A Brief Overview of Modeling Topics

By MARAMA

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Learning Objectives

The participant will use the information learned to:

- Correctly use model names and acronyms in discussion or written materials
- Identify the types of modeling needed to develop attainment demonstrations for SIPs for various pollutants
- Identify useful dispersion models for point source analysis
- Identify useful photochemical grid models for SIP planning
- Recognize key meteorological models and how they are used
- Define source apportionment modeling and receptor modeling and their role in identifying source contribution to air pollution
- Know the setps needed to develop emissions inventories fror SiP development
- Know where to find more detailed information when needed.

Introduction?

Five modeling types will be introduced in this document as shown in the following table. Each model type has a distinctly different purpose and structure. They are all called "models" because they attempt to pull from a variety of sources to build a representation of the complex system that intersects sources, meteorology, and topography.

Type	Uses
Photochemical Models	Estimate ozone and reactive particulate matter. Designed to predict long range transport and atmospheric chemical transformations over hundreds and even thousands of miles.
Dispersion Models	Estimate the effect of local sources on the local atmosphere of pollutants that are not affected by chemical transformation.
Meteorological Models	Describe the meteorology for the modeled area.
Receptor Models	Identify the primary sources of individual pollutants measured at a given location.
Emissions Models	Calculate emissions for particular sectors of the inventory.

Which models are used for different purposes?

The modeling approach taken will depend on the question being asked. For NAAQS attainment demonstrations, photochemical modeling is generally required due to the chemical transformations in the atmosphere. Fine particulate and haze are complicated, involving 18 different sub-species that must be summed. However, for permit applications, including PSD permit application, dispersion modeling is generally what is required. If the source is within 100 miles of a Class 1 area, more detailed modeling may be required.

	Model type	Pollutants involved
PM SIP	Receptor, Dispersion, Photochemical	PM2.5, SO_2, NO_X, CO, Ammonia, a variety of other species.
Ozone SIP	Photochemical	VOC, NO_X, CO
Haze SIP	Receptor, Dispersion, Photochemical	All of the above
Conformity	Emissions	NO_X and CO, and PM
Source permitting	Dispersion	Source specific
NO_X 1 hour attainment demonstration	Dispersion	NO_X
SO_2 1 hour attainment demonstration	Dispersion	SO_2

What is Photochemical Modeling?

Photochemical air quality models are large-scale air quality models that simulate the changes of pollutant concentrations in the atmosphere using a set of mathematical equations characterizing the chemical and physical processes in the atmosphere. These models are applied at multiple spatial scales from local, regional, national, and global. They have become widely and routinely utilized tools for regulatory analysis and attainment demonstrations by assessing the effectiveness of control strategies.

There are two types of photochemical air quality models commonly used in air quality assessments: the **Lagrangian** trajectory model that employs a moving frame of reference, and the **Eulerian** grid model that uses a fixed coordinate system with respect to the ground. Earlier generation modeling efforts often adopted the Lagrangian approach to simulate the pollutants formation because of its computational simplicity. The disadvantage of Lagrangian approach, however, is that the physical processes it can describe are somewhat incomplete. The current operational photochemical air quality models have adopted the three-dimensional Eulerian grid modeling mainly because of its ability to better and more fully characterize physical processes in the atmosphere and predict the species concentrations throughout the entire model domain. The following models all employ an Eulerian grid.
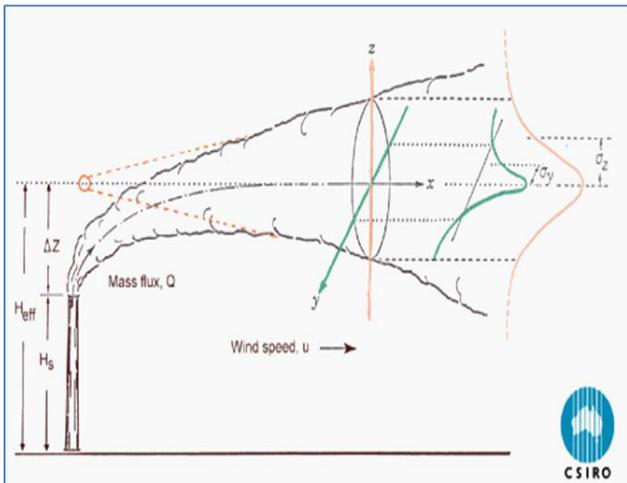
Figure 1 - Lagrangian Modeling Scheme

Figure 2- Eularian Modeling Scheme

Community Multi-scale Air Quality (CMAQ) - EPA's CMAQ modeling system is supported by the Community Modeling and Analysis System (CMAS) Center. The CMAQ model includes state-of-the-science capabilities for conducting urban to regional scale simulations of multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation.

