Group Exercise (Tropospheric Ozone)
ATMO 469A/569A CHEE 569A
Air Pollution: Gases
Due Date (Dec 13, 2019 5pm)
Submit softcopy via D2l or email to me)
(100 points, 25% of final grade)

Project Description:

The overall goal of your term project is to enhance your understanding of tropospheric ozone chemistry. Here, you will use a state-of-the-art box model of ozone chemistry called BOXMOX (see BOXMOX related documents such as Boxmox_Download.pdf, Boxmox_Readme.pdf and BoxMox_Reference.pdf in D2L Project Section). You will use this model to: a) determine the main drivers of ozone concentration for a typical ambient planetary boundary conditions (Case 1), and urban plume environment (Case 2), and/or b) understand the photochemistry of an air sample in a chamber experiment (Case 3).

You are given one directory for each case. Each directory will contain csv files (e.g., use excel to read/edit these files) which are the inputs to BOXMOX. For this project, we will use one of the chemical mechanisms (i.e., set of reactions) used in current chemistry transport models (i.e., MOZART). Aside from csv input files, you also have BOXMOX.nml which you can view using any text editor. This namelist file includes starting (TSTART) and ending (TEND) time and time step (DT) of your simulation (you don't have to change or edit this file). View the README file for each case directory to get more information on the case study.

a) For each case, first transfer/save your csv and nml files to your local machine and to a directory you created for this project. This is your default configuration (see last page of this document for some notes on running BOXMOX)

b) Now, run BOXMOX by typing in the prompt ./MOZARTT1.exe and hitting enter:

   For example, if you are group 1:

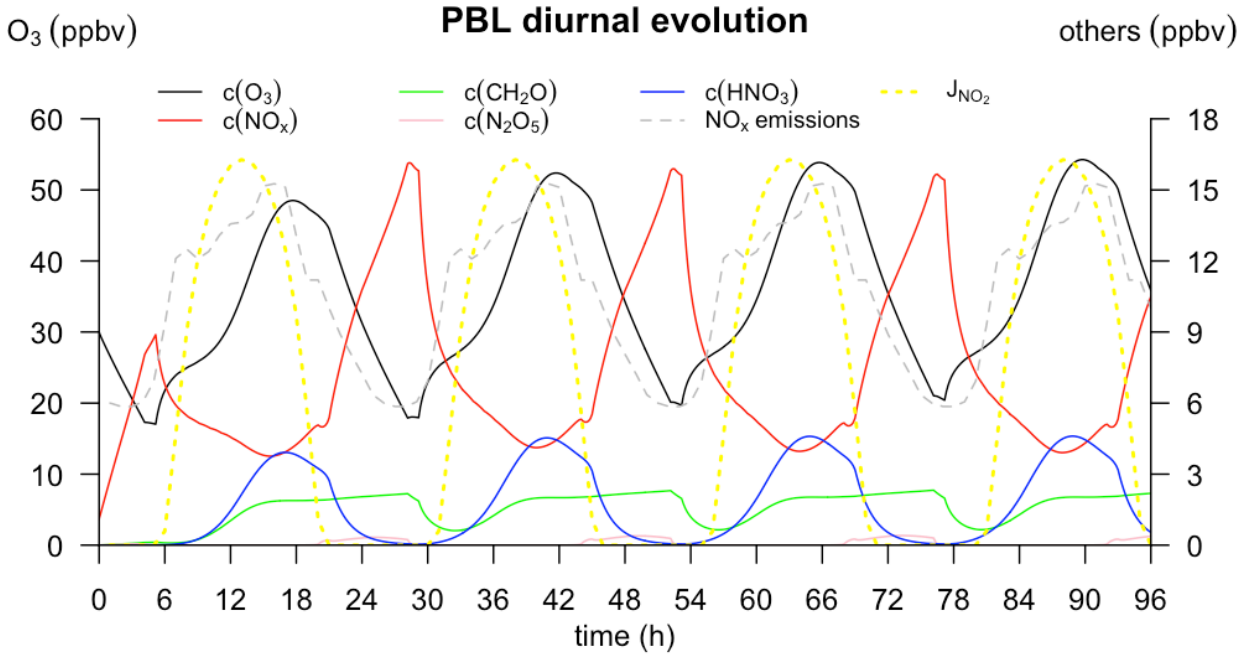
   [atmo569a_1@master case1]$ ./MOZARTT1.exe

