DEPT. OF EARTH & ENVIRONMENTAL SCIENCES, UNIVERSITY OF ROCHESTER

Atmospheric Research
EES 306

Mauna Loa Observatory, Hawai'i

Fall 2021
Syllabus

Last Updated: August 23, 2021

Contents

1 Course Overview

Lecture Location: Wegmans Hall 1009 (subject to COVID-19 safety protocols)
Lecture Time: Tu/Th 11:05 AM-12:20 PM Eastern
Lab Location: Hutchison Hall B03
Lab Time: TBD on first day of class

Co-Instructor: Prof. Vasilii V. Petrenko
Personal Pronouns: he/his/him
E-mail: vasilii.petrenko@rochester.edu
Office Location: Hutchison 228
Office Hours: W 7:30-8:30 PM on Zoom, or by e-mail appointment

Co-Instructor: Prof. Lee T. Murray
Personal Pronouns: he/his/him
E-mail: lee.murray@rochester.edu | @leetmurray
Office Location: Hutchison 479
Office Hours: Tu/Th 12:30-1:30 PM, or by e-mail appointment

1.1 Description

The atmosphere enables life as we know it to exist on Earth. However, the atmosphere has undergone enormous change in recent decades due to human activity that is changing the Earth's climate and threatens public and ecological health. In this course, students will get a hands-on introduction to cutting-edge atmospheric research via involvement in ongoing projects in the EES department. The course will include reading and presenting research literature that introduces the research projects, learning and applying experimental techniques for analysis of atmospheric composition, and working with models of atmospheric physics and chemistry to help interpret the measurements. Students will write a brief paper on the obtained results and their interpretation. This course fulfills a closure requirement for Environmental Science and Environmental Studies majors.

1.2 Pre-requisites

Required, unless granted permission by instructor:

- CHEM 131 or equivalent and MATH 141-142 or equivalent

1.3 Main Learning Goals

The overarching goals of this class are:

- Understand the role of hydroxyl radicals (OH) in tropospheric chemistry
- Understand how measurements of trace gases such as ^{14}CO and methyl chloroform can be used to characterize OH abundance and variability
- Understand the processes that affect ^{14}CO concentration in the atmosphere

- Understand and be able to work with atmospheric box models
- Learn and be able to independently perform volumetric gas mixing as well as measurements of carbon monoxide mole fraction in air samples
- Be able to use measurement results to calculate the true ^{14}CO concentration in air samples
- Understand and be able to apply in your work with data the concepts of calibration, uncertainty, precision, signal-to-noise ratio, blanks and statistical significance
- Understand how inverse modeling (Bayesian optimization) works in both theory and practice, its relative strengths and limitations, and be able to apply such tools to use atmospheric observations of ^{14}CO and methyl chloroform to constrain OH
- Be able to lead an effective presentation / discussion on a research article
- Be able to write an effective research synthesis report

2 Readings

Readings indicated on the syllabus must be completed prior to coming to lecture for which the reading is indicated. Note, students do not need to purchase any course materials. All readings may be accessed from their blue links or will be posted on Blackboard. However, some may require you to be on the campus network or VPN if off campus (see University IT for directions).

2.1 Required

Books

Brasseur, G. P., and D. J. Jacob (2017), *Modeling of Atmospheric Chemistry*, Cambridge University Press, Cambridge, UK, doi:10.1017/9781316544754.

Jacob, D. J. (1999), *Introduction to Atmospheric Chemistry*, 1st ed., Princeton University Press, Princeton, NJ, http://acmg.seas.harvard.edu/publications/jacobbook/index.html.

Rodgers, C. D. (2000), *Inverse Methods for Atmospheric Sounding: Theory and Practice*, 2 ed., 240 pp., World Scientific, Singapore, https://www.worldscientific.com/worldscibooks/10.1142/3171#t=toc.

Wilks, D. S. (2011), *Statistical Methods in the Atmospheric Sciences*, Elsevier Science & Technology, ProQuest Ebook Central, online at https://ebookcentral.proquest.com/lib/rochester/detail.action?docID=689817.

Articles and Excerpts

Brenninkmeijer, C. A. M., M. R. Manning, D. C. Lowe, G. Wallace, R. J. Sparks, and A. Volz-Thomas (1992), Interhemispheric asymmetry in OH abundance inferred from measurements of atmospheric 14CO, *Nature*, *356*(6364), 50–52, doi:10.1038/356050a0.

