Carnegie Mellon ENGINEERING

06-100: Introduction to Chemical Engineering

Climate and CO_2 - Part II

September 25th, 2013

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Announcements

- Office Hours today
  - 2:30 pm – 4:00 pm
  - Cyert Hall B6A
- Friday Lecture (09/27)
  - **Homework 4** and **Recitation 3** due: **beginning** of class
  - Majors Information Session for Engineering Intro Courses
- Recitation 3 help material on Blackboard
  - Help slides + Additional information on part (d)
- Scott Institute for Energy Innovation
  - http://www.cmu.edu/energy/
  - Energy Experts → By Topic Area

Outline

- Quantitative Analysis
  - Concentrations and fractions (emphasis on air)
  - Ideal gas
- Basic Calculations
  - Molecular weight of dry air
  - Mass of C corresponding to 1 ppm of CO_2 in the atmosphere (homework)
- Software Workshop
  - Reading and graphing pollution data in MATLAB
  - Plot CO_2 emissions in Mauna Loa (homework)

Concentrations and Fractions

- Mass- or mole-based concentrations

$\frac{\mu g}{m^3}$	$\frac{\text{mass of species}}{\text{volume of air}}$
$\frac{\text{mol}}{m^3}$	$\frac{\text{mole of species}}{\text{volume of air}}$

- In air, fractions are usually expressed on a *molar* or *volume* basis (equivalent for ideal gases)

%	1 part species per 100 parts solution
ppm	1 part species per 10^6 parts solution

also ppmv (on a volume basis), ppb, ppt…

Example: 5 ppb of benzene in air means there are 5×10^{-9} moles of benzene in 1 mole of air

Ideal Gas Law

- First of all, an “ideal gas” does not exist!
- Simple model of *P*-*V*-*T* relations of a gas
  - Works well at low *P* and high *T*
  - Neglects molecular size and intermolecular interactions
- In almost every case in environmental engineering, air can be treated as an ideal gas

$$PV = nRT$$

or

$$P\hat{V} = RT$$

where $\hat{V} = \dfrac{V}{n}$ is the specific molar volume

Ideal Gas Mixtures

- Ideal gas law for species *i*

$$p_i V = n_i R T$$

- Partial pressure and molar fraction

$$p_i = \frac{n_i}{n} P = y_i P$$

- Average molecular weight of *any* mixture with *C* components

$$\overline{MW} = y_1 MW_1 + y_2 MW_2 + \ldots + y_C MW_C = \sum_{i=1}^{C} y_i MW_i$$

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Exercise: MW of Dry Air

- Given the composition of air, calculate its molecular weight

Species	MW [g mol^{-1}]	Percent
Nitrogen (N_2)	28	78.08
Oxygen (O_2)	32	20.95
Argon (Ar)	40	0.93
Carbon Dioxide (CO_2)	44	0.035

Answer:

$$\overline{MW}_{\mathrm{air}} = y_{\mathrm{N_2}} MW_{\mathrm{N_2}} + y_{\mathrm{O_2}} MW_{\mathrm{O_2}} + y_{\mathrm{Ar}} MW_{\mathrm{Ar}} + y_{\mathrm{CO_2}} MW_{\mathrm{CO_2}}$$

$$\overline{MW}_{\mathrm{air}} = [(0.7808)(28) + (0.2095)(32) + (0.0093)(40) + (0.00035)(44)]\,\mathrm{g\ mol^{-1}}$$

$$\boxed{\overline{MW}_{\mathrm{air}} = 28.95\,\mathrm{g\ mol^{-1}} \approx 29\,\mathrm{g\ mol^{-1}}}$$

Homework: Problem 1

- Calculate the mass of C that corresponds to 1 ppm of CO_2 in the atmosphere

Answer: 2.2 Gt (giga tons) = 2.2×10^9 t = 2.2×10^{12} kg

- Hints:
  - Estimate mass or moles of the atmosphere
  - Calculate 1 ppm (amount of CO_2) from the answer above
  - Calculate mass of C (how many moles of C are in one mole of CO_2?)
- You may find useful to know
  - Mean radius of the earth: R = 6370 km
  - Pressure at the surface: $P = 1.01325 \times 10^5$ Pa = 1.01325×10^5 N m^{-2}

