

# *Air PSE (Problem Solving Environment)*

## **MODELLING OF AIR POLLUTION IN THE LOS ANGELES BASIN WITH AIR PSE**

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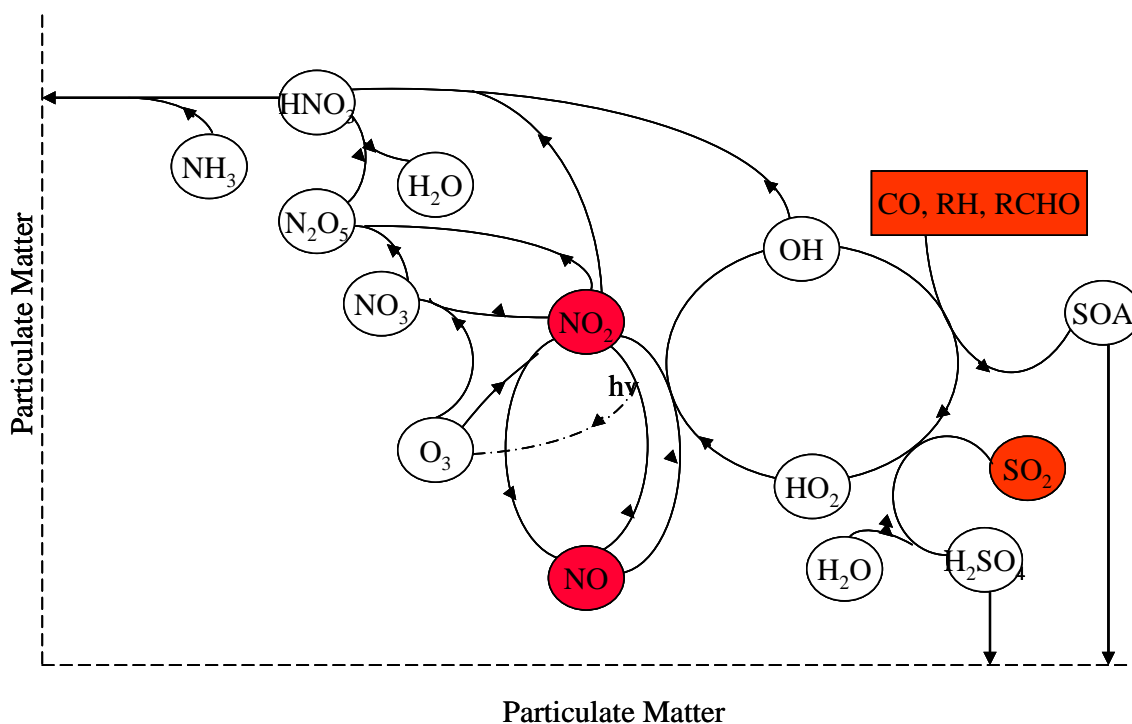
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## THE BASICS OF ATMOSPHERIC COMPUTER MODELS

An air pollution model is a computer program that computes how the different chemical species in the atmosphere move and mix, and how they react with one another. The results from these computations produce a simulation to what is happening in the real world. The model creates a virtual world where virtual experiments can be performed. This is important since there are many experiments that cannot be performed in the real world. For example, the model can compute answers to questions like “what if factories put out half as much carbon monoxide”, or “what if car traffic is reduced by one-third”. Using the model results from these experiments, policy makers can determine the effect of reducing industry emissions or decreasing car use. An air pollution model is never exact in its attempt to simulate the atmosphere, but a well-designed air pollution model provides an approximation to the real atmosphere that is accurate enough to be very useful.

There are many components that affect air pollution. Winds, temperature, anthropogenic and biogenic emissions, and amount of sunlight are a few of these components. The model takes these components from measurements and observations as the input parameters and calculates the concentration of the species of interest in the simulated atmosphere. To take all the needed measurements for the Air PSE is a big job, so these measurements are only available for a relatively small number of days.

## THE BASICS OF ATMOSPHERIC CHEMISTRY



Formation of ozone involves complex processes and chemical reactions. Ozone precursors are Volatile Organic Compounds (VOC) and Nitrogen Oxides (NO<sub>x</sub> = NO + NO<sub>2</sub>).

Formation of ozone is driven by solar radiation, and hence, peak ozone concentration occurs during the day. Higher temperatures also favor ozone formation. As a result, the highest ozone concentrations occur typically during the summer.