Duncan, B. N., J. A. Logan, I. Bey, I. A. Megretskaia, R. M. Yantosca, P. C. Novelli, N. B. Jones, and C. P. Rinsland (2007), Global budget of CO, 1988–1997: Source estimates and validation with a global model, *Journal of Geophysical Research*, *112*(D22), doi:10.1029/2007jd008459.

Jacob, D. J. (2019), *How to write a scientific paper and how to deal with the review process*, http://acmg.seas.harvard.edu/presentations/2019/gsf_paper.pptx.

Jöckel, P. (2002), The seasonal cycle of cosmogenic ^{14}CO at the surface level: A solar cycle adjusted, zonal-average climatology based on observations, *Journal of Geophysical Research*, *107*(D22), doi:10.1029/2001jd001104.

Lelieveld, J., F. J. Dentener, W. Peters, and M. C. Krol (2004), On the role of hydroxyl radicals in the self-cleansing capacity of the troposphere, *Atmospheric Chemistry and Physics*, *4*(9/10), 2337–2344, doi:10.5194/acp-4-2337-2004.

Lelieveld, J., et al. (2006), New Directions: Watching over tropospheric hydroxyl (OH), *Atmospheric Environment*, *40*(29), 5741–5743, doi:10.1016/j.atmosenv.2006.04.008.

Levy, H. (1971), Normal atmosphere: large radical and formaldehyde concentrations predicted., *Science*, *173*(3992), 141–143, doi:10.1126/science.173.3992.141.

Manning, M., D. Lowe, R. Moss, G. Bodeker, and W. Allan (2005), Short-term variations in the oxidizing power of the atmosphere., *Nature*, *436*(7053), 1001–1004, doi:10.1038/nature03900.

Michalak, A. M., L. Bruhwiler, and P. P. Tans (2004), A geostatistical approach to surface flux estimation of atmospheric trace gases, *Journal of Geophysical Research: Atmospheres*, *109*(D14), doi:https://doi.org/10.1029/2003JD004422, https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2003JD004422.

Montzka, S., M. Krol, E. Dlugokencky, B. Hall, P. Jöckel, and J. Lelieveld (2011), Small interannual variability of global atmospheric hydroxyl., *Science*, *331*(6013), 67–69, doi:10.1126/science.1197640.

Murray, L. T., A. M. Fiore, D. T. Shindell, V. Naik, and L. W. Horowitz (2021), Large uncertainties in global hydroxyl projections tied to fate of reactive nitrogen and carbon, *Proc Natl Acad Sci USA*, in review.

Naik, V., et al. (2013), Preindustrial to present-day changes in tropospheric hydroxyl radical and methane lifetime from the Atmospheric Chemistry and Climate Model Intercomparison Project (ACCMIP), *Atmospheric Chemistry and Physics*, *13*(10), 5277–5298, doi:10.5194/acp-13-5277-2013.

Patra, P., et al. (2014), Observational evidence for interhemispheric hydroxyl-radical parity., *Nature*, *513*(7517), 219–223, doi:10.1038/nature13721.

Petrenko, V. V., A. M. Smith, E. M. Crosier, R. Kazemi, P. Place, A. Colton, B. Yang, Q. Hua, and L. T. Murray (2021), An improved method for atmospheric ^{14}CO measurements, *Atmospheric Measurement Techniques*, *14*(3), 2055–2063, doi:10.5194/amt-14-2055-2021.

Riedel, K., and K. Lassey (2008), Detergent of the atmosphere, *Water & Atmosphere*, *16*(1), https://niwa.co.nz/sites/niwa.co.nz/files/import/attachments/detergent.pdf.

Rigby, M., et al. (2013), Re-evaluation of the lifetimes of the major CFCs and CH3CCl3 using atmospheric trends, *Atmospheric Chemistry and Physics*, *13*(5), 2691–2702, doi:10.5194/acp-13-2691-2013.

Spivakovsky, C. M., et al. (2000), Three-dimensional climatological distribution of tropospheric OH: Update and evaluation, *Journal of Geophysical Research: Atmospheres*, *105*(D7), 8931–8980, doi:10.1029/1999jd901006.

Stevenson, D. S., et al. (2020), Trends in global tropospheric hydroxyl radical and methane lifetime since 1850 from AerChemMIP, *Atmospheric Chemistry and Physics*, *20*(21), 12,905–12,920, doi:10.5194/acp-20-12905-2020.

Volz, A., D. H. Ehhalt, and R. G. Derwent (1981), Seasonal and latitudinal variation of ^{14}CO and the tropospheric concentration of OH radicals, *Journal of Geophysical Research*, *86*(C6), 5163, doi:10.1029/jc086ic06p05163.