CO_2 Levels in MLO: Text Data

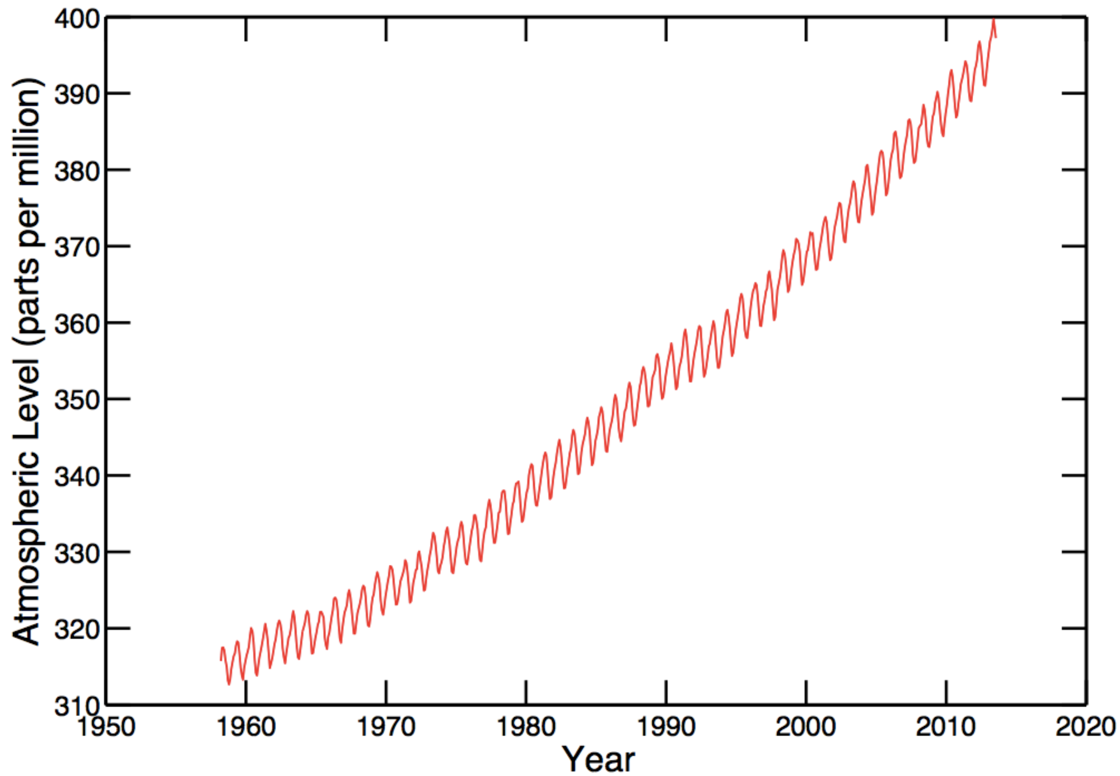
- Yearly CO_2 measurements in Mauna Loa (volcano in Hawai'i)
  - Text file by the Earth System Research Laboratory (ESRL) at the National Oceanic & Atmospheric Administration (NOAA) (http://www.esrl.noaa.gov/)

```
# NOTE: In general, the data presented for the last year are subject to change,
# depending on recalibration of the reference gas mixtures used, and other quality
# control procedures. Occasionally, earlier years may also be changed for the same
# reasons.  Usually these changes are minor.
#
# CO2 expressed as a mole fraction in dry air, micromol/mol, abbreviated as ppm
#
#  (-99.99 missing data;  -1 no data for #daily means in month)
#
#            decimal     average   interpolated    trend    #days
#             date                             (season corr)
1958   3    1958.208      315.71      315.71      314.62     -1
1958   4    1958.292      317.45      317.45      315.29     -1
1958   5    1958.375      317.50      317.50      314.71     -1
1958   6    1958.458      -99.99      317.10      314.85     -1
1958   7    1958.542      315.86      315.86      314.98     -1
1958   8    1958.625      314.93      314.93      315.94     -1
1958   9    1958.708      313.20      313.20      315.91     -1
1958  10    1958.792      -99.99      312.66      315.61     -1
1958  11    1958.875      313.33      313.33      315.31     -1
1958  12    1958.958      314.67      314.67      315.61     -1
1959   1    1959.042      315.62      315.62      315.70     -1
```