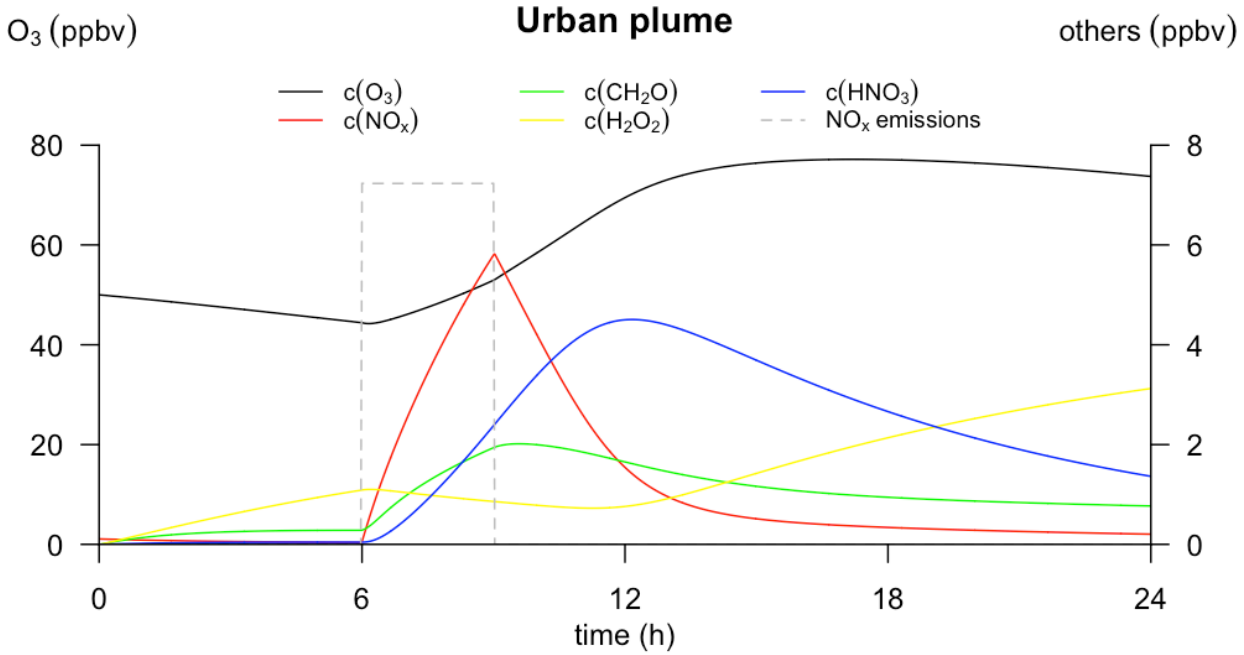
c) After running BOXMOX, you will have new dat files generated. These are the output files of BOXMOX. For this project, the output file you will use is MOZARTT1.dat. You can use excel to read this file (or any other editor you choose). This file contains several columns (corresponding to time and species) and rows (corresponding to the time stepping from TSTART to TEND).

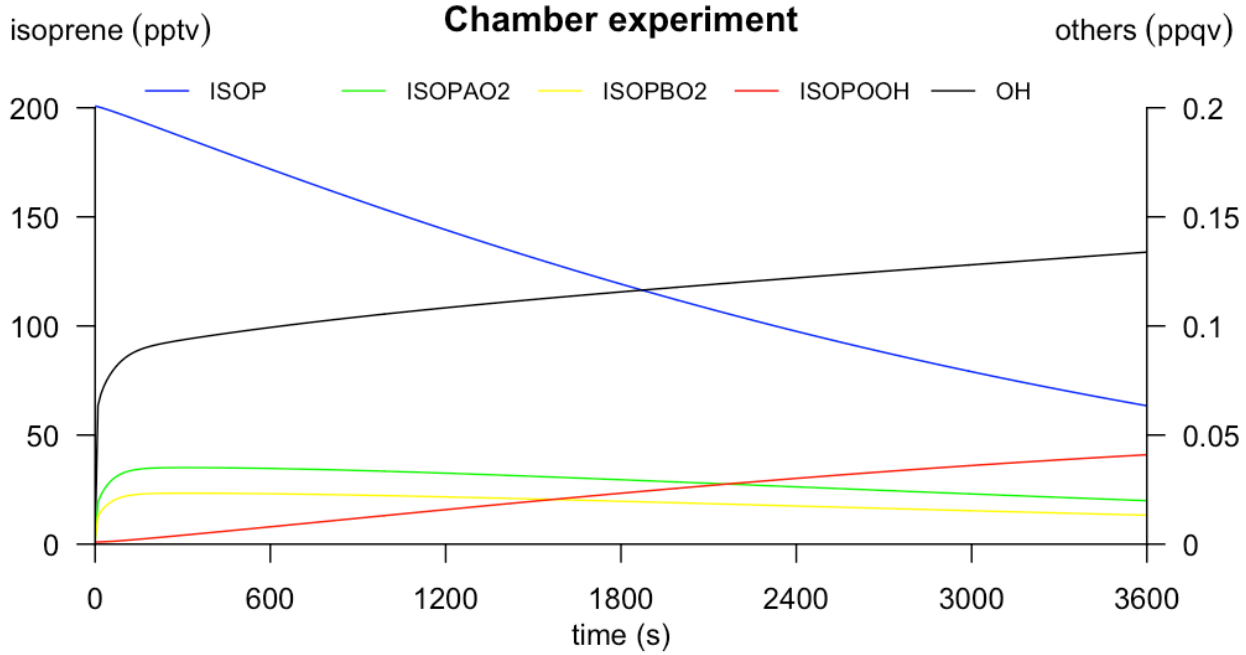
d) Transfer/save MOZARTT1.dat to your local machine and directory.

