Air Quality Modeling for Teachers

THE SHODOR EDUCATION FOUNDATION, INC.

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The Shodor Education Foundation, Inc.

Ozone

O3 creation

O Molecules

Ozone Guess

impact of cl

normal decay

O3 per cl radical

Post 1994 message

depletion
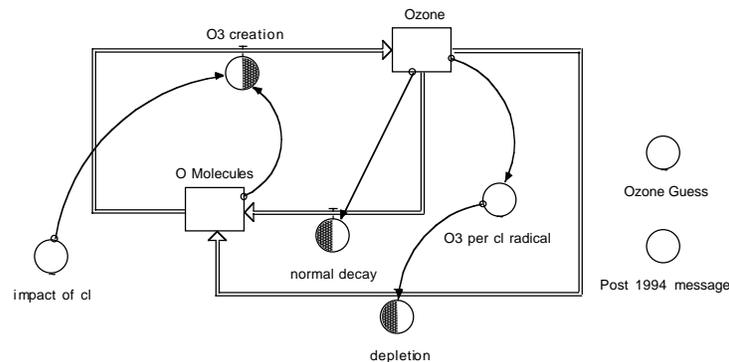
Notes:

Welcome to this presentation on air quality modeling for teachers! This presentation looks to:

1. Introduce you to the basic concepts of atmospheric science, atmospheric chemistry, and basics of air quality models (AQMs)

2. Present (for further discussion via the Web on January 30th!) an Environmental Protection Agency (EPA) air quality regulatory model available to you and your students free of charge via the Web.

3. Discuss activities for the classroom in the use of this online model.

This presentation requires roughly 30-40 minutes to complete. Thanks for your time and effort in viewing this presentation!
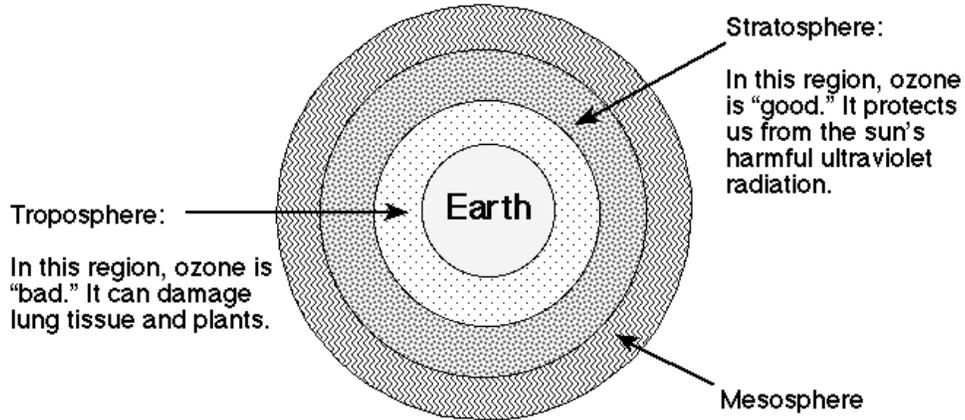
The Atmosphere
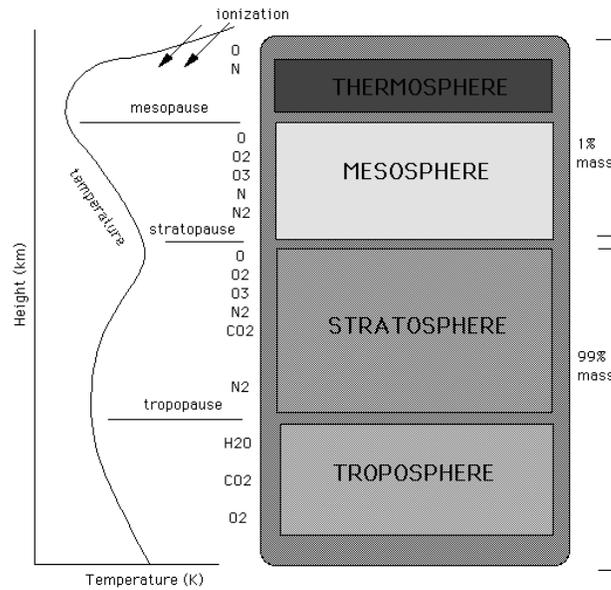
Notes:

The first slide of this presentation focuses on basic atmospheric science. We can divide the atmosphere into four sections: the troposphere, the stratosphere, the mesosphere, and the thermosphere. For all practical purposes, we are only concerned with the troposphere in air quality modeling, since the troposphere is that part of the atmosphere that we interact with the most. The troposphere has a height of roughly 11 km (or a little less than seven miles), and, when combined with the stratosphere, contains 99% of the Earth's atmosphere. Between the troposphere and the stratosphere is the "tropopause", a dividing line if you will between the two lower atmospheric spheres. The height of the tropopause is variable, and is determined by several techniques, mostly through readings (called "soundings") taken by balloons released from many locations twice a day. You might notice that the tropopause starts where the temperature line begins to increase!

While we are not unconcerned with air quality in the stratosphere (as you will see on the next slide), for purposes of this particular air quality model (AQM), we focus our attention in this model on the troposphere.

Ozone in the Earth's Atmosphere

Stratosphere:

In this region, ozone is "good." It protects us from the sun's harmful ultraviolet radiation.

Troposphere:

In this region, ozone is "bad." It can damage lung tissue and plants.

Earth

Mesosphere

## Ozone in Earth's Atmosphere

Notes:

The particular model presented here looks at predicting the amount of ozone, or O3, formed in the troposphere. Ozone is a secondary pollutant -- that is, it is a pollutant that is formed through a variety of chemical reactions of primary pollutants. Primary pollutants are those that are emitted into the atmosphere from a variety of sources, which we will discuss later.

In the troposphere, ozone is a harmful, yet odorless, gas. It has particular implications for those with respiratory illnesses, children, senior citizens, and those active in the outdoors. Ozone also has damaging effects on plants. Fundamentally, ozone in the troposphere is "bad", and millions of dollars are spent each year trying to reduce ozone concentrations in the lower atmosphere.

Conversely, ozone in the stratosphere is "good", as it serves as a barrier to ultraviolet (UV) rays from the sun, which are known to cause cancer. We're all familiar with the "ozone hole", particularly the one laying over Antarctica. Unfortunately, we can't "export" ozone from the troposphere to the stratosphere, so we work to reduce ozone in the troposphere while trying to keep it in the stratosphere!