  - Let's plot the data to detect trends…

CO_2 Levels in MLO: Graph

- Yearly CO_2 measurements in Mauna Loa (volcano in Hawai'i)
  - Text file by the Earth System Research Laboratory (ESRL) at the National Oceanic & Atmospheric Administration (NOAA) (http://www.esrl.noaa.gov/)



Scatter Plots in MATLAB

```
>> x = [2008 2009 2010 2011 2012 2013]
>> y = [310 350 370 400 410 440]
>> scatter(x, y)
```

or

```
>> scatter(x, y, 'fill')
```

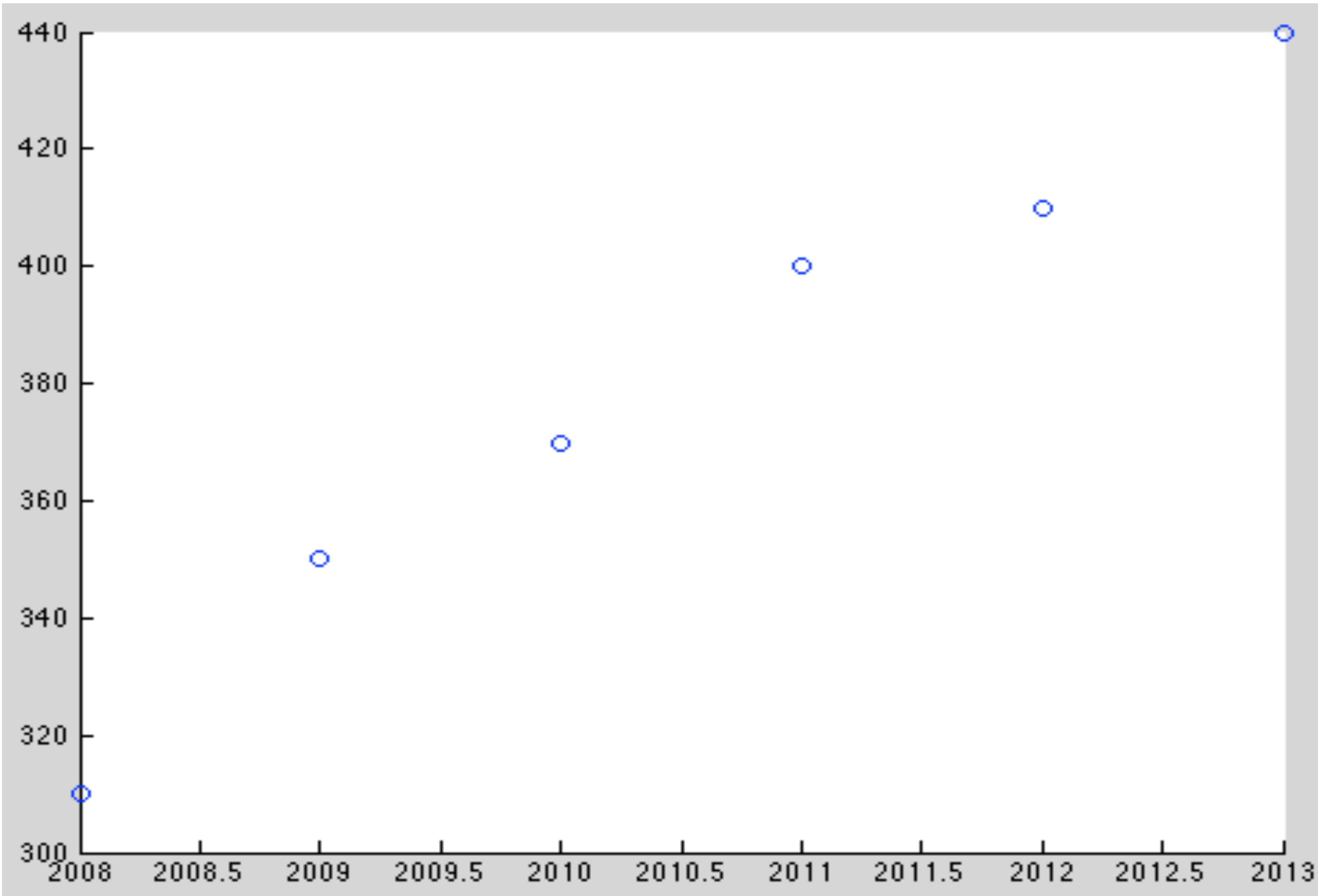
or

```
>> scatter(x, y, markertype)
```