Comprehensive Air quality Model with extensions (CAMx) - The CAMx model simulates air quality over many geographic scales. The model treats a wide variety of inert and chemically active pollutants, including ozone, particulate matter, inorganic and organic PM2.5/PM10, and mercury and other toxics. CAMx also has plume-in-grid and source apportionment capabilities.

Regional Modeling System for Aerosols and Deposition (REMSAD) - REMSAD was designed to calculate the concentrations of both inert and chemically reactive pollutants by simulating the physical and chemical processes in the atmosphere that affect pollutant concentrations over regional scales. It includes those processes relevant to regional haze, particulate matter and other airborne pollutants, including soluble acidic components and mercury.

Basic Photochemical Air Quality Model Diagram
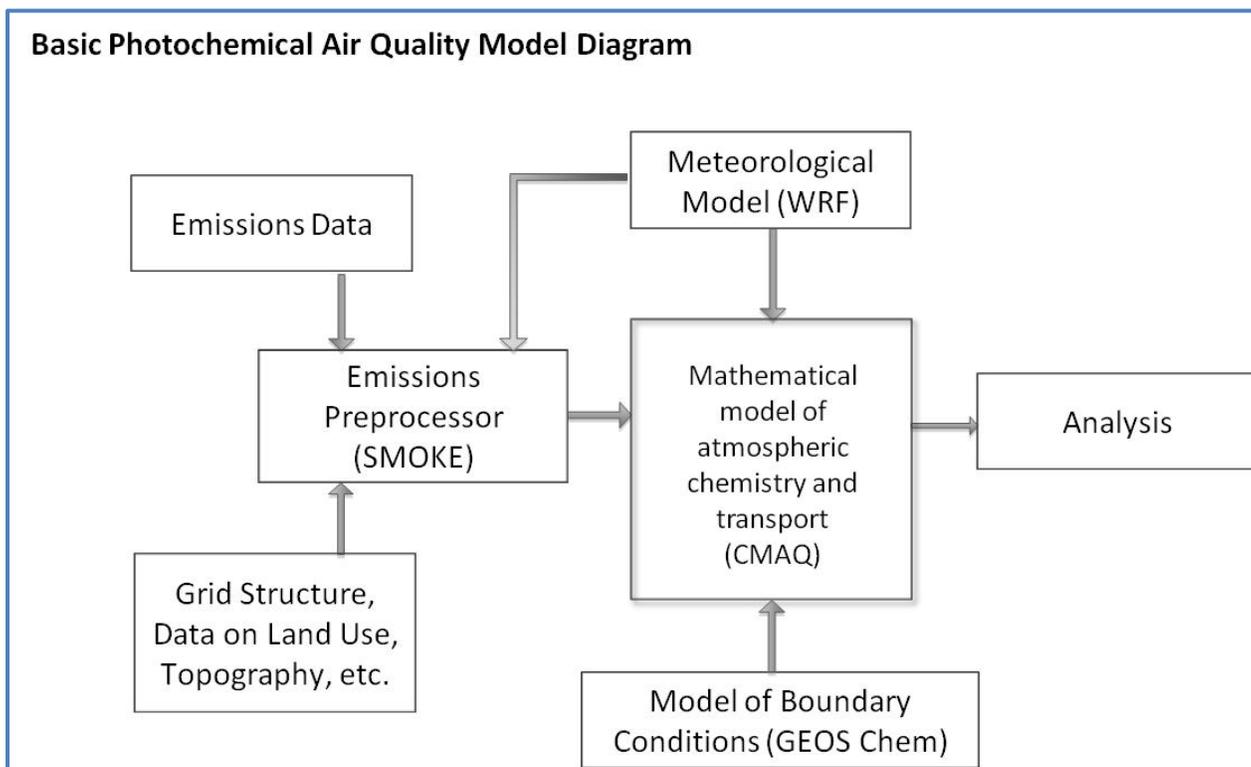
Urban Airshed Model Variable Grid (UAM-V ®)- The UAM-V Photochemical Modeling System was a pioneering effort in photochemical air quality modeling in the early 1970s and has been used widely for air quality studies focusing on ozone. It is a three-dimensional photochemical grid model designed to calculate the concentrations of both inert and chemically reactive pollutants by simulating the physical and chemical processes in the atmosphere that affect pollutant concentrations. This model is typically applied to model air quality "episodes" - periods during which adverse meteorological conditions result in elevated ozone pollutant concentrations.[1]