Ozone Production

Precursor chemicals + hν = Ozone (O3)

NOx + VOCs + (CO) -------> O3 + PAN, etc.
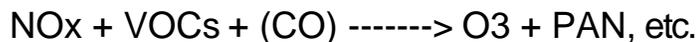
- NOx: a family of chemicals known as oxides of nitrogen
- VOCs: volatile organic compounds that include carbon (C), hydrogen (H), and oxygen (O)
- PAN: peroxyacetyl nitrates (strong irritants, toxics)

Notes:

The chemistry of ozone formation in the troposphere is quite complex. Some descriptions, or mechanisms, of the chemistry of the troposphere only have 60 unique chemical reactions -- other mechanisms have close to 180! The graphic above shows a very simplistic snapshot of how ozone is formed in the troposphere.

There exist two families of primary pollutants: NOx and VOCs. Both of these are consider the main culprits in the formation of tropospheric ozone. NOx (pronounced "knox") can be chemicals such as NO, NO2, etc. VOCs are, as described, a large class of organic compounds, i.e., those that contain carbon, hydrogen, and sometimes oxygen. We call these chemicals primary pollutants or, less often, precursor pollutants. Put these two families together in the presence of "hv" (a shorthand representation for sunlight, go ask your physics or chemistry friends for a definition!), and you have ozone (O3) formed. In addition, a number of secondary chemicals, such as peroxyacetyl nitrates (PAN), are typically formed. For the chemists out there, there are some interesting examples of kinetics, limiting reagents, free radical chemistry, and other commonly-taught principles in introductory chemistry that can be demonstrated with ozone production reactions.

Lagrangian Transport Schematic
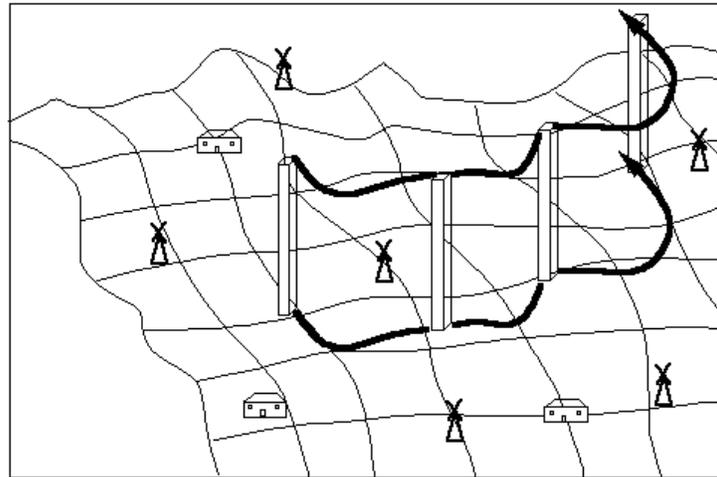
Notes:

This graphic gives a rough characterization of what we will be trying to do with our air quality model. The graphic represents a community, with various buildings, trees, powerlines, etc., badly drawn. Imagine if you will a column of air, extending from the ground to some height in the troposphere. This column of air moves about (hence the name "Lagrangian") from one location to another over the modeling area (note: if the column was fixed, and stuff moved in and out of the fixed column, we would call it an "Eulerian" schematic). What goes in this column of air? In our case, we're interested in the quantity and type of primary pollutants -- NOx, VOCs, others -- that get into this column of air as it moves around. We're also interested in how much ozone gets formed in this column of air. Too much ozone, and the community is in "non-compliance" with federal air quality standards, and subject to fines (never mind the fact that the air isn't very healthy either!). As you will see in the model, the movement of this column of air depends greatly on the meteorology of the area, as well as the terrain, type and heights of buildings, and other factors.
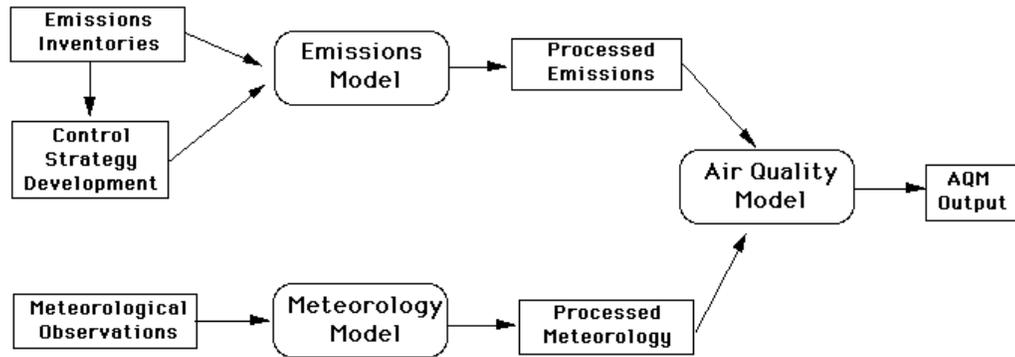
Notes:

This graphic shows an excellent overview of air quality models in general. As you can see, there are fundamentally two parts to the model: an emissions model, which focuses on the type and amount of emissions (primary pollutants) that go into the model, and the meteorological model, driven by a wide variety of meteorological observations and data, such as temperature, relative humidity, mixing heights, and others.

The emissions part of the model is defined by the emissions inventory, a collection of the various types of chemicals that are emitted and their amounts (either as raw amounts or as fractions of the whole amount). These inventories are keyed in, and, at runtime, go to the emissions model, where they are processed and outputted to the air quality model. The user can also introduced a control strategy to the model. For example, after the emissions inventory is entered, the user can say "suppose we reduce this particular emission by 20%, how would that affect our air quality?". This is what we will ask you to do with our model -- develop a control strategy, given a particular emissions inventory. You can also, of course, enter in your own emissions inventory, but we're not expecting your students to do this.

Likewise, we can collect meteorological data, enter it, and have it processed by the met model. This processed data is delivered to the AQM, where it is combined with the emissions output to produce a final output file for your analysis.

EKMA/OZIP

- ∟ OZIP is an early-generation (late 70s) ozone concentration modeling program
- ∟ EKMA: Empirical Kinetics Modeling Approach
    - » Empirical: using experimental data from the field
    - » Kinetics: based on rates of chemical reactions in the atmosphere
- ∟ OZIP: Ozone Isopleth Plotting Program
    - » Isopleth: a chart showing equal ("iso") concentrations ("pleths") of ozone

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Notes:

The model that you are presented with on our web page is the "EKMA/OZIP" model, a late 70s/early 80s regulatory model developed by the EPA. This model is still in use, although it has been replaced for regulatory usage by other more sophisticated and elaborate models. For educational purposes it is still, however, a good learning tool, as the input and output for this model are "typical" of many of the newer models.

