PFOS. In addition, species from different trophic levels with different feeding

Purpose and rationale

This figure helps readers understand the sampling, which translates to

understanding results. This is not always necessary, but is a useful aid in this paper

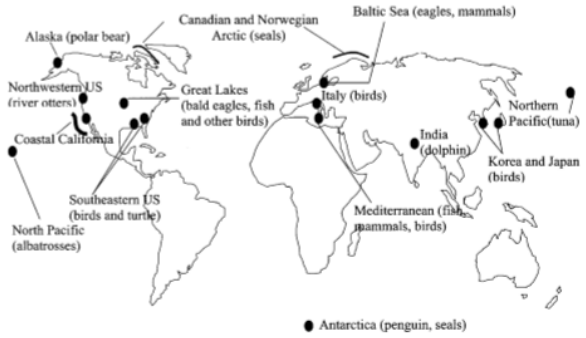

FIGURE 2. Sampling locations of wildlife to monitor fluorinated organic compounds.

Here, materials and methods are written as one large section. If you'd like you can use subheadings such as "sampling location", "materials", "extraction methods", "instrumental conditions", "quality control", or whatever makes sense for your paper

Sample information. Notice that they refer to their figure

strategies were selected to provide some insight into potential environmental pathways.

Materials and Methods

Tissues of various species of aquatic mammals, birds, fish, and amphibians were collected as part of earlier monitoring studies conducted by Michigan State University, East Lansing, Michigan. Samples were collected under permits from state and federal agencies. Tissues of most individuals of aquatic mammals were obtained from stranded dead animals. Samples were also obtained from archived tissues from federal and state agencies. Samples collected in the 1990s were used. Samples were obtained to represent various geographical locations including the Arctic and the Antarctic Oceans (Figure 2).

Extraction procedures + sample prep

Concentrations of PFOS and other FOCs in liver, egg yolk, muscle, or blood plasma were determined by use of high-performance liquid chromatography (HPLC) with electrospray tandem mass spectrometry (*9*). The PFOS used as standards and for matrix spikes was purchased as the potassium salt (Fluka, Milwaukee, WI). The purity of the PFOS standard was 86%. The reported concentrations were not corrected for the purity. The internal standard, 1*H*,1*H*,2*H*,2*H*-perfluorooctane sulfonate (THPFOS) was purchased from ICN (Costa Mesa, CA). One mL of sera, 5 μL of internal standard (250 ng), 1 mL of 0.5 M tetrabutylammonium hydrogen sulfate (TBA) solution, and 2 mL of 0.25 M sodium carbonate buffer (adjusted to pH 10) were added to a 15-mL polypropylene tube for extraction. After the solution was thoroughly mixed, 5 mL of methyl-*tert*-butyl ether (MTBE) was added, and the mixture was shaken for 20 min. The organic and aqueous layers were separated by centrifugation, and an exact volume of MTBE (4 mL) was removed from the solution. The aqueous mixture was rinsed with MTBE and separated twice; all rinses were combined in a second polypropylene tube. The solvent was allowed to evaporate under nitrogen before being reconstituted in 1 mL of methanol. The extract was vortex mixed for 30 s and passed through a 0.2-μm nylon mesh filter into an autosampler vial. For the extraction of liver samples, a liver homogenate of 1 g of liver in 5 mL of purified (milli-Q) water was prepared. A 1-mL aliquot of the homogenate was added to a polypropylene tube, and the sample was extracted according to the procedure described above.