where *markertype* can be `'o'`, `'+'`, `'*'`, `'d'` etc.

- Plot data measurements as scatter points
- Plot functions (models) as lines

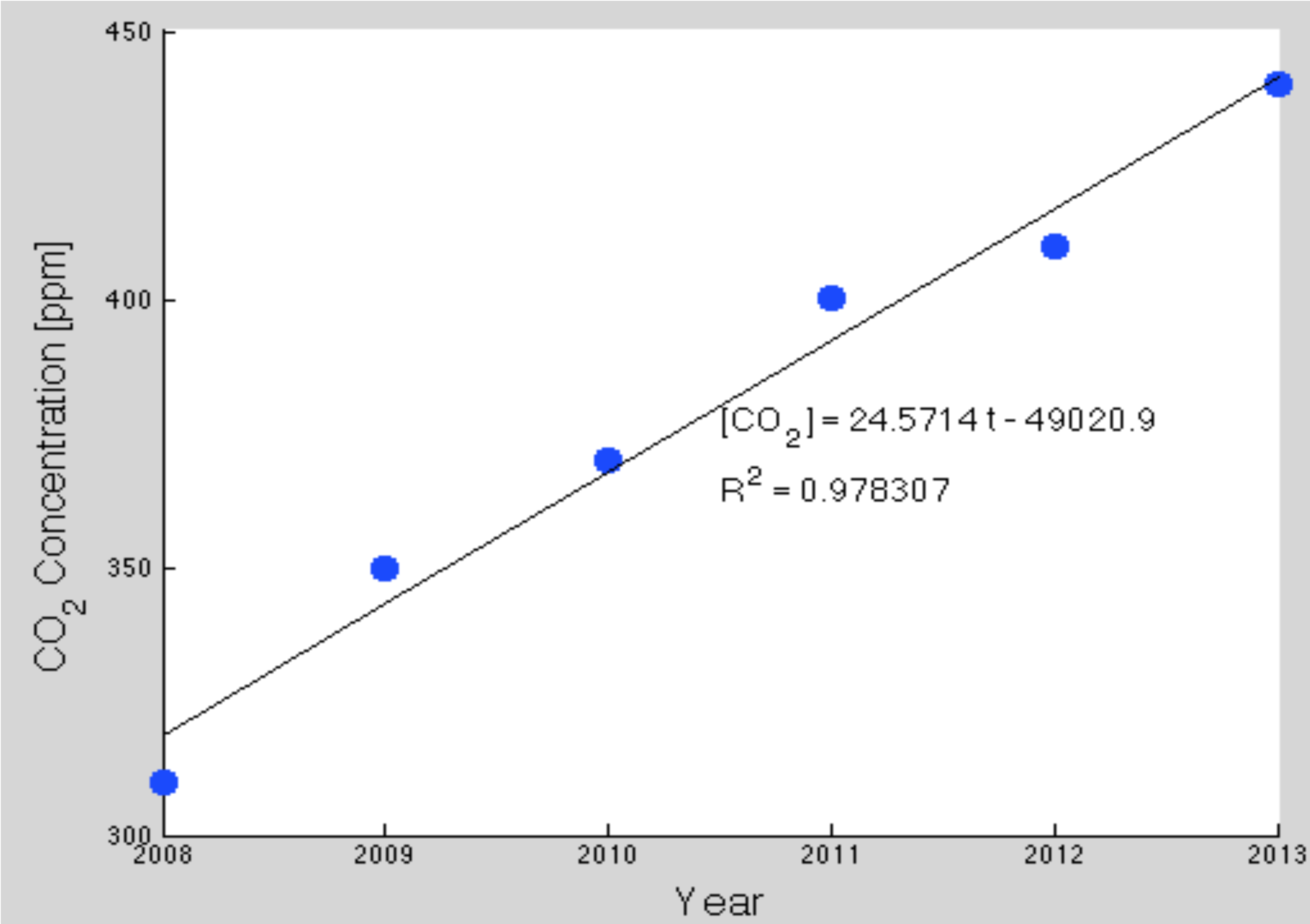
Scatter Plots in MATLAB



Some Few Improvements…

```
% Data
x = [2008 2009 2010 2011 2012 2013];
y = [310 350 370 400 410 440];

% Fit 1st degree polynomial (straight line) through the data (trendline)
p = polyfit(x,y,1); % p = p(1)*t + p(2)

% Obtain R^2 value (Coefficient of Determination)
rsq = rsquared(x,y,p);

% We will plot two sets of data on the same figure, so use hold on/off for every plot statement or hold all/off
hold all

% Plot data as scatter points
markersize = 100;
scatter(x,y,markersize,'fill')

% Plot trendline in black
plot(x,polyval(p,x),'k')

% Display trendline equation and R^2
xmiddle = mean(x);
ymiddle = mean(y);
% Note that p(2) is negative, so to make it pretty I add the negative sign
% in the string and display the absolute value of p(2)
text(xmiddle,ymiddle - 5,sprintf('[CO_2] = %g t - %g',p(1),abs(p(2))),'FontSize',14)
text(xmiddle,ymiddle - 15,sprintf('R^2 = %g',rsq),'FontSize',14)

% Change labels
xlabel('Year','FontSize',16)
ylabel('CO_2 Concentration [ppm]','FontSize',16)

% Change tick marks on x-axis
set(gca,'XTick',x)
```

Some Few Improvements…



Read Data from Text File

- Use MATLAB's function `dlmread`

```
M = dlmread(filename)
```