The name "EKMA/OZIP" captures both the theory behind the model (the modeling "approach") and the output of the model. EKMA, as described in the slide, defines the approach that the developers used to create this model. When you investigate the model, you will hopefully take the opportunity to explore the various components, especially the chemical mechanisms underlying the model (the "kinetics" part of the model).

Likewise, the OZIP part of the name represents the type of data that emerges. Unlike the newer, fancier models that display three-dimensional color graphics and animations, this model creates an ozone isopleth graph, showing the concentrations of primary pollutants and the resulting concentration of ozone. We'll explore how to interpret this graph in subsequent slides.

OZIP: Ozone Isopleth Plotting Program

1 25 FORTRAN programs, working in series
  » only calculates ozone concentrations for a single day (vs. multiple-day of newer models)
    – UAM: Urban Airshed Model
    – MODELS-3
  » requires understanding of
    – chemical reactions of the troposphere
    – emissions inventories
    – meteorology
    – various simulation scenarios

Notes:

A brief description of the modeling environment is in order. Our version of OZIP uses 25 FORTRAN programs, all compiled to run as a single program. Unlike the newer models, OZIP only calculates ozone values for a single day, whereas newer models can calculate ozone formation over a longer period of time. EPA's current regulations strongly suggest that modelers use these newer models with their multi-day capabilities (not to mention their more sophisticated data analysis and visualization capabilities!)

To use these models, the user needs an understanding of the underlying chemistry, have data for the emissions inventory, know how to collect and enter meteorological data, and then have some ideas of what types of scenarios might be of interest. That's a lot to know and understand. In recognition of the difficulty in doing that for teachers and students, we have two versions of the program, one that allows the user to input everything into the model, and another that "hides" some of the input, and presents the user with a narrow list of options to be changed. We'll recommend, of course, the use of the more limited model in the classroom. However, for longer projects, both models use the same code, so students could opt to learn about the larger input interface.

Shodor's Approach to EKMA/OZIP

1 in support of EPA, Shodor has:
  - » installed OZIP on its high-performance workstation (SGI)
  - » constructed a Web-interface with user support
  - » provided full documentation to the user
  - » created a realistic scenario based on current (November 1996) national air quality standards and regulations

Notes:

A little bit about our interface. EKMA/OZIP, at the time we were doing this project, existed only as the FORTRAN programs, requiring users to install their own code, create input files from scratch (in perfect FORTRAN format), and run the code from a command line prompt in UNIX. What we did in support of a funded project was to build a Web interface with built-in user support. The interface provides a way for the user to input the data easily, and, upon hitting the "Submit" button, packages the data up in the correct format, ships it to Shodor's Silicon Graphics Indigo 2 scientific workstation, runs the code, creates an output Web page, and displays it on the users screen. The user still has to understand the science of the input data, and be able to do the analysis work. The interface just works to make the model runs significantly easier.

In addition to putting all of the documentation online, and creating some useful online calculators, we also created a scenario based on a real-world situation. Students, working in teams, can use this scenario to function in the role of air quality consultants. In working with a variety of universities and high schools, we have seen that the scenario is an effective "platform" from which to have students understand air quality modeling from a variety of perspectives -- chemistry, meteorology, emissions, computational science, and public policy.

Notes:

You should now consider visiting the modeling site, at the URL listed above. The graphic in this slide shows you a snapshot of the main page, so you can convince yourself that you are in the correct location!

A short description of the page layout. On the left are all of the materials that students need to solve a sample scenario that we created. In this scenario, students work in teams of five and simulate being air quality consultants under contract to a utilities company in danger of non-compliance with air quality standards. In the scenario materials, we present getting started instructions, a sample "scope of work", EPA memos that the students will need, links to various datasets, and other materials that the students can use if they think they are helpful.

On the right is a complete set of documentation on the use of the model. We don't expect students to read these unless they are doing the entire scenario. However, at the bottom of the column, there are two links, one to the "basic" version of the model interface, and one to the "advanced" version of the interface. We'll be recommending the use of the basic interface for our start.

Ozone Isopleth Plotting Program (OZIP) Web Interface
(Basic Interface)

DISCLAIMER! The OZIP model available through this Web page is NOT to be used for regulatory, research, legal, or scientific purposes. It is intended SOLELY as an educational tool. Y

Need help with using this interface? Read the Quick Guide to Using an Air Quality Model

Title and Initial Settings:

Title of the simulation: `TITLE HERE (your name, or the`   Location: `CITY AND STATE`

Latitude : `35.59982`   Longitude : `77.37439`   Time Zone: `Eastern Daylight Time`

Year : `2000`   Month : `3`   Day : `24`

Base and Future Conditions

1. Base Case

   O_3 daily design value: `0.160` ppm

   Design Ratio :

   `15.0` parts of VOCs to one part of NO_x

2. Future

   Decrease in NO_x emissions (percentage) : `-0.000`   Decrease in CO emissions (percentage) : `-0.000`

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Notes:

If you scroll to the bottom right of the main page, you will see a link for the "Basic Interface". Clicking on this link results in the screen you see above. You should also investigate the "Advanced" interface, so that you are aware of the differences, specifically the items that we "hide" from the student. In the basic interface, there is a "Quick Guide" that we recommend you read, either online or as a printout.

The input boxes that you first see should be fairly self-explanatory. The hardest item is the latitude and longitude. Clicking on either lat or long will bring up a navigator that will help you to determine your coordinates.   Why might you think this is important in an air quality model?

The title box can be anything, such as your name. The city/state box is just for documentation purposes. You should notice that the model is specific for your time zone and the specific day and month.

The graphic above doesn't show the entire interface. You should scroll on your Web browser to see the entire interface. Notice the "Run OZIP" button at the bottom of the interface. Clicking on this sends your data to Shodor for computation.

OZIP: Ozone Isopleth Plotting Program

You can look at three different files for this run:

- Your input file
- Your output file
- Your isopleth file: (note: if you size your window to see four columns of numbers, the pattern will be more clear). The first number is the VOC concentration in ppm, the second number is NO_x concentration in ppm, and the third number is the ozone concentration in ppm. The fourth number is not needed in this scenario.