Voulgarakis, A., et al. (2013), Analysis of present day and future OH and methane lifetime in the ACCMIP simulations, *Atmospheric Chemistry and Physics*, *13*(5), 2563–2587, doi:10.5194/acp-13-2563-2013.

Weinstock, B. (1969), Carbon monoxide: residence time in the atmosphere., *Science*, *166*(3902), 224–225, doi:10.1126/science.166.3902.224.

3 Schedule

3.1 Lectures

Below is the tentative class schedule, with topics for each class, associated readings, and problem set and exam due dates. The schedule is subject to change pending course progress and any changes in University operations (e.g., due to COVID-19 restrictions).

Tuesday	Thursday
Aug 24th	26th **1** **Overview (P & M)** Key Topics 1. Course Description and Expectations 2. Lab Tour 3. Lab Scheduling Reading • Syllabus
31st **2** **Introduction to Research Project (P & M)** Key Topics 1. Project Background and Description Reading • NSF Proposal **Lab Group 1 - Training**	Sep 2nd **3** **Overview of Measurements (P)** Key Topics 1. CO mole fraction 2. CO separation 3. ^{14}C measurement Reading • *Petrenko et al.* (2021)

TUESDAY	THURSDAY
7th **4** **Gaussian Statistics and Bayes' Theorem (M)** Key Topics 1. Normal Distribution 2. Conditional Probability 3. Bayes' Theorem Reading • Ch. 1-2 of *Wilks* (2011) • Appendix E.7 of *Brasseur and Jacob* (2017) **Lab Group 2 - Training**	9th **5** **Atmospheric Science Overview (M)** Key Topics 1. Global Energy Budget 2. Atmospheric Transport 3. Atmospheric Chemistry Reading • Ch. 2-3 of *Brasseur and Jacob* (2017)
14th **6** **Measures of Atmospheric Composition (P)** Key Topics 1. Mole fraction 2. Number density Reading • Ch. 1 of *Jacob* (1999) **Lab Group 3 - Training**	16th **7** **Calculation of ^{14}CO Concentration (P)** Key Topics 1. ^{14}C units and notation 2. Dilution and blank corrections **PS1 Due by start of class**
21st **8** **CO Budget Overview (M)** Key Topics 1. Emissions 2. *In situ* production 3. Sinks Reading • *Duncan et al.* (2007) **Lab Group 1 - Training**	23rd **9** **Box Models (P)** Key Topics 1. Sources and sinks 2. Lifetime and reservoir size Reading • Ch. 3 of *Jacob* (1999) **PS2 Due by start of class**
28th **10** **Multi-Box Models (M)** Key Topics 1. Transport 2. Solving Linear Systems of Equations Reading • Ch. 3 of *Jacob* (1999) **Lab Group 2 - Training**	30th **11** **Linear Algebra Overview (M)** Key Topics 1. Scalars, Vectors and Matrices 2. Matrix Multiplication 3. Matrix Inversions Reading • Appendix E.1-6 of *Brasseur and Jacob* (2017) • Appendix A of *Rodgers* (2000) **PS3 Due by start of class**

<table>
<tr><th>TUESDAY</th><th>THURSDAY</th></tr>
<tr><td>Oct 5th 12
Accuracy and Signal-to-Noise (P)
Key Topics
1. Needed accuracy
2. Signal-to-noise ratio
Reading
• TBD
Lab Group 3 - Training</td><td>7th 13
Calibration (P)
Key Topics
1. The need for calibration
2. Constructing a calibration scale
Reading
• TBD
PS4 Due by start of class</td></tr>
<tr><td>12th
Fall Break</td><td>14th 14
Hydroxyl Radicals (P)
Key Topics
1. OH production
2. Key reactions and OH cycling
3. OH distribution and spatial and seasonal variability
Reading
• Levy (1971)
• Spivakovsky et al. (2000)
• Lelieveld et al. (2004)
• Riedel and Lassey (2008)
• Lelieveld et al. (2006)</td></tr>
<tr><td>19th 15
Hydroxyl Radicals (M)
Key Topics
1. Model estimates of OH
2. Long-term OH variability and key controls on OH
3. Uncertainties in the OH budget
Reading
• Naik et al. (2013)
• Voulgarakis et al. (2013)
• Stevenson et al. (2020)
• Murray et al. (2021)
PS5 Due by start of class
Lab Group 1 - Training</td><td>21st 16
Inverse Modeling Part I (M)
Key Topics
1. Inverse Problem for Scalars
2. State Vector
3. A priori and a posteriori
Reading
• Ch 11.1-3 of Brasseur and Jacob (2017)</td></tr>
</table>