Analyte separation was performed using a Hewlett-Packard HP1100 liquid chromatograph modified with low dead-volume internal tubing. Extract (10 μL) was injected onto a 50 × 2 mm (5 μm) Keystone Betasil C_{18} column with a 2 mM ammonium acetate/methanol mobile phase starting at 45% methanol. At a flow rate of 300 μL/min, the gradient was increased to 90% methanol before reverting to the original conditions after 9 min. Column temperature was maintained at 25 °C. The HPLC system was interfaced to a Micromass (Beverly, MA) Ultima or Quattro II atmospheric pressure ionization tandem mass spectrometer operated in the electrospray negative ion mode. In all cases, the capillary was held between 1.6 and 3.2 kV. Cone voltage was 20−60 v and collision energy was 30−45 v. The source temperature was maintained at 250 °C. Instrumental parameters were optimized to transmit the [M-H], [M-K], or [M-NH_4] ion for analytes. When possible, multiple daughter ions were monitored, but quantitation was based on a single product ion. In the electrospray tandem mass spectrometry (ESMSMS) system, the 499 Da → 80 Da transition can be optimized to provide a stronger signal than the 499 Da → 99 Da transition of PFOS. However, in the analysis of tissue samples collected from some species of animals, an unidentified interferent was present in the 499 Da → 80 Da transition. Although this interferent was rarely observed, to ensure complete selectivity, quantitation was based on the 499 Da → 99 Da transition. To further ensure that no interferent compromised the quantitation of PFOS, the transitions 499 Da → 80 and 499 → 99 were compared. If a quantitative deviation of >20% was observed, a third transition, 499 Da → 130 was also monitored. In all cases, the validity of the 499 Da → 99 transition was confirmed by one of the other transitions. Samples were evaluated versus an averaged $^1/_x$ weighted, unextracted external calibration curve. Because of the variety of matrices analyzed, with respect to both species and tissues, and because of evolving analytical methods, the limit of quantitation (LOQ) was variable. Data quality assurance and quality control protocols included matrix spike, surrogate spike, laboratory blank, surrogate matrix blanks, and continuing calibration verification. Recoveries of target analytes spiked to rabbit sera or liver and passed through the analytical procedure ranged from 85 to 101% (*9*). Concentrations of target analytes were not corrected for recoveries of the surrogate standard or matrix spike recoveries.

Analytical methods and instrumental conditions. In this paper, they provide a lot of detail because it is a

very new analysis method. In your reports, you can put some of this into the SI. For example, mass spec transitions can go into SI. Make sure

to refer to the SI in the main text

Quality control information

This table has a descriptive heading, that includes the different units that concentrations are reported in

All of the information reported in this table is relevant, and aids readers in understanding the results. Here, their LOQs are different for different matrices, therefore they report "less than" different values based on the species and tissue type.

This data could also be presented in a bar graph, but because of the many different types of samples, a table is more appropriate. Notice that the table is neatly formatted.

TABLE 1. Ranges of Concentrations of PFOS (ng/g, wet wt, for Liver and Muscle Tissues and ng/mL for Blood Plasma) in Wildlife; Mean Concentrations Are Given in Parentheses