Go back to sample runs file

NOTE: You may need to wait for several minutes to get the ouput HTML file. If if doesn't appear, revisit this page or use the RELOAD button.

Isopleth Graph

The graph of the isopleth is shown below. This is a plot of the intial concentrations of VOCs and NO_x plotted against the concentration of ozone. An isopleth is a graph of "equal (iso) concentrations (pleth)".

For an ozone value of 0.09 ppm, for example, the line shows every value of VOCs and NO_x that combine to form that concentration (0.09 ppm) of ozone. One way to use this graph is to pick ONE value of VOC, such as 1.0 ppm, then move up and down the NO_x axis and observe at what value(s) of NO_x you intersect with the desired ozone concentration. For example, holding VOCs constant at 1.0 ppm, you might find that you intersect the 0.09 ppm O_3 isopleth at two different concentrations of NO_x. That means that when VOCs are 1.0 ppm and NO_x are at **either** of those two NO_x values, you will produce 0.09 ppm of ozone.

VOCs (in parts per million, or ppm) are plotted along the x-axis

NO_x values are plotted on the y-axis in ppm. Concentrations plotted are 0.08, 0.09, 0.10, 0.11, and 0.12.

On the isopleth the lowest concentrations begin on the left side of the graph, and move from left to right. The concentration 0.08 is the first dotted line beginning at the left, followed by 0.09, 0.10, and so on.

Ozone Isopleth Plot

Notes:

The graphic above shows a partial screenshot of a sample run. Clicking on the input file link shows you the input file submitted to Shodor, in proper FORTRAN format, not very interesting except for debugging purposes (why am I getting such weird answers?). The output file is a <u>long</u> and detailed file that provides the "answer" to your model run. The raw numerical data is also available in case you wish to export this data to a spreadsheet or other computational tool for analysis.

At the bottom of the results page (only the header is shown in the graphic above) is the ozone isopleth plot for this run. This plot is also described in text in the output file, and we'll suggest you use the text-based results rather than the isopleth file. It is, however, useful and instructive to learn how to read and interpret the isopleth graph, which we will now do in the next series of slides.
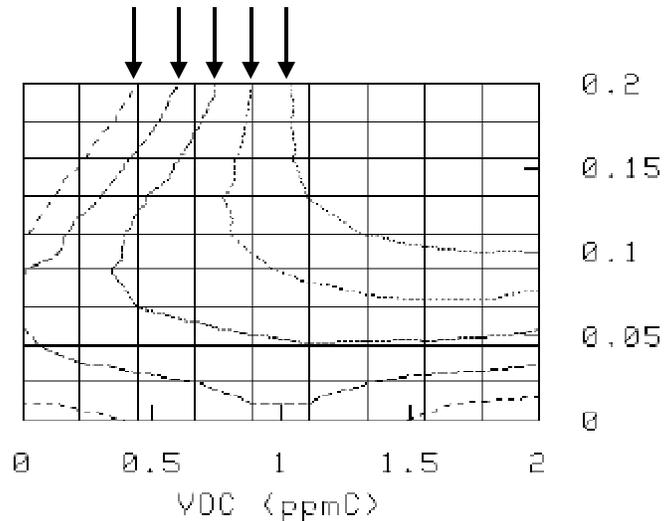
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Sample Isopleth Chart

ℓ NOx is plotted on the y-axis

ℓ Values of ozone

    0.08 ppm
    0.10 ppm
    0.12 ppm
    0.14 ppm
    0.16 ppm

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Notes:

The graphic above shows a sample ozone isopleth. On the bottom (x) axis the graph shows the concentration of volatile organic compounds (VOCs) in units of parts per million of carbon. A concentration of 10 parts per million (ppm) says that there are 10 molecules of pollutant for every 1 million molecules of air. The VOC ppmC scale for this chart goes from 0 ppmC to 2 ppmC. The model allows you to adjust this scale if needed. On the y-axis, we have plotted NOx, also in units of parts per million. On this particular graph, we plot from zero to 0.2 ppm. Again, that is adjustable in the model interface.

The actual curvy lines on the graphs represent the concentrations of ozone, in units of parts per million. Starting from the left and moving to the right, there are five lines, beginning with 0.08 ppm, then 0.10 ppm up to 0.16 ppm. Again, the user can decide what concentrations s/he would like to see plotted. The value of 0.08 ppm is the current national air quality standard for ozone, a recent change from 0.12 ppm, hotly contested by the nation's business and transportation communities, all the way up to the Supreme Court. Reaching a standard of 0.08 ppm ozone is much more difficult and expensive than 0.12 ppm!

Sample Isopleth Chart

At this intersection, the O3 level is at 0.10 ppm

REDUCE NOx, O3 levels GO UP!

0.10 ppm   0.12 ppm
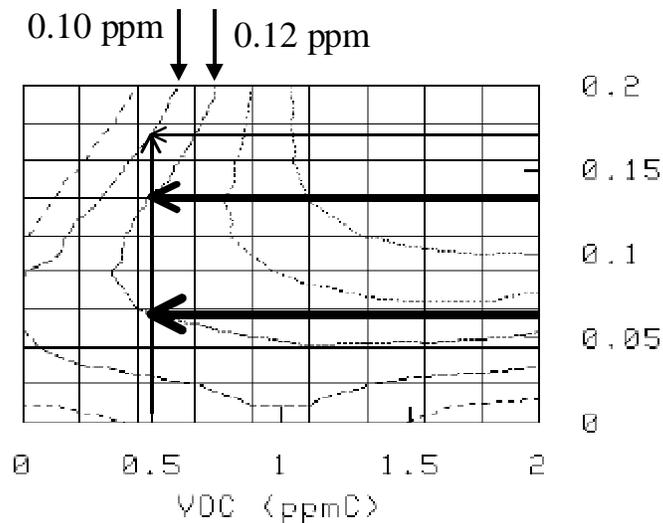
Notes:

This next graphic works better if you are viewing this from the PowerPoint SlideShow option on your desktop. What we are trying to show with this slide is a very interesting phenomenon. One might think the following: "IF I reduce either NOx or VOC concentrations (or both), then my ozone concentration should come down". Simply speaking, put less stuff in the air, then ozone should be better. This slide tries to convey that that is not always the case. For example, suppose we have a concentration of 0.5 ppmC of VOCs, and it does not change. Suppose the concentration of NOx is 0.18 ppm. Looking at the thin red horizontal arrow at the very top, we read that the concentration of ozone is 0.10 ppm. Now let's reduce the concentration of NOx to something like 0.13 ppm (the second, fatter red line). What is the new concentration of ozone? It's 0.12 ppm! In this case, reducing the concentration of NOx actually increased the concentration of ozone. This has to do with the very nonlinear behavior of the reaction mechanisms in the troposphere. While it's not always true that a reduction in one or more of the primary pollutants will result in higher ozone levels, it is important to ensure that students understand that fixing the ozone problem isn't a simple issue of putting less bad stuff in the air.

l   Each red dot represents a monitoring station

l   Monitoring stations measure NOx and VOCs being transported downwind

l   Design ratio: a ratio of VOC concentration (in ppm) to NOx concentration (in ppm)
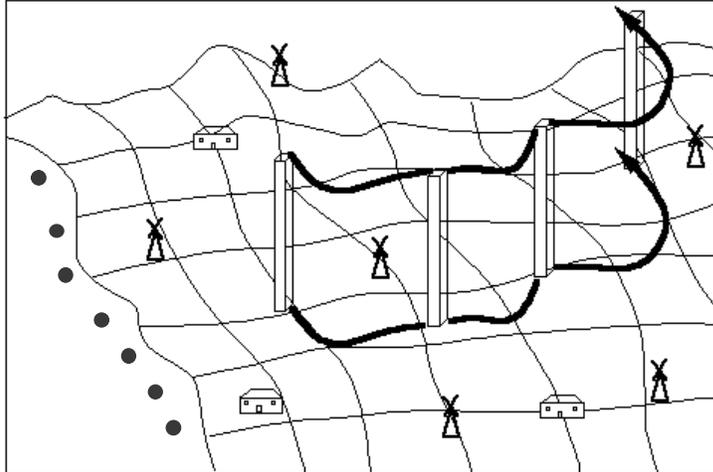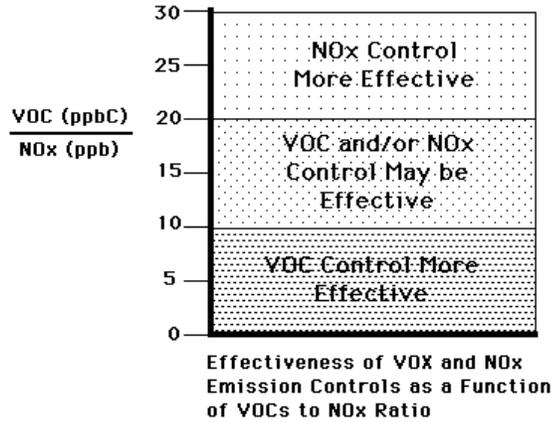
Notes:

There are two main values to be used in exploring ozone levels with the basic version of the interface: the design ratio and the daily design value. The next several slides discuss the design ratio.

The design ratio is an EPA-approved measure of the amount of VOCs and NOx pollutants being transported into a community. Some communities, usually larger cities, will have monitoring stations that measure concentrations of these emissions as they move downwind. In the graphic above, we have used red dots to represent monitoring stations, on the westward (upwind) side of the community. These monitoring stations collect data on the transport of primary and secondary pollutants from polluting sources upwind.

The ratio is simply a division of VOCs to NOx concentrations. Why does this number matter? It matters because the model uses this number to determine how a control strategy -- a reduction in one or more of the primary pollutants -- will result in a change in ozone concentrations.

Design Ratios and Control Strategies

l   measured through the use of monitoring stations for some locations in the US

l   For non-monitored locations, estimates of the daily design ratio are made. EPA must approve the estimates before they can be used in AQMs (see the EPA memo under the Scenario Materials)

$$\frac{VOC\ (ppbC)}{NOx\ (ppb)}$$

NOx Control More Effective

VOC and/or NOx Control May be Effective

VOC Control More Effective

Effectiveness of VOX and NOx Emission Controls as a Function of VOCs to NOx Ratio
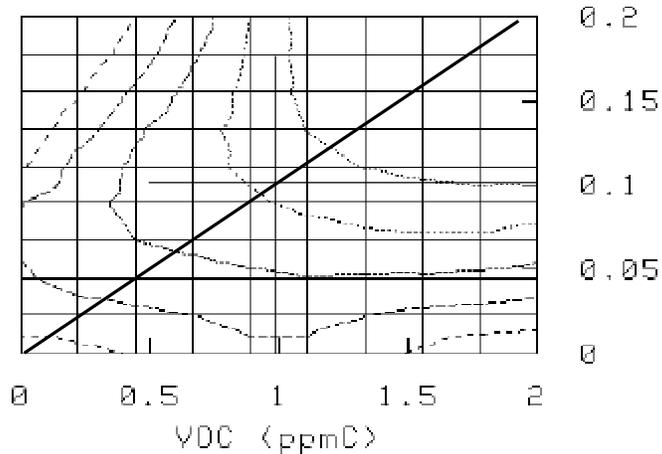
Notes:

As described in the previous slide, we can measure or estimate the design ratio for a given community. Often the choice of this ratio is a legal consideration between the community and the Environmental Protection Agency. The choice of a design ratio has a number of implications, the most important being the design of a control strategy for reducing the amount of primary pollutants in the hope that the ozone levels will also come down. The graphic above presents a guideline that suggests how an air quality modeler might design his or her control strategy, based on the design ratio that has been measured and/or estimated and approved for use by the EPA.

For example, in the graphic above, it is suggested that if the design ratio is determined to be below 10:1 (units are given here in ppb, but it is the same for ppm), then it makes more sense to try to reduce VOCs in order to reduce ozone concentrations. Likewise, ratios above 20:1 suggest that controlling NOx makes more sense. Between 10 and 20, it's a coin-toss as to which one to try to control. Needless to say, most design ratios fall between 10:1 and 20:1, making the task of the air quality modeler more difficult.

l Design ratio line is drawn at 10 to 1 (VOCs to NOx)

Notes:

The graphic in this slide simply shows a drawing of the design ratio, based on a 10:1 ratio. We used 1 ppmC of VOCs and 0.1 ppm NOx as our guideposts, as you can see from the red guidelines. We'll use this design ratio line to do a sample hand calculation of a control strategy using the isopleth chart. This is a useful activity to have students do, since it helps them to better understand the underlying mathematics of the calculations being done by the computer, and also works to ensure that they have a feel for design ratios and daily design value (presented in the next slide). A sample hand calculation using the isopleth is provided after the next slide.