TUESDAY	THURSDAY
26th **17** **Inverse Modeling Part II (M)** Key Topics 1. Inverse Problem for Vectors 2. Error-covariance matrices 3. Jacobian matrix 4. Averaging kernel matrix Reading • Ch 11.4-5 of *Brasseur and Jacob* (2017) **Lab Group 2 - Training**	28th **18** **Uncertainty Estimation (P)** Key Topics 1. Measurement uncertainties 2. Error propagation Reading •
Nov 2nd **19** **Leaks, Mixing, Dilutions (P)** Key Topics 1. Volumetric mixing 2. Leak tolerance **PS6 Due by start of class** **Lab Group 3 - Training**	4th **20** **Student Presentations I** Key Topics 1. Methyl chloroform Reading • *Montzka et al.* (2011) • *Patra et al.* (2014)
9th **21** **Cosmic Rays (P & M)** Key Topics 1. Origin and nature of cosmic rays 2. Cosmogenic nuclides and ^{14}CO Reading • TBD **PS7 Due by start of class** **Lab Group 1 - Test**	11th **22** **Inverse Modeling Part III (M)** Key Topics 1. Error characterization 2. A practical example Reading • Ch 11.4-5 of *Brasseur and Jacob* (2017) • *Rigby et al.* (2013)
16th **23** **Writing a Scientific Report/Paper (M)** Key Topics 1. Structure and Tone 2. Giving Proper Credit 3. Graphics Reading • *Jacob* (2019) **Lab Group 2 - Test**	18th **24** **Blanks, Sample Memory (P)** Key Topics 1. Procedural blanks and corrections 2. Sample memory **PS8 Due by start of class**
23rd **25** **Data Quality Control, Stat. Significance (P)** Key Topics 1. Quality control and outlier rejection 2. Statistical significance Reading • TBD	25th **Thanksgiving Break**

TUESDAY	THURSDAY
30th **26** **Inverse Modeling Part IV (M)** Key Topics 1. Adjoint Methods 2. Geostatistical Methods 3. Data Assimilation Reading • Ch. 11.4.4, 11.6-11.9 of *Brasseur and Jacob* (2017) • *Michalak et al.* (2004) **Lab Group 3 - Test**	Dec 2nd **27** **Student Presentations II** Key Topics 1. ^{14}CO Reading • *Weinstock* (1969) • *Volz et al.* (1981) • *Brenninkmeijer et al.* (1992) **PS9 Due by start of class**
7th **28** **Student Presentations III** Key Topics 1. ^{14}CO Reading • *Jöckel* (2002) • *Manning et al.* (2005)	9th **Reading Period**
14th **Exam Period**	16th **Group Report Paper Due: Dec 17 at 5PM.** **Exam Period**

3.2 EES 306 Lab

In addition to lectures, there will be a course lab component. Part of this will be in Prof. Petrenko's laboratory and focused on learning atmospheric measurement techniques. Students will be divided in groups of 2, and only 1 group per week will be in the laboratory. The other students will meet and work on the group coding assignments in a location of their preference.

4 Grading

Students will have their grade determined as follows:

EES 306	
Participation in Discussions:	15 %
Problem Sets:	30 %
Lab Exam:	15 %
Student Presentations:	15 %
Group Report:	25 %
Total:	100 %

4.1 Problem Sets

There will be approximately weekly problem sets assigned on material covered in previous lectures and readings.

The aim of the problem sets is to help you learn the course concepts. Working together with your classmates is thus encouraged, although problem sets should always be solved and written up individually. **If you collaborate, write with whom you worked on your submission**.

For problems involving calculations, show all work, explaining in sufficient detail how you arrived at the answer. Describe the rationale behind each step using language like "Convert from kg to molecules" or "Apply the blank correction." Partial credit for ultimately wrong answers will be assigned based on work shown. Make sure to show units throughout the problems. If a problem or problem set contains multiple problems / parts of a problem that require an identical approach / calculation, it is sufficient to refer to the equivalent earlier problem (e.g., write "this problem is solved the same way as problem 1.2" and then provide the answer).

For long-answer questions not requiring calculations, ensure that everything is clearly readable, all parts of the answer are logically and concisely argued and the answer stays focused on the question and does not go off on tangents.

No partial credit problems: We will try to include some problems where you do not get any partial credit if you do not get the correct answer. This is intended as practice for your future careers, in which you do not get "partial credit" for work that yields an incorrect answer, and, in the worst-case scenario, you can get a situation like the Mars climate orbiter being lost due to confusion about units.

Problem Sets will be submitted digitally through GradeScope.