What is CB05? - An important component of air quality models (AQMs) is the photochemical
mechanism that describes how volatile organic compounds (VOCs) and oxides of nitrogen (NOx) interact to produce ozone and other oxidants. Three of the most commonly used chemical mechanisms in current AQMs for both regulatory and research applications include the Carbon Bond 4 (CB4) (Gery et al., 1989), SAPRC-99 (Carter, 2000), and CB05 (an update to CB4, Yarwood et al., 2005). All three mechanisms have been evaluated against measurements from a large number of chamber experiments and have been demonstrated to be reasonably successful in predicting ozone and related species from complex mixtures in 'typical' urban atmospheres.[2]

Carbon Bond mechanism developed in 2005 (CB05) is a mechanism of atmospheric oxidant chemistry that provides a basis for computer modeling studies of ozone, particulate matter (PM), visibility, acid deposition and air toxics issues. CB05 accounts for156 reactions involving 51 species. It is considered to be a condensed version of what is known to occur in atmospheric ozone chemistry which is intended to cover the most prevalent reactions but condensed to allow a reasonable model runtime. [3]

Who does photochemical modeling?

For the most part, regional photochemical modeling is done by regional planning organizations. This is because the pollutants originate from sources located across broad geographic areas. As a result, initially to address visibility, EPA encouraged States and Tribes to work regionally and provided funding to five regional planning organizations to address regional haze and related issues. This impetus has shifted over time to include other air quality issues besides visibility. And in some cases, the state groupings have shifted. For example, Virginia works with both the northeastern and the southeastern states. The current modeling organization is described below.

Northeastern United States

A loose consortium of states and other organizations under the leadership of the Ozone Transport Commission prepare regional modeling that is used by the northeastern states. States and groups performing the modeling include New York, New Jersey, Virginia, New Hampshire and NESCAUM. MARAMA plays a supporting role by preparing the emissions inventory and running emissions models.

Southeastern United States

The Southeastern Modeling, Analysis, and Planning (SEMAP) project is overseen by Metro 4 and SESARM. It is designed to meet the following goals:

- leverage the resources and capabilities of local and state agencies in the ten southeastern states
- assess regional air quality in relation to national ambient air quality standards and regional haze goals
- determine possible emission controls that will reduce transport and assist states in meeting Clean Air Act requirements
- offer interaction with stakeholders having various interests in the project
- provide documentation and data to support submittal to EPA of State Implementation Plans

The SEMAP project is organized as follows:

- State and Tribal Air Directors (STAD) – sets policies for the project and provides management oversight
- Coordinating Committee – oversees general operations and coordinates the project
- Technical Analysis Work Group – conducts detailed technical work with the assistance of various contractors
- Teams
- Emissions and Air Quality Modeling Team
- Emissions Inventory Team
    - EGUs Subgroup
    - Fires Subgroup
    - MOVES Subgroup
    - Meteorological Modeling Team

Upper Midwest

Lake Michigan Air Directors Consortium (LADCO) performs photochemical modeling for Ohio, Michigan, Wisconsin, Illinois and Indiana.

Central States

Central Regional Air Planning Association (CENRAP) coordinates photochemical modeling for this region

Western States

The Western Regional Air Partnership (WRAP) coordinates interstate technical analyses.

California and Texas

These two states perform their own photochemical modeling.

What is Dispersion Modeling?