Question 1 (20 points) Plot specific species as a function of time. For example, you may reproduce the plots below for Case 1 (PBL_DIURNAL_CYCLE), Case 2 (URBAN_PLUME), and

Case 3 (CHAMBER_EXPERIMENT). You can use excel, matlab, R, or any software of your choice. Describe the evolution of ozone as a function of main precursors and oxidants.







Now that you have plotted the chemical evolution for each case, conduct the suggested experiments below. Make sure you have a different sub-directory for each experiment in your local machine so you will not overwrite the files of your default configuration (and the other experiments). Coordinate with your group members to make sure you are not running simultaneously with each other (otherwise, you will have different input files, etc). The best way to do this is to work as a group.

Case 1: (40 points)

a) Explore Emission.csv. See section 3 of BOXMOX_README.pdf for some description of this file. Briefly, this file (and the other csv files) constitute the representation of the components of the continuity equation we discussed in class.

b) Conduct a suite of sensitivity analysis for this csv file (at least 2 including the default) by decreasing/increasing by some percentage (e.g., 50%) some select variables in the csv file. For example, what is the impact on ozone concentration when CO and/or NOx (NO or NO2 or both) and/or ISOP and/or CH2O is increased or decreased? You are free to play around with the variables to answer the questions:

Question 2 (20 points): What are the main precursor emissions driving the changes in ozone? How does ozone change? You do not have to explore ALL variables in each csv file. Pick familiar variables we used in class. Explain your answers by showing plots of your analysis and a brief description of your results. You do not have to plot ALL variables. Are you in VOC-limited or NOx limited regime? Briefly explain.

c) Now, go to PIMA DEQ website (http://envista.pima.gov/) check the current values of ozone and precursors and environmental variables (temperature, etc) in Childrens Park

AQ site. Edit InitialConditions.csv and Environment.csv to reflect the values for this site. Run BOXMOX and Plot the evolution of ozone.

Question 3 (20 points): Determine if you can reproduce the ozone evolution in Childrens Park. Why or why not? Briefly explain.

Choose between Case 2 and Case 3:

Case 2: (20 points)

d) Similar to Case 1, explore the csv file: Emissions.csv, InitialConditions.csv, Environment.csv, and/or PhotolysisRates.csv. See section 3 of BOXMOX_README.pdf for some description of these files.

e) Conduct a suite of sensitivity analysis for each csv file by decreasing/increasing by some percentage (e.g., 50%) of select variables in the csv file you choose to study. For example, what is the impact on ozone concentration in the urban plume when initial condition of CO and/or O3 and/or NOX is increased or decreased?

Question 4 (20 points): What are the main precursors driving the changes in ozone? How does ozone change? You do not have to explore ALL variables in each csv file. Pick familiar variables we used in class. Explain your answers by showing plots of your analysis and a brief description of your results. You do not have to plot ALL variables.

Case 3: (20 points)

f) Similar to Cases 1 and 2, explore the csv files: InitialConditions.csv, Environment.csv, and/or PhotolysisRates.csv. See section 3 of BOXMOX_README.pdf for some description of these files.

g) Conduct a suite of sensitivity analysis for each csv file by decreasing/increasing by some percentage (e.g., 50%) of select variables in the csv file. For example, what is the impact on OH and O3 when photolysis rates of NO2 and/or CH2O and/or H2O2 is increased or decreased?

Question 4 (20 points): What are the main photolysis driving the changes in OH? How does OH change? Explain your answers by showing plots of your analysis and a brief description of your results. You do not have to explore ALL variables in each csv file. Pick familiar variables we used in class.