species	location	tissue	n	PFOS
	Aquatic Mammals			
ringed seal	Canadian Arctic	plasma	24	<3–12
ringed seal	Baltic Sea	plasma	18	16–230 (110)
ringed seal	Norwegian Arctic	plasma	18	5–14 (9)
gray seal	Baltic Sea	plasma	26	14–76 (37)
gray seal	Canadian Arctic	plasma	12	11–49 (28)
California sea lion	Coastal California	liver	6	<35–49
elephant seal	Coastal California	liver	5	<35
harbor seal	Coastal California	liver	3	<35–57
river otter	Northwestern USA	liver	5	34–990 (330)
sea otter	Coastal California	liver	8	<35
northern furseal	Coastal waters of Alaska	liver	14	<35–120
polar bear	Alaska, USA	liver	17	180–680 (350)
mink	Midwestern USA	liver	18	970–3680 (2830)
bottlenose dolphin	Mediterranean Sea	liver	5	170–430 (270)
striped dolphin	Mediterranean Sea	liver	4	65–160 (100)
weddel Seal	Terra Nova Bay, Antarctica	liver	1	<35
Ganges river dolphin	Ganges River, India	liver	2	<35–81
	Birds			
double-crested cormorant	Lake Huron, Great Lakes	plasma	6	1–270 (170)
herring gull	Lake Huron, Great Lakes	plasma	2	66–79 (73)
polar skua	Terra Nova Bay, Antarctica	plasma	2	<1–1.4
black-tailed gull	Hokkaido, Japan	plasma	24	2–12 (6)
double-crested cormorant	Lake Winnepeg, Canada	egg yolk	4	130–320 (210)
ring-billed gull	Lake Huron, Great Lakes	egg yolk	3	<35–150
Laysan and black-footed albatrosses	Midway Atoll, North Pacific	liver	9	<35
common loon	North Carolina, USA	liver	8	35–690 (290)
brown pelican	Mississippi, USA	liver	2	290–620 (460)
common cormorant	Italy	liver	12	33–470 (96)
black-tailed gull	Korea	liver	15	70–500 (170)
Laysan and black-footed albatrosses	Midway Atoll, North Pacific	plasma	3	9–26 (18)
double-crested cormorant	Lake Huron, Great Lakes	plasma	3	110–430 (260)
herring gull	Lake Huron, Great Lakes	plasma	2	280–450 (370)
bald eagle	Midwestern USA	plasma	26	1–2570 (360)
Laysan and black-footed albatrosses	Midway Atoll, North Pacific	plasma	10	3–39 (9)
	Fish			
lake whitefish	Michigan waters, USA	eggs	2	150–380 (260)
brown trout	Michigan waters, USA	eggs	3	49–75 (64)
Chinook salmon	Michigan waters, USA	liver	6	33–170 (110)
lake whitefish	Michigan waters, USA	liver	5	33–81 (67)
brown trout	Michigan waters, USA	liver	10	<17–26
yellow-fin tuna	Northern North Pacific Ocean	liver	12	<7
blue-fin tuna	Mediterranean Sea	liver	8	21–87 (48)
carp	Saginaw Bay, Michigan, USA	muscle	10	60–300 (120)
Chinook salmon	Michigan waters, USA	muscle	6	7–190 (110)
lake whitefish	Michigan waters, USA	muscle	5	97–170 (130)
brown trout	Michigan waters, USA	muscle	10	<6–46
	Turtles and Frogs			
yellow-blotched map turtle	Mississippi, USA	liver	6	39–700 (190)
green frogs	Southwest Michigan, USA	liver	4	<35–290
snapping turtle	Lake St. Clair, Michigan, USA	plasma	5	1–170 (72)

Brief summary of experiment

Results and Discussion

Samples were scanned for four FOCs: PFOS, perfluorooctane sulfonylamide (PFOSA), perfluorohexane sulfonate (PFHS), and perfluorooctanoate (PFOA). However, all concentrations of PFHS were less than the LOQ (LOQ range = 1 to 86 ng/g, wet wt) and only a few samples contained PFOA or PFOSA at levels greater than the LOQ of 2.5 to 180 ng/g, wet wt, and 1 to 38 ng/g, wet wt, respectively. Therefore, only the results for PFOS are presented (Table 1).

When a method detection limit of 1 ng/g, wet wt, was attained, PFOS was detectable in most samples including those from remote marine regions. Concentrations of PFOS in the blood of ringed and gray seals from the Canadian and Norwegian Arctic were in the range of 3 to 50 ng/mL. PFOS concentrations were 2–10 times greater (14–230 ng/mL) in seals from relatively more urbanized locations,such as the Baltic Sea, than those from the Arctic Ocean. Blood plasma of Laysan and black-footed albatrosses collected from remote oceanic locations, such as Midway Atoll in the North Pacific Ocean, contained concentrations of PFOS ranging from 3 to 26 ng/mL. PFOS concentrations in the blood of cormorants and herring gulls from the Great Lakes were approximately 10-fold greater than those in albatrosses from Midway Atoll. Although the liver of yellow-fin tuna from the northern North Pacific did not contain quantifiable concentrations of PFOS (<7 ng/g, wet wt), blue-fin tuna from the Mediterranean Sea contained up to 87 ng/g, wet wt, PFOS in the liver. Livers of polar bears from Alaska contained concentrations of PFOS between 180 and 680 ng/g, wet wt. Although PFOS is distributed in remote marine environments including polar regions, concentrations of PFOS in these regions were severalfold less than those from relatively more industrialized

Refers to specific concentration values and compared between different samples. Refer to table/figure when applicable.

locations such as the Baltic Sea and the Great Lakes.