- `M` is a matrix with as many rows and columns there are in the text file whose name is `filename`
- Example: File "data.txt"

```
2000   10
2050   20
2100   30
```

- Read data into variable called `X`

```
X = dlmread('data.txt')
```

Homework: Problem 2

- Given a text file ("CO2_MLO_data.txt" from NOAA ESRL) containing annually mean CO_2 concentration measurements (ppm) in Mauna Loa (MLO), plot and fit a 2^{nd} degree polynomial to the data. Display the polynomial equation and the R^2 in the figure.

- Hints
  - You will have to ask `polyfit` to center and scale the *x* values, or MATLAB will issue a warning message
  - After centering and scaling, the polynomial coefficients are obtained with respect to the centered and scaled *x* values and not the original ones. So whenever you have to use the coefficients, make sure to use the centered and scaled *x* values.

Air Quality at CMU

- Center for Atmospheric Particle Studies (CAPS)
  – http://caps.web.cmu.edu/members/index.html
  – ChemE faculty
    - Prof. Neil Donahue (Chem)
    - Prof. Spyros Pandis (EPP)
    - Prof. Peter Adams (CivE, EPP)
  – Other faculty members
    - Prof. Allen Robinson (MechE, EPP)
    - Prof. Ryan Sullivan (Chem, MechE)
    - Prof. Albert Presto (MechE)
- Prof. Kris Dahl and I are very grateful for the ideas, materials and guidance from Prof. Neil Donahue in implementing the *Climate Change Module* in 06-100 (Introduction to Chemical Engineering).