Practical Application. Imagine you are a consultant for Tucson Electric Power (TEP). The electric company is interested to know the following:

a) **Question 5 (10 points).** How will ozone change in Tucson in a warmer world (under global warming conditions in the future)? Assume reasonable values of warmer temperature. Use BOXMOX (Case 1) to answer this question.

b) **Question 6 (10 points).** TEP is also shifting from coal to natural gas in the near future. This means less CO2 but potentially more CH4 and VOCs and slightly higher NOx. Using your Case 1 Childrens Park conditions in BOXMOX, what would be the impact of this shift in this fuel mixture to ozone in Tucson. Again, assume some reasonable values of CH4, Ethane (representing VOCs) and NOX emissions.

Notes on Running BOXMOX:

You will run BOXMOX (i.e., MOZARTT1.exe) in a Linux machine (stratus.has.arizona.edu). Each group will have an account to remotely access the machine.

Group 1: Joe, Genie, and Emmanuel:
(Username) atmo569a_1 (Password) air_pol1
Group 2: Xiaojian, Adriana, and Lindsey
(Username) atmo569a_2 (Password) air_pol2
Group 3: Kellie, Sunyi, Eva-Lou, Brenna
(Username) atmo569a_3 (Password) air_pol3

You need to have three software applications:

1) Ability to remotely login to stratus and run MOZARTT1.exe (e.g., SSH, Putty)
2) Ability to transfer files from your local machine to stratus and vice versa
3) Ability to open/edit/save csv and dat files and plot several time series (e.g., excel, matlab, R)

SSH to stratus: Using Putty e.g.,

For Group 1:

$ ssh atmo569a_1@stratus.has.arizona.edu
atmo569a_1@stratus.has.arizona.edu's password: air_pol1

[atmo569a-1@master ~]$

typing 'ls' and hitting enter will show

[atmo569a_3@master ~]$ ls

BoxMox_Download.pdf BoxMox_Readme.pdf BoxMox_Reference.pdf Cases dat_files

These are the files (and subdirectories) in this main directory.

Type 'cd Cases' and then type 'ls'.

case1 case2 case3 exp0 src

These are the subdirectories in this Cases directory.

For your experiments (case 1, case 2 and case 3), go to the specific directory:

e.g.,

type 'cd case1' to go to case1 directory (i.e.,

[atmo569a_1@master Cases]$ cd case1

Now, see the contents of this directory by typing 'ls' and hitting enter. You'll see:

BOXMOX.nml Environment.csv MOZARTT1.exe MOZARTT1_rates.dat plot.R
Deposition.csv InitialConditions.csv MOZARTT1_hessian.dat pbl_diurnal_cycle.png README
Emissions.csv MOZARTT1.dat MOZARTT1_jacobian.dat PhotolysisRates.csv Xtrainment.csv

If you're ready, run BOXMOX by:

typing './MOZARTT1.exe' and hitting enter (i.e.,

[atmo569a_1@master case1]$ ./MOZARTT1.exe

wait until diagnostics are done printing (i.e. until

BOXMOX successfully completed.

[atmo569a_1@master case1]$

is displayed in your terminal. Check if you have new dat files by

[atmo569a_1@master case1]$ ls –alt

this will print all information for each file sorted from most recent file to oldest file modified/created. You should see MOZARTT1.dat as the first file listed with date and time corresponding to the most recent time you invoke MOZARTT1.exe.

SFTP from or to stratus: Using WinSCP, you can have a GUI to easily transfer files. All you need to do is type the remote machine's address: stratus.has.arizona.edu, your username, and password. Once you're logged in, you can drag files from or to stratus. Make sure you create a dedicated directory in your local machine prior to transferring files.

If you choose to use the terminal (linux commands):

Open two terminals:
On the first terminal, ssh to stratus and go to the desired case experiment directory (see SSH steps above).

In the second terminal, go to your local directory where your case experiment is located:

For Mac:

a) To transfer files from stratus to your local machine:
[~]$ cd /Users/afarellano/Documents/Teaching/ATMO_569A/Projects/Cases/case1/exp0
this is the directory I used for my experiment 0 (default run).

[~]$ scp atmo569a_1@stratus.has.arizona.edu:/st8/atmo569a_1/Cases/case1/*.* .

it will ask for your password (type your password and hit enter) and then this will transfer all files having extensions (e.g., *.csv, *.nml, *.dat).

b) to transfer csv files to stratus from your local machine (assuming you are in exp0 for example):

scp *.csv atmo569a_1@stratus.has.arizona.edu:/st8/atmo569a_1/Cases/case1/

it will ask for your password (type your password and hit enter) and then this will transfer all files having extensions csv to stratus in case 1 directory. Note that this will replace your csv files in that directory.

WHEN USING WINSCP OR LINUX COMMANDS, MAKE SURE YOU SAVE/ARCHIVE EACH CSV AND DAT FILE TO A SEPARATE EXPERIMENT DIRECTORY.

Before doing another experiment, make sure that the csv file is the updated file and make a separate directory for each of your experiment or sensitivity tests.