All problem sets will be weighted equally.

4.2 Lab Test

Toward the end of the course, each student will be observed and evaluated in their performance of the laboratory procedures. The evaluation will be based on how correctly the procedure is followed, the number and severity of any mistakes (i.e., is the procedural mistake an imperfection that might slightly affect the measurement, or does it result in a major error in the result, or in loss of the sample), as well as on the student's understanding of the procedure (i.e., why are we doing the steps that we are doing).

4.3 Student Presentations

Every student will be required to do a presentation / lead a discussion on a research article (or two) that we read in the course. The instructors will do similar presentations earlier in the course to provide some examples. The presentations will be evaluated based on the following criteria:

- Is the presentation clear and logical?
- Is there a good balance between time devoted to presenting the main concepts and discussion? (should be about half and half, as everyone should have carefully read the paper)
- Does the presentation / discussion fit well within the allotted time (about 35 min per presenter)?
- Are the needed key background concepts explained (if any)?

- Are the main concepts and questions raised by the paper adequately discussed?
- Does the presenter have a good understanding of the paper?
- Does the presenter do a good job at actively involving the others in the discussion, by, for example: posing stimulating questions, encouraging a dialogue and / or setting very short in-class problems designed to help students understand the concepts

4.4 Group Report

In lieu of a final exam, the class will generate a final group summarizing the project. The report will synthesize relevant background and motivation, measurement methodology and results, and an interpretation of the measurements using the model tools built in the problem sets. Students will work with the instructors to design an outline. Then, each student will be lead author on a different section of the report. Students will provide constructive feedback and edits to their peers' sections of the report. Each student's individual grade will be weighted equally between the quality of their own section and the overall quality and the cohesiveness of the report.

The report paper **must be written following the Style Guide and Reference Format of the American Geophysical Union**, including proper in-line citations consistent with the university Academic Honesty policies.

5 Classroom Policies

5.1 Diversity and Inclusion

This class is an inclusive and welcoming learning environment for all students regardless of background or ability, consistent with University policy, state and federal laws and the instructors' personal beliefs. Students must respect the different experiences, identities, beliefs and values expressed by their peers, and refrain from derogatory comments about other individuals, cultures, groups, or viewpoints.

Please make sure that we are pronouncing your name correctly, and let us know if you have any preferred nicknames and/or pronouns that you would like us to use.

In the event you encounter any barrier(s) to full participation in this course due to the impact of a disability, please contact the Office of Disability Resources. The access coordinators in the Office of Disability Resources can meet with you to discuss the barriers you are experiencing and explain the eligibility process for establishing academic accommodations. You can reach the Office of Disability Resources at: disability@rochester.edu; (585) 276-5075; Taylor Hall; `http://www.rochester.edu/college/disability`.

5.2 COVID-19

You are expected to adhere to all University policies regarding the COVID-19 pandemic (vaccination, masking, distancing, staying home if you have any symptoms, etc.). Please make sure you stay up to date on these policies, as they continually evolve.

Given the extraordinary circumstances of the COVID-19 pandemic, we acknowledge that students may be subject to a host of pressures and difficulties that will make learning this semester especially difficult. We encourage you to meet with one or both of us about any concern or situation that affects your ability to complete your academic work successfully.

6 Academic Honesty

All assignments and activities associated with this course must be performed in accordance with the University of Rochester's Academic Honesty Policy. A comprehensive description of the University of Rochester's Academic Honesty Policy is available at: `http://www.rochester.edu/college/honesty`. For this course, the lab test and presentation need to be completed individually, but we encourage collaboration on the problem sets. The final project report is a group assignment.

7 Credit Hour Policy

This course follows the College credit hour policy for four-credit courses, which stipulates that students are expected to complete an "extra period" in addition to the course instructional time of two or three class periods per week. In this course, students will mainly use this "extra period" for hands-on lab and coding sessions. Students will also use this "extra period" for meeting with the instructor about their presentations and problem sets, as well as for other enriched independent study, including reading, preparing presentations and working on problem sets and group reports.

8 Feedback

We want you to get the most out of this class.

Students are encouraged to offer feedback at any time about the course and our instruction to either of us in person, through e-mail to vasilii.petrenko@rochester.edu or lee.murray@rochester.edu, or via an anonymous note placed in either of our departmental mailboxes located in Hutchison Hall 227.

We note that this is the first time we are offering this course, so (despite our best efforts to make to run as smoothly as possible) there are bound to be glitches and imperfections. So your feedback is extremely important in helping us improve the course in the future.

At the end of the course, we would greatly appreciate if you fill out the course review.