The chemical mechanisms associated with ozone production are so complex that emission reductions of ozone precursors may not necessarily decrease the ozone production rate, depending on the area where these reductions are applied. We'll see some examples of it later.

## ***FACTORS THAT AFFECT POLLUTANT CONCENTRATIONS***

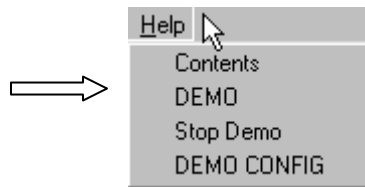
- **Initial conditions:** initial values for concentration of all species are needed to start the calculations.
- **Boundary conditions:** concentrations of species at the boundaries of the modeling domain are needed to account for influx of pollutants from outside the basin.
- **Wind field:** wind velocity profiles are needed to determine the transport of pollutants from one region to another. In the Los Angeles area, prevailing winds transport pollution from Los Angeles to inland locations. The San Bernardino Mountains located in the northern and eastern part of the basin act as a trap for pollutants.
- **Diffusion:** the magnitude of diffusion forces, driven solely by the difference in concentrations, is needed for the transfer of pollutants from areas of high to low concentrations. In the horizontal direction, transportation by wind (advection) is significantly more important than diffusion.
- **Deposition:** deposition is needed to determine the rate of removal of pollutants from the atmosphere through pollutant uptake by surfaces. Deposition velocity depends on the nature of each species.
- **Emissions:** pollutants directly emitted into the atmosphere (primary pollutants, e.g. NO) are needed to calculate the concentration of secondary pollutants formed as products of chemical reactions involving primary pollutants (e.g. O<sub>3</sub>, PAN, etc.).
- **Temperature:** temperature is needed because reaction rates are strongly dependent on it. Hence, reactions that produce and destroy ozone are affected by temperature changes. As a result, temperature affects ozone concentration.
- **Humidity:** humidity is needed since there are species that react with or dissolve into water, so water acts as a sink for these species. However, water can also be a source for other species, such as the OH radical, which is the most important atmospheric oxidant during daytime.
- **Ultra Violet (UV) radiation:** UV radiation drives the photochemical reactions that lead to the formation of ozone. Consequently, ozone concentration peaks during the day.

# GETTING STARTED

## USING THE DEMO

The following description of the DEMO gives an instructive overview geared for new users.

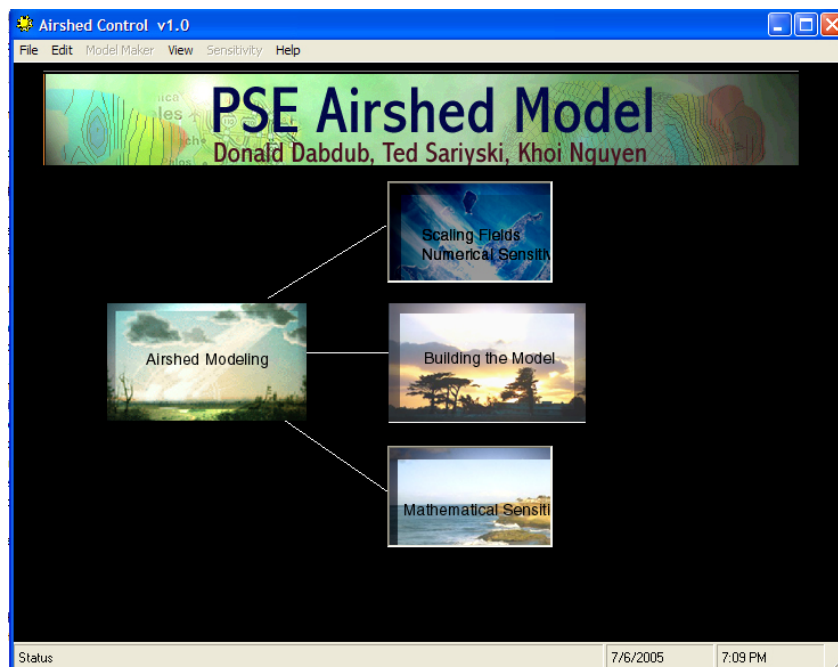
After reading “the basics of atmospheric computer models”, you are ready to start using Air PSE. The best way for a new user to be introduced to the PSE Air is to watch the demo. Access the DEMO by selecting *Help* on the menu bar, and then clicking on *DEMO*.