Among various bird species analyzed, blood plasma of bald eagles from the midwestern U.S. contained PFOS concentrations of up to 2570 ng/mL (mean: 360). All plasma samples were obtained from bald eagle chicks less than 200 days old. Other fish-eating water birds such as common loons and brown pelicans contained quantifiable concentrations of PFOS in the liver. All the bird tissues from Canada, Italy, Japan, and Korea contained quantifiable concentrations of PFOS. PFOS concentrations in the blood of black-tailed gulls (2−12 ng/mL) from Hokkaido in Japan were less than those found in albatrosses from Midway Atoll. Occurrence of PFOS in these birds suggests that their potential source of exposure is the fish diet. Tissues of fish from the Great Lakes and the Mediterranean Sea contained measurable concentrations of PFOS. The highest PFOS concentrations observed in fish (300 ng/g, wet wt) were in the muscle of carp from Saginaw Bay, Michigan.

Mink from the midwestern U.S. contained significant concentrations of PFOS in their livers (970−3680 ng/g, wet wt). Mink are opportunistic predators but do eat fish as part of their diet. When mink were fed carp from Saginaw Bay, Michigan, containing an average concentration of 120 ng PFOS/g (wet wt), under laboratory conditions, the estimated biomagnification factor based on the concentrations of PFOS in livers of mink was approximately 22.

Although the results of this study have demonstrated for the first time that PFOS is widely distributed on a global scale and can be persistent and bioaccumulative in various food chains, little information is available on possible toxic effects of PFOS to wildlife. PFOS and related perfluorinated compounds have been shown to affect cell−cell communication, membrane transport and process of energy generation, and proxisome proliferation (*11*, *12*). Currently available data (unpublished reports to U.S. EPA; Docket No. FYI-0500-01378) indicate that concentrations of PFOS in wildlife are less than those required to cause significant adverse effects in laboratory animals. However, as more species-specific information becomes available, a more refined assessment of the risks to wildlife will be possible.

Acknowledgments

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ES001834K

This paper was the first time PFOS was measure in wildlife, so there is not much literature to refer to. Every time you write a paper or report, you must compare what you have seen to what is published in the literature. If there is no literature, you should mention that as well. For the purpose of CHM410, mention at least one literature value, but don't spend too much time looking into this

This paper concludes that more information and measurements are required. For your reports, make sure you are repeating the purposed of the experiment and then stating your overall conclusion

References must be formatted consistently with all relevant information. Choose a journal's format and stick to it. You can use the Environmental Science & Technology or Journal of the American Chemical Society if you'd like.

A minimum of 5 reference is required, at least 3 should be peer-reviewed.

Some examples of visualizing data

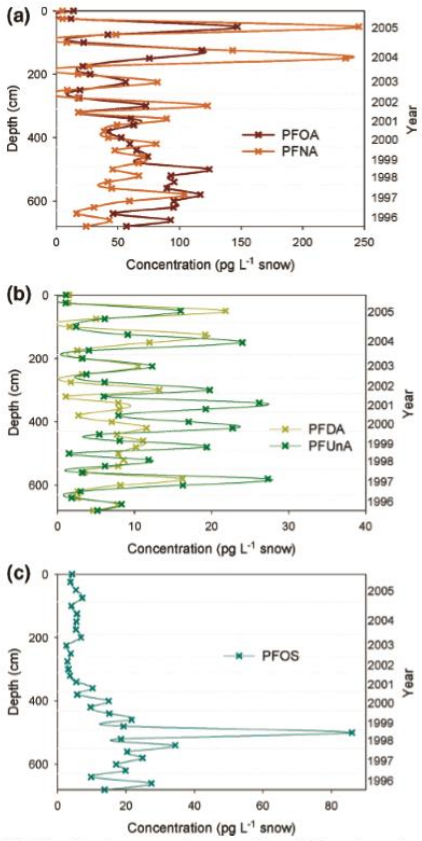

FIGURE 1. Density-corrected concentrations of PFAs on Devon Ice Cap since 1996: (a) PFOA and PFNA; (b) PFDA and PFUnA; and (c) PFOS.

This paper reported concentrations of 5 analytes at various depths of an ice core. These three graphs show the

concentrations in snow versus the depth of the ice (which is also plotted as the year on the right y-axis).

This 3-panel graph is appropriately labeled with lower-case letters that are referred to in the figure caption.

In this figure, the fluxes of each analyte are plotted in a bar graph versus year. Notice that they have

plotted the standard error of the mean (n=3) as error bars.

