ATMS/CHEM 458 Atmospheric Chemistry Data Set Analysis

Cornelia Fort, Nashville, TN Southern Oxidants Study

Preliminary Instructions and Definitions

1. Download the matlab file (sos99_data_subset.mat or sos99_data_subset.xls) from the course website. Let me know if you have any trouble.

2. Check that the following variables are present in the workspace (e.g. by typing: **who** in Matlab).

sos_time: running time vector in units of day-of-year, fractional day
sos_tod: time of day vector (midnight-to-midnight)

airT : outside air temperature in Kelvin

j_no2: j-value for NO_2 photolysis to $NO + O$
j_o3:j-value for O_3 photolysis to $O(^1D) + O_2$
j_h2co: j-value for Formaldehyde photolysis to $H+HCO$

oh_ppt: OH mixing ratio

no_ppb: NO mixing ratio
no2_ppb: NO_2 mixing ratio measured by Laser-Induced Fluorescence

h2co_ppb: Formaldehyde mixing ratio
o3_ppb: Ozone mixing ratio

General TIPS

1) **Be careful about using the word "*noisy*"**, or not analyzing a plot fully because there is a lot of scatter. Your eye is very good at discerning trends and averages. There is a big difference between real atmospheric variance and instrumental precision. Just because a measurement shows lots of ups and downs doesn't mean the measurements are imprecise. In fact, what usually looks like "noise" in measurements is actually interesting variations in the atmosphere from which we can learn about the chemistry.

2) **UNITS UNITS UNITS UNITS UNITS UNITS UNITS UNITS UNITS UNITS. If they aren't right, you'll have a hard time interpreting the data. Always check your units by hand before you type the calculation into matlab and make plots. Also double check that the values you are plotting actually make sense! E.g. is it really possible that $P_{O3} = 1 \times 10^{26}$ molec cm^{-3} s^{-1}??**

3) **Zooming in on sections of a plot** can be very helpful, as can using the "grid" feature in matlab for estimating averages and trends. If the data looks like a flat line near zero with a few points having very large values, you should zoom in on the flat looking part.

4) You might encounter **divide by zero warnings**, don't worry, just plot the vector and realize that it might be blowing up to infinity and that you'll have to zoom in on the region of interest.

5) Rate constants, or expressions for their calculation, can be found in many places. Textbooks such as Seinfeld and Pandis, Finlayson-Pitts and Pitts, etc (some of which are on reserve), and databases such as the IUPAC kinetics database online at **http://www.iupac-kinetic.ch.cam.ac.uk/** and the JPL (NASA) handbook also available online at **http://jpldataeval.jpl.nasa.gov/** are all good places to look.