Daily Design Values

l   The current level of ozone in a given community, based on measured ozone levels over a three-year period

»   The daily design value is the fourth highest ozone value over a three-year period of time.

»   The daily design value is the starting point for a model run.

Hypothetical Case (two O3 sites in an area, each year at least 75% complete)

FOUR HIGHEST DAILY MAXIMUM VALUES

		Max	2nd Hi	3rd Hi	4th Hi
SITE 1	1986	.127	.123	.122	.110
	1987	.129	.124	.121	.116
	1988	.142	.136	.134	.115

The design value for Site 1 is 0.129 ppm, the fourth highest daily maximum value during the three year period.

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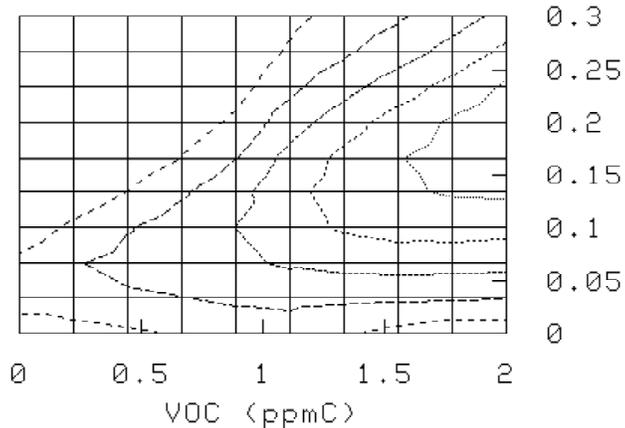
Notes:

The other value of interest in the basic interface is the daily design value. This the starting point for the model; this is the value that characterizes the level in a given community that is not in compliance. For example, looking at the hypothetical case above, the daily design value is 0.129 ppm, not bad, but not in compliance with the (new) federal standard of 0.08 ppm! In our model use, we will want to design a control strategy that instructs this community how to reduce its ozone levels from 0.129 ppm to 0.08 ppm. We suspect that this will require some reduction in VOCs and some reduction in NOx, with some reduction in carbon monoxide (CO) emissions thrown in for good measure.

1 Given:
  » Design ratio = 15:1
  » Daily design value=0.16 ppm O3
  » Control strategy - reduce NOx by 20%
  » Calculate: percent reduction in VOCs to reach 0.12 ppm (old federal standard)

VOC (ppmC)

0.3
0.25
0.2
0.15
0.1
0.05
0

0   0.5   1   1.5   2

Notes:

In this slide we present a simple problem that a student might do by hand, using a computed ozone isopleth chart. The student is given the design ratio of 15:1, which suggests that the control strategy could involve <u>either</u> a reduction of VOCs or NOx, or both. We have given the student the daily design value of 0.16 ppm ozone, a pretty high value.

The student is given part of the control strategy -- a reduction of NOx by 20%. S/he needs to use the isopleth to determine the other part of the control strategy, namely, what accompanying percent reduction in VOCs will produce a new ozone value of 0.12 ppm. We chose 0.12 ppm rather than 0.08 ppm to make the calculation easier for the first-time calculation.

Sample hand calculation

- Red line is the design ratio line
- Plotted isopleths are: 0.8 (far left) to 0.16 (far right)
- Steps (click to show in sequence):
  - Draw design ratio
  - Find value of NOx at intersection of 0.16 ppm and design line. Estimated at 0.13 ppm
  - Find value of VOCs at intersection of 0.16 ppm and design line. Estimated at 1.85 ppm
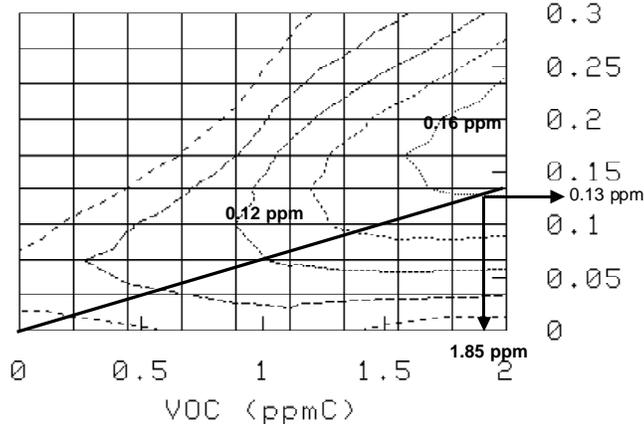
Notes:

These next several slides show how to use an ozone isopleth to determine a control strategy. Given the data from the previous slide, we wish to determine by how much we need to reduce VOCs IF we reduce NOx by 20%. We're starting with a daily design value of 0.16 ppm, we have as our target 0.12 ppm, and we're working with a design ratio of 15:1.

First we draw our design ratio line. I used the two points (0,0) and (1.5 VOCs, 0.15 NOx) to draw the line. Next find where the design ratio line and the daily design value intersect. Read across to the y-axis, read off NOx in ppm. Using the "eyeball" approach, I get 0.13 ppm.

Do the same thing going down from the intersection of the design ratio line and the daily design ratio. Again, by eyeball I get a value of 1.85 ppm for VOCs.

Sample hand calculation

Steps (continued):

» Reduce NOx by 20% (control strategy): 0.13 x (1-0.20)=0.104

» Extend NOx line to 0.12 ppm isopleth (target value)

» Arrow down to find value of VOCs. Estimated is 0.8 ppm

» Calculate VOC reduction needed: (1-(0.8/1.85)) x 100 = 56.8%
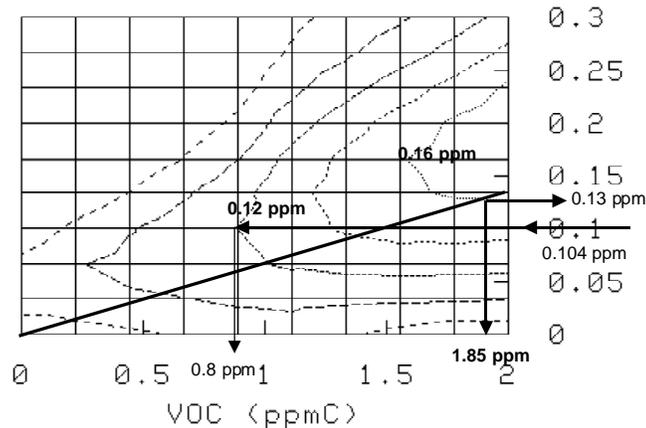
Notes:

Reduce the NOx value by 20% (mathematically, multiply it by 0.80). I get 0.104, roughly 0.1 ppm.