Notice that all of these plots are neat and have fully labelled axis, in units that make sense for the values

reported. Colour helps visualization, but if you are printing in black and white, make sure you are using different shapes or patterns.

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Perfluorinated Acids in Arctic Snow: New Evidence for Atmospheric Formation

CORA J. YOUNG,† VASILE I. FURDUI,† JAMES FRANKLIN,‡ ROY M. KOERNER,§ DEREK C. G. MUIR,|| AND SCOTT A. MABURY*,†

Department of Chemistry, University of Toronto, 80 St. George Street, Toronto, Ontario, Canada M5S 3H6, CLF-Chem Consulting, 28 Rue Edouard Olivier, Brussels, Belgium BE-1170, Geological Survey of Canada, 601 Booth Street, Ottawa, Ontario, Canada K1A 0E8, and Water Science and Technology Directorate, Environment Canada, 867 Lakeshore Drive, Burlington, Ontario, Canada L7R 4A6

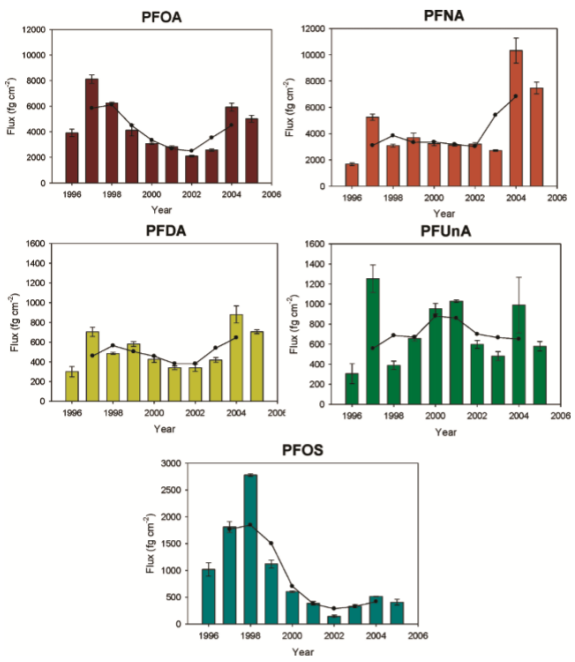

FIGURE 2. PFA fluxes to Devon Ice Cap by year. Mean fluxes with standard error of three replicates indicated by bars. Lines reflect a 3-year moving average.

CHM410-1410 Grading Scheme for the Air Sampling Lab

Title (2)	(2)	Appropriate and descriptive title
Abstract (10)	(2)	State objectives and hypothesis of your study
	(2)	Brief description of methodology (what was done)
	(2)	Summary of major findings (results)
	(2)	Support main result statement with numbers
	(2)	State principle conclusion
Introduction (15)	(4)	Background information on the methods used and their relevance to the experiment
	(4)	Background information on the analyte(s) of interest
	(4)	Introduction gave the reader the appropriate background to understand the results and discussion
	(3)	Rationale for present study (purpose)
Materials & Methods (7)	(2)	Sampling details
	(2)	Sensor Details
	(3)	Data analysis details
Results & Discussion (38)	(3)	Begin with brief overall description of experiment
	(7)	Presentation of data: Judicious use of tables & figures that summarize the important results
	(5)	Referred to and used tables or figures when discussing results
	(5)	Addressed hypothesis with specific reference to data
	(5)	Compared data to background literature
	(3)	Addressed the effect of sampler resolution
	(10)	Overall well-structured and presented story
Conclusions (4)	(4)	Hypothesis and final conclusion
Future Directions (4)	(4)	Explain what you would do as a follow up study
References (5)	(5)	Proper and thorough (minimum 3) with in-text citations
Supplemental Information (5)	(3)	Appropriate use of the SI with specific analytical details (additional instrumental conditions and details, sample chromatograms), raw data, or calibration curves
	(2)	Sample calculations
Clarity and writing style (7)	(5)	Concise and clear
	(2)	Proper and consistent verb tenses
Word limit (3)	(3)	2000 works text for Labs 2&3, 3000 words text for the Field Trip. The word count does not include references or supplemental information, and **MUST be provided underneath your title**, if not you will receive zero. Minus one mark for every 100 words over the 3000 word limit.