Atmospheric dispersion modeling is the mathematical simulation of how air pollutants disperse in the ambient atmosphere. It is performed with computer programs that solve the mathematical equations which simulate the pollutant dispersion as a result of winds, rain, and random motion. Most modern dispersion models also account for wet and dry deposition on surfaces. The dispersion models are used to estimate or to predict the downwind concentration of air pollutants or toxins emitted from sources such as industrial plants, vehicular traffic or accidental chemical releases. The important difference between a dispersion model and a photochemical model is that dispersion models do not account for any chemical transformation of pollutants. Another practical difference is that most dispersion models are Lagrangian while most photochemical models are eulerian
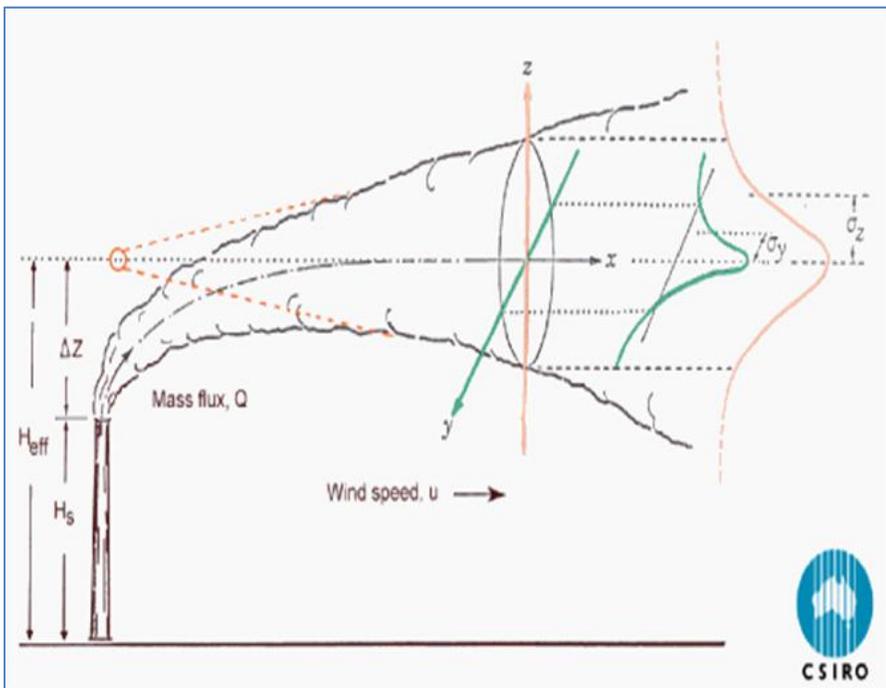
Figure 1 - Lagrangian Modeling Scheme

Unlike photochemical modeling, where larger regions band together to perform modeling, dispersion modeling is generally done by all states to evaluate proposed projects that might impair air quality. Dispersion models are typically employed to determine whether existing or proposed new industrial facilities are or will be in compliance with the National Ambient Air Quality Standards (NAAQS). The models also serve to assist in the design of effective control strategies to reduce emissions of harmful air pollutants.

Air dispersion models are also used by public safety responders and emergency management personnel for emergency planning of accidental chemical releases. Models are used to determine the consequences of accidental releases of hazardous or toxic materials from fires, spills or explosions. The results of dispersion modeling, using worst case accidental release source terms and meteorological conditions, can provide an estimate of location impacted areas, ambient concentrations, and be used to determine protective actions appropriate in the event a release occurs.

The dispersion models vary depending on the mathematics used to develop the model, but all require the input of data that may include:

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- Meteorological conditions such as wind speed and direction, the amount of atmospheric turbulence (as characterized by what is called the "stability class"), the ambient air temperature, the height to the bottom of inversions aloft that may be present, cloud cover and solar radiation.
- Emissions or release parameters such as emission rate, location and height, type of source (i.e., fire, pool or vent stack) and exit velocity, exit temperature and mass flow rate or release rate.
- Terrain elevations at the source location and at the receptor location(s), such as nearby homes, schools, businesses and hospitals.
- The location, height and width of obstructions (such as buildings or other structures) in the path of the emitted gaseous plume, surface roughness or the use of a more generic parameter "rural" or "city" terrain.

Many dispersion modeling programs include a pre-processor module for the input of meteorological and other data, and many also include a post-processor module for graphing the output data and/or plotting the area impacted by the air pollutants on maps. The plots of areas impacted may also include isopleths showing areas of minimal to high concentrations that define areas of the highest health risk. The isopleths plots are useful in determining protective actions for the public and responders.

Dispersion models are also known as atmospheric diffusion models, air dispersion models, air quality models, and