Using 0.104 ppm on the NOx scale, draw a line over to the 0.12 ppm isopleth. Read down to the VOCs scale, I get an eyeball value of 0.8 ppm VOCs.

Calculate what percentage reduction this is, using the formula:

Percent VOC reduction = (1 - (finalVOC/initial VOC)) x 100

For example:

Percent VOC reduction = (1- (0.8/1.85)) x 100 = 56.8%

Using EKMA/OZIP

- l http://www.shodor.org/ekma
- l Click on "Basic Interface"
- l Change screen as shown below
- l Hit "Run OZIP" button
- l Wait for run to complete (5-10 minutes)

Base and Future Conditions

1 Base Case

O_3 daily design value: 0.160 ppm

Design Ratio :

15.0 parts of VOCs to one part of NO_x

2. Future

Decrease in NO_x emissions (percentage) : -20.00   Decrease in CO emissions (percentage) : -0.000

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Notes:

This slide shows how to do this same calculation using the online program. Once you have gone to the Web page, click on the basic interface. The run that I did uses the default values for latitude and longitude, day, year, month, and time zone. If you change these, you won't get the same numbers I did!

In the section entitled "Base and Future Conditions", enter your data for O3 daily design value -- 0.16 ppm -- and the design ratio -- 15.0. You do not need to enter 15:1, the program knows what you are entering!

Once you have made this simple change, scroll down and hit the "Run OZIP". Go find something else to do while the model runs, depending on other things happening on the machine, it will take between three and 10 minutes!

Sample Output

- l From output screen, click on "Your output file"
- l Scroll down to see the output as shown
- l Target: 0.12 ppm
  - » For a 20% reduction in NOx, and 0% reduction in CO, we need a 60% reduction in VOCs to reach 0.1211 ppm, or 70% reduction to reach 0.1090 ppm
- l Use interpolation calculator to determine percent reduction at 0.12 ppm

```
predicted changes in ozone for future changes in hc
```

voc	nox	co	o3	%-chg voc	%-chg nox	%-chg co	%-chg o3
1.818	0.097	1.700	.1483	0.0	-20.0	0.0	-7.4
1.636	0.097	1.700	.1465	-10.0	-20.0	0.0	-8.5
1.454	0.097	1.700	.1439	-20.0	-20.0	0.0	-10.1
1.273	0.097	1.700	.1405	-30.0	-20.0	0.0	-12.3
1.091	0.097	1.700	.1358	-40.0	-20.0	0.0	-15.2
0.909	0.097	1.700	.1295	-50.0	-20.0	0.0	-19.1
0.727	0.097	1.700	.1211	-60.0	-20.0	0.0	-24.4
0.545	0.097	1.700	.1090	-70.0	-20.0	0.0	-31.9
0.364	0.097	1.700	.0921	-80.0	-20.0	0.0	-42.5
0.182	0.097	1.700	.0736	-90.0	-20.0	0.0	-54.0
0.000	0.097	1.700	.0587	-100.0	-20.0	0.0	-63.3

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Notes:

This slide provides a snapshot on how to find and extract data from the model run. The output file, shown as a clickable link on the output page, provides several pages of data. We focus here on the most interesting section, found about halfway down the text-based output file. Look for the section entitled "predicted changes in ozone for future changes in hc", where hc stands for hydrocarbons, the same as VOCs. Looking at the O3 column, we look for 0.12 ppm. The closest we can find is 0.1211 ppm. Reading across, we see that a 60% reduction in VOCs, a 20 percent reduction in NOx, with no reduction in CO, is required to reach 0.1211 ppm, starting from 0.16 ppm with a design ratio of 15:1. If you wish to hone in on the numbers for 0.12 ppm, you can use the online interpolation calculator as described on the next slide.

Notice that, if we wish to reach the 0.08 ppm standard, we will need roughly an 85% reduction in VOCs.

Using the interpolation calculator

- l Hit the "Back" button, click on interpolation calculator
- l Enter values from text-output run
- l Click "Evaluate" to determine percent reduction

Input Value(s):

Target value	0.1200
First ozone value	0.1211
First percent reduction	-60.0
Second ozone value	0.1090
Second percent reduction	-70.0

[Reset Values] [Evaluate]

Result(s):

Interpolated percent	-60.9

Notes:

We have provided a simple Javascript calculator to allow students to interpolate a target value, given a high and low value. For example, in the dataset on the previous slide, we see that we have ozone values of 0.1211 ppm with a 60% reduction in VOCs and a 0.1090 ppm ozone level tied to a 70% reduction in VOCs. The interpolation calculator allows us to interpolate between these values to find the VOC percentage reduction for the target value of 0.12 ppm of ozone. The calculator should be fairly self-explanatory and easy to use.

Alternatively, you might wish to have the students create their own interpolation tool, using a spreadsheet or some programming language.

Sample Projects

l   Project 0: run "SmogCity"
l   Project 1: effect of design ratio
l   Project 2: control strategy design
l   Project 3: Using the full scenario

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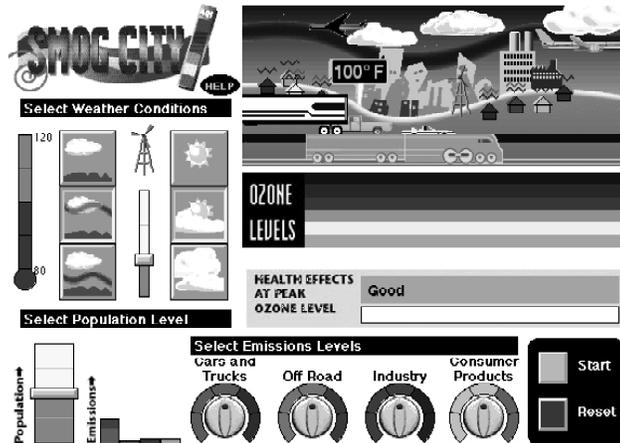
Notes:

There are a number of projects that students can do using these online materials, and we hope that some of you might consider creating a new project that incorporates these materials.

In the next set of slides, we describe four projects, starting with one that uses an online Java applet developed by air quality modelers in California. Each of these projects can be done as "stand-alone" projects, or in sequence for a longer unit.