The DEMO describes the three major steps involved in a model run.

1. Create a new command file that contains the information about the changes made to the model from the default values.
2. Run the model with the new command file.
3. View the results of the model run.

The following is a description of the steps that are performed by the DEMO. (After viewing the DEMO once or twice, it is recommended that the user replicate the steps without the DEMO).



## DEMONSTRATIONS

### INITIAL STEP

A – Select the *Scaling Fields/Numerical Sensitivity* box (this allows access to the menu headers needed to do a model run).

### CREATE A NEW COMMAND FILE:

B – Under *File* on the menu bar, select *New*. Note that nothing visual happens here (the file will be saved later).

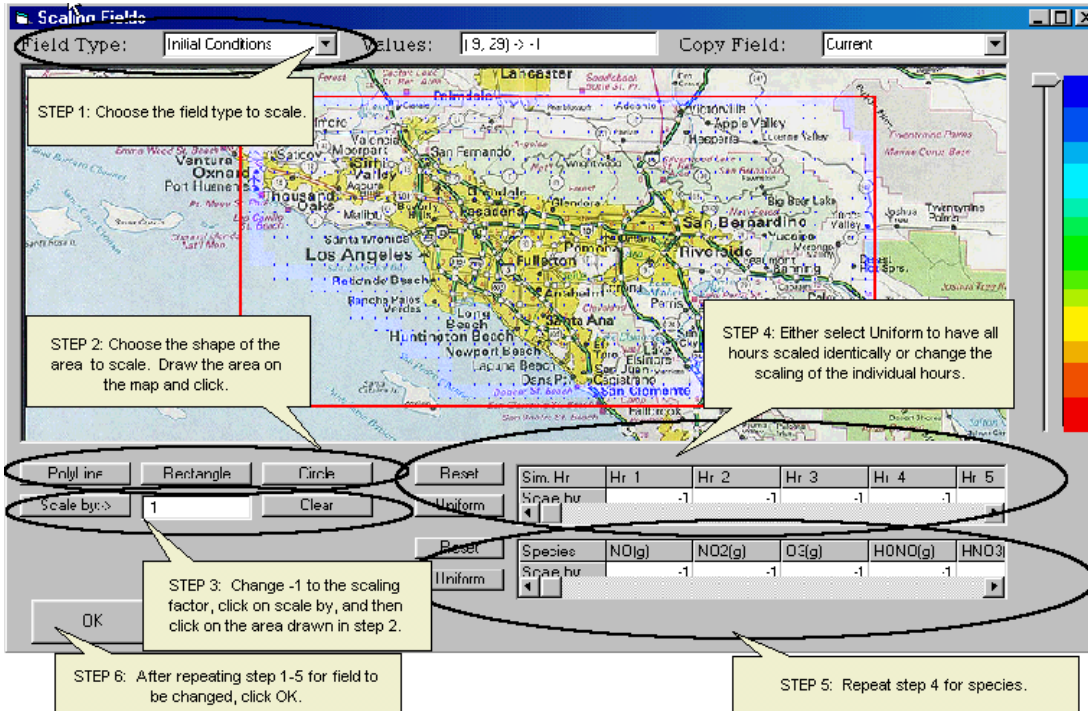
C – Under *Edit* on the menu bar, select *Choose Operators*. The DEMO will turn off Aerosol Dynamics since it is very time consuming to compute.

D – Under *Edit* on the menu bar, select *Scaling Fields*. This is where the majority of changes to the model inputs are made. Each input change requires five steps. The order of these steps is important!

1. Choose the *Field Type* to be changed. A description of the field types is given in the “Explanation of Terms” section of this manual.
2. Choose a region where the field will be modified. This can be done in two ways. First, a new area can be defined by clicking on *PolyLine*, *Rectangle*, or *Circle*. *PolyLine* defines an irregular polygon by its vertices, *Rectangle* defines the region by its diagonal corners, and *Circle* defines the region by its center and perimeter. After the shape is drawn, click on the area and a red line will outline the area. Alternatively, *Copy Field* will define a region that has been used in the modification of another field.
3. Enter the factor the field is to be scaled by (e.g. enter 5 to have all values of the field increased by a factor of 5). Then, click on *Scale by*, followed by a click on the region defined in step 2. Hash marks should appear inside the region.
4. Choose the hours in which the field will be scaled. To have all hours scaled by the scale factor from step 3, click on *Uniform*. This will change the hourly scale factor to “1” for every hour. If only some hours are to be scaled, enter the scale factor individually for each hour.
5. If desired, choose the species that will be scaled. This works identically to the hour selection in step 4. A description of all the species is given in the “Chemical Species” section of this manual.

*NOTE: The final scale by value takes the primary scale by value in step 3, multiplies it by the hour scale by value in step 4 and the species scale by value in step 5.*

These 5 steps are repeated for each field that is to be scaled. Again, the order is important. The scale by value for each of the modified fields can be double-checked by hovering the mouse over the regions of interest, and the number in the *values* box should change accordingly.



When all desired fields have been scaled, click on *OK*.

E – Under *File* on the menu bar, select *Save* and save your command file.

### **RUN THE MODEL USING THE NEW COMMAND FILE**

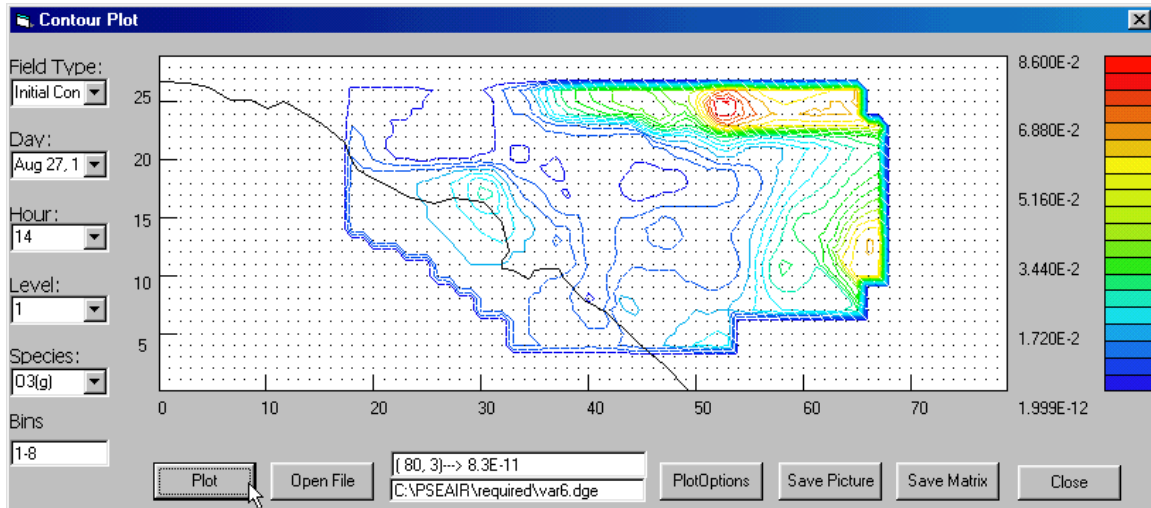
F – Under *File* on the menu bar, select *Execute Gas* (this could take a while).

### **VIEW THE RESULTS**

G – Under *View* on the menu bar, select *Contour*.

1. Click on *Open File* and choose the file that has the same prefix as the model run to be investigated.
2. Choose *Output Concentrations* under *Field Type*.
3. Choose the *Hour* (from a 24-hour clock) and *Level* to be plotted.  
(Note: there is only one option for the *Day*.)

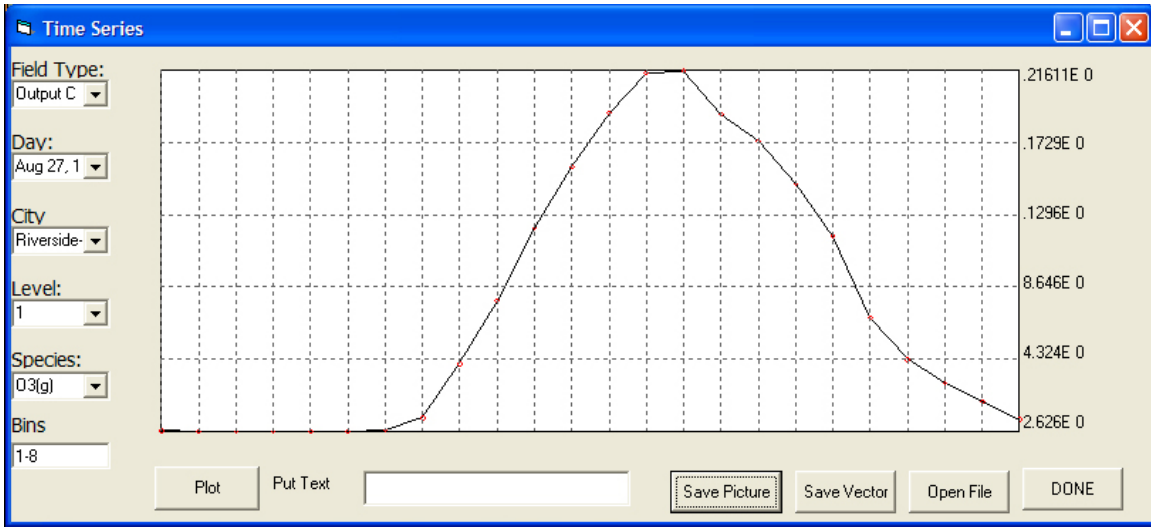
4. Choose the *Species* to be plotted. (A full list of species is given under “Chemical Species” section of this manual).
5. If you wish to see the locations of cities on the plot, click on *PlotOptions* and select the cities.
6. Click on *Plot*.



Fields from the base case can also be plotted, including emissions, temperature and initial conditions. This can be done by selecting a field other than output concentrations from the fields. Opening a file is not necessary to view these fields.

H – Under *View* on the menu bar, select *Time Series*.

1. Click on *Open File* and choose the file that has the same prefix as the model run to be investigated.
2. Choose *Output Concentrations* under *Field Type*.
3. Choose the *City* and *Level* to be plotted.  
(Note: there is only one option for the *Day*.)
4. Choose the *Species* to be plotted. (A full list of species is given under “Chemical Species” section of this manual).
5. Click on *Plot*.



The plotting provided in the Air PSE is intended for a quick viewing of results. For more advanced viewing the *Save Matrix* or *Save Vector* buttons will save your results to a file that can be accessed by a plotting program.





- 2) **What happens on a really hot day?** Let's examine the effects of changing the temperature profile of the domain.

Procedures:

1. Create a new file.
2. Turn off *Aerosol Dynamics*.
3. Under *Edit* on the menu bar, select *Scaling Fields*. Under *Field Type*, select *Temperature*. Increase the temperature field by a factor of 2 over the entire domain.
4. Save the file as *hightemp*.
5. Run the "gas" model.
6. View the output for ozone on *Level 1* for *Hour 16*.

Questions:

- What is the maximum ozone concentration? Where?
  - How are the ozone concentration contours different from the base case?
- 3) **A completely clean day.** Suppose a miracle happens and the air is completely clean. Set all the initial concentrations to zero and run the model. Look at the ozone concentration contours for this "clean" day.
- What is the maximum ozone concentration? When does this occur? Where is this peak located?
  - How does this compare to the base case? Is it what you would have expected?

**4A) Holiday.** Try to model a busy holiday.

- What input fields would you expect to change on a busy holiday?
  
- How would you estimate and implement these changes in the named input fields?

Put these changes into the model and run a “holiday” case. Look at ozone concentration through the day

- What is the maximum ozone concentration? At what hour does this occur? Where is this peak located?
  
- How does the holiday case compare to the base case?

**4B) Cloudy Day.** Try to replicate a cloudy day

- What model input parameters will be affected by a cloudy day?
  
- How would you estimate and implement the change in these parameters?
  
- Which parameter would you expect to have the biggest effect on max ozone concentration? Why?

Run a model case with for each parameter you think will vary, changing only that one parameter for that model run. Then run a model case with all the parameters changed included. Examine the ozone concentration contours for all model runs.

- Which individual parameter had the biggest effect on ozone concentration? How does this vary geographically?
  
- Did the model with all the changes do what you would expect from looking at the models with the individual changes? Explain.

**5) Save the planet!** If you were in charge of making a policy to decrease (max) ozone concentration, but could only vary 1 input field, which one would it be? You may scale any input field by  $\frac{1}{2}$  or 2. Look at the chemical mechanism and try to consider all the factors that affect air pollution presented above (Prelab pages 2-3).

- How did the maximum ozone concentration change? Try to explain the change.

# THE DETAILS

## LISTING OF OPERATIONS

The following is a listing of all the operations that can be performed within the PSE Air.

### File

- **New**  
-Opens a new command file. (You don't see anything here)
- **Open**  
-Opens an existing command file.
- **Save**  
-Saves a command file under the name given by the user.
- **Execute Air Model**  
-Executes the model with aerosols?
- **Execute Gas Model**  
-Executes the model.
- **Exit**  
-Exit the program.

### Edit

- **Scale Fields:**  
Field Type: Choose the field type to be modified.  
Values: States the field value at the current location of the cursor.  
Copy Field: Allows the modification area for one field to be copied to another field.  
Poly Line / Rectangle / Circle: Three types of modification areas that can be drawn.  
Scale by: This is the primary scale by field.  
Hours:  
    Reset: Sets all hours to -1 (no scaling).  
    Uniform: Sets all hours to 1 (scale by primary value).  
    Scale by: Allows individual hours to be scaled.  
Species:  
    Reset: Sets all species to -1 (no scaling).  
    Uniform: Sets all species to 1 (scale by primary value).  
    Scale by: Allow individual species to be scaled.
- **Choose Operators**  
Deselect any operators that are not desired with the model run.

### Model Maker

This feature is currently not operational.

## View

- **Contours**

Field Type:

Day: Set the day to be plotted.

Hour: Set the hour to be plotted.

Level: Set the level to be plotted.

Species: Choose the species to be plotted

Bins:

Plot: Plot the chosen field

Open File: Open the file with output concentrations.

Plot Options: Add city dots to the plot.

Save Picture: Save graphics

Save Matrix: Save data (to be used in another program)

Close:

- **Time Series**

Most options are identical to Contours, with the following exception:

City: Choose the location to be plotted

## Sensitivity

## Help

- **Contents**

Gives a description of the model

- **Demo**

Runs a demonstration of PSE Air

- **Stop Demo**

Stops the demonstration run.

- **Demo Config**

Allows modification to the demonstration run.

## **EXPLANATION OF TERMS**

**Field Type:** There are 11 elements (fields) of the original model that can be changed using PSE Air for experimental purposes.

- 1) **Initial Conditions** are the concentrations of species at the beginning of the model run.
- 2) **Boundary Conditions** are the concentrations of species at the edges of the model area.
- 3) **Wind Fields** are the wind speeds throughout the model run.
- 4) Horizontal diffusion
- 5) Vertical Diffusion
- 6) **Deposition** is the rate at which species are deposited on the ground.
- 7) **Area Emissions** are the emissions of species during the model run primarily from cars.
- 8) **Point Emissions** are the emissions of species during the model run primarily from industry.
- 9) **Temperature**
- 10) **Humidity**
- 11) **Ultra Violet Radiation**



## CHEMICAL SPECIES

### Gas phase species:

NO - NITRIC OXIDE  
NO<sub>2</sub> - NITROGEN DIOXIDE  
O<sub>3</sub> - OZONE  
HONO - NITROUS ACID  
HNO<sub>3</sub> - NITRIC ACID  
HNO<sub>4</sub> - PERNITRIC ACID  
N<sub>2</sub>O<sub>5</sub> - NITROGEN PENTOXIDE  
NO<sub>3</sub> - NITRATE RADICAL  
HO<sub>2</sub> - HYDROPEROXY RADICAL  
CO - CARBON MONOXIDE  
HCHO - FORMALDEHYDE  
ALD<sub>2</sub> - LUMPED ALDEHYDE  
MEK - METHYL ETHYL KETONE  
MGLY - METHYLGLYOXYL  
PAN - PEROXYL ACYL NITRATE  
RO<sub>2</sub> - TOTAL RO<sub>2</sub> RADICALS  
MCO<sub>3</sub> - CH<sub>3</sub>CO<sub>3</sub> RADICAL  
ALKN - ALKYL NITRATE  
ALKA - >C<sub>3</sub> ALKANES  
ETHE - ETHENE  
ALKE - >C<sub>2</sub> ALKENES  
TOLU - TOLUENE  
AROM - AROMATICS  
DIAL - UNKNOWN DICARBONYLS  
NPHE - NITROPHENOLS  
NH<sub>3</sub> - AMMONIA  
NIT - AEROSOL NITRATE  
ISOP - ISOPRENE  
APIN - a-PINENE  
BPIN - b-PINENE  
MYRC - MYRCENE  
CARN - d<sub>3</sub>-CARENE  
LIMO - LIMONENE  
MEOH - METHANOL  
ETOH - ETHANOL  
MTBE - METHYL TERT-BUTYL ETHER  
OSD - O SINGLET D  
O - O ATOM  
OH - HYDROXYL RADICAL  
RO<sub>2</sub>R - GENERAL RO<sub>2</sub> #1  
R<sub>2</sub>O<sub>2</sub> - GENERAL RO<sub>2</sub> #2  
RO<sub>2</sub>N - ALKYL NITRATE RO<sub>2</sub>  
RO<sub>2</sub>P - PHENOL RO<sub>2</sub>  
BZN<sub>2</sub> - BENZALDEHYDE N-RO<sub>2</sub>  
BZO - PHENOXY RADICAL  
H<sub>2</sub>O<sub>2</sub> - HYDROOGEN PEROXIDE  
H<sub>2</sub>O - WATER VAPOR  
O<sub>2</sub> - OXYGEN  
H<sub>2</sub> - HYDROGEN  
SO<sub>2</sub> - SULFUR DIOXIDE  
SO<sub>3</sub> - SULFUR TRIOXIDE (RAPIDLY FORMS H<sub>2</sub>SO<sub>4</sub>)  
M - THIRD BODY  
HCL - Hydrochloric acid  
ATO1 - Condensable vapor 1 from toluene  
ATO2 - Condensable vapor 2 from toluene  
AAR1 - Condensable vapor 1 from higher aromatics  
AAR2 - Condensable vapor 2 from higher aromatics  
AAP1 - Condensable vapor 1 from mono-terpenes  
AAP2 - Condensable vapor 2 from mono-terpenes

### Aerosol species:

Na, sodium  
SO<sub>4</sub>, sulfate  
NH<sub>4</sub>, ammonium  
NO<sub>3</sub>, nitrate  
Cl, chloride  
K, potassium  
Ca, calcium  
Mg, magnesium  
H<sub>2</sub>CO<sub>3</sub>, carbonic acid  
H<sub>2</sub>O, water  
*Other inorganic species:*  
EC, elemental carbon  
TA, toluene product 1  
TB, toluene product 2  
AA, higher aromatic product 1  
AB, higher aromatic product 2  
PA, mono-terpene product 1  
PB, mono-terpene product 2  
OO, other organic species.

## **USE AS AN EDUCATIONAL TOOL**

This section contains a sample of problems that could be used in the classroom to help students make discoveries about air pollution and air pollution models.

### **Problem 1: Tree Pollution**

When he was president, Ronald Reagan stated that trees cause as much air pollution as cars. While not totally correct, there is truth in this statement. Trees are the major producer of isoprene. Should we then cut down trees to reduce pollution? That's what this problem is about. What would happen if 75% of the trees in the LA basin were cut down? That can be tested in the AirPSE by reducing the isoprene by 75% for both the area emissions and the initial conditions. Students can explore the effects of trees on ozone.

### **Problem 2: NO<sub>x</sub> from Point Emissions**

Power plants and factories all over the U.S. were required to reduce their NO<sub>x</sub> emissions by 25% between the years 1990-2001. Nine states on the east coast were required to reduce their NO<sub>x</sub> emissions by 60% over a similar time period (See [www.epa.gov/airmarkets/cmprpt](http://www.epa.gov/airmarkets/cmprpt) ). What affect would the additional reduction have for the L.A. basin? This can be tested in the AirPSE by reducing the point emissions of NO and NO<sub>2</sub> by .75 and by .6 all over the basin and comparing the differences.

### **Problem 3: Emission Reduction from a Single Source**

The web site [www.scorecard.org](http://www.scorecard.org) records emissions from different sources across the US. (They are organized by zip code). The information from this web site makes it possible to approximate the affects of a single source. For example, an Arco in Carson produces large amounts of NO<sub>x</sub> and CO. On the PSE grid, Carson is located at approximately the point (36,12). By drawing a small circle around (36,12) and reducing NO<sub>x</sub> and CO by .5, students can get an idea of how much a single source of pollution affects the entire LA Basin.

### **Problem 4: NO<sub>x</sub> /Ozone Relationship**

Study the relationship between NO<sub>x</sub> and ozone. Does a decrease in NO<sub>x</sub> always mean a decrease in ozone?