In describing the projects in the next several slides, we provide the goal of the project, a sample instructional strategy, and our best guess as to the duration of the project, based on our experiences and those of others.

l http://www.smogcity.com
  » Animated simulation, based on actual model runs, of ozone levels
  » Helps students to understand various factors, including emissions
  » Non-mathematical/non-quantitative
  » NOTE: this is a simulation, not a model
l Duration: one class period

Notes:

Smog City (http://www.smogcity.com) is a Java-based simulation that is a useful pre-EKMA activity for preparing students to interact with the air quality model. Given time constraints, we might suggest the use of this tool over the actual online EPA model. However, this is a simulation, the options for changes are limited, and students don't really get a sense of the types of data that go into an actual model. We tend to be a little "leery" of simulations such as these -- while they do help the students engage in a number of "what if" situations, these simulations do not provide some of the "teachable moments" that can be generated by the "real McCoy". For example, I have been unable to get this simulation to suggest, as is true in the real world, that a reduction in primary emissions sometimes results in an <u>increase</u> in ozone levels. Regardless, this is a great tool to use to help the student begin to understand that meteorology (as represented by temperature, inversions, wind speed, and cloud cover) and emissions (as represented by population and the four types of emissions sources) are the critical determinants of ozone levels.

Sample Project: Effect of Design Ratio

- Goal: determine effect of one variable (design ratio) on the impact of VOC and NOx reduction
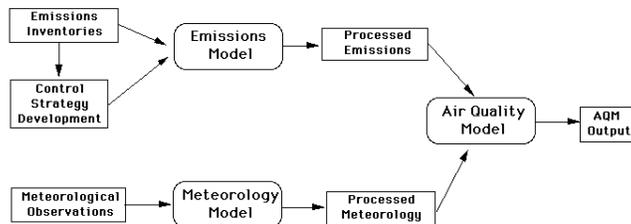- Strategy: five runs
  - » Design ratio
    - 6 VOCs : 1 NOx
    - 12:1
    - 18:1
    - 24:1
    - 30:1
  - » compare relative impact of VOC versus NOx reduction
- Duration: one or two class periods for runs

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Notes:

This activity is best done in a team-approach, having each student do one of the runs. In this activity, the students are investigating the effect of different design ratios. The "discovery" activity is the creation of the graphic shown on Slide 16, so you may wish to <u>not</u> show them that graphic if you are using these slides for presenting this activity. Optionally, you can discuss that graphic, then have them do a "verification" type of activity.

What I have done in the past that works well is to plot VOC and NOx reduction percentages using a bar graph in Excel or Appleworks. From that graph it's pretty easy to see which primary pollutant is the best one to change for a given design ratio. Probably the "best" results are shown starting with a daily design value of 0.16 ppm in a summertime environment, but you can experiment with various scenarios.

Sample Project: Control Strategy Design

- Goal: given a design ratio, design a balanced control strategy
- Tool: OZIP, using the EKMA approach
- Strategy: multiple runs
  - » Form groups of students
  - » Each group investigate one <u>fixed</u> NOx percentage reduction (I.e. 10%, 20%, etc.)
  - » Include CO reduction to investigate its effect
  - » Once "decided", does the control strategy "work" in different seasons in different locations?
- Duration: short project, but can take several days to several weeks, depending on number of runs

Notes:

Given a little more time, another project is to have students, preferably working in groups, explore different control strategies. Hopefully they will have seen, verified, and/or discovered the "control strategies guideline" chart shown on Slide 16, and will use that to determine some starting points for their control strategy.

For example, you might have one group of students be the "10% NOx" group, where they set NOx reduction at a fixed value, then let the model explore different values of VOCs. Additionally, they might wish to see if CO (carbon monoxide) has an effect on the overall control strategy, and if so, what that effect might be.

Once the students "settle" on a control strategy that they think works, they might want to try to apply that control strategy to different times of the year at different locations in the United States. They should not try to run the model for locations outside of the US, the photochemical parameters are set for North America.

Sample Project: Using the Full Scenario

- Goal: use the full scenario as described on the left side of the main web page
- Tool: requires use of advanced version of the interface
- Strategy: teams of five students
  - » Each student has a role: computer modeler, chemist, meteorologist, emissions inventory specialist, public policy specialist
  - » Task: prepare a technical memo for the CEO of "LotsoNOx, Inc." regarding his/her options, with cost amounts, for reducing emissions from his coal-burning plant to reach compliance
- Duration: several weeks

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Notes:

We have had several universities and high schools participate in the "full" scenario as described in the Scenario section on the main Web page. In this scenario, students form a consulting company that is contracted to provide a recommendation to the CEO of a large pollution-producing company. The students are asked to deliver a technical memo to the CEO that describes a control strategy that will help the CEO to ensure that the community surrounding his/her plant is "in compliance" with federal air quality standards. The students are provided $1 million to work with, that is, the cost of their recommended reductions must not exceed that amount. Approximate costs for each percentage reduction of each of the three primary pollutants are provided in the scenario materials.

This is a lengthy activity. We have worked with several high schools that have used this with great success in AP Environmental Science classes over a period of several weeks to a month (not, of course, to the exclusion of other activities). In all of these groups, Shodor has served as online consultants, providing technical support and playing the role of EPA program officer, offering legal and technical opinions.

Note that the full scenario requires the use of the advanced interface, not described in this presentation!

l Run times:
  » Typical run times: 3-8 minutes, depending on load
l Advising Shodor prior to runs
  » Notifications are helpful
    – Online, real-time technical help
    – "runaway jobs"
    – System debugging

Notes:

We conclude this presentation with some technical notes. In designing your instructional program, you should know that each run can take three to eight minutes, longer if multiple students are doing runs. You need to remember that this model is numerically-intensive. Even running on a reasonably powerful scientific workstation, there are a lot of calculations to be done. Students need to work together to ensure that lots of them are not submitting jobs at the same time! Towards that end, it's helpful if you, as the instructor, let us know a day or two ahead of time that your students will be doing runs.   We can help by monitoring the system, making sure that "runaway jobs" are killed, and generally keep track of how things are doing and provide advice back to you and/or the students.

Given an appropriate amount of lead time, we can also work directly with your students through online chats or videoconferencing as they work their way through the model. We strongly recommend this if students are doing the full scenario!

Thanks for taking the time to work through this presentation, and hope to see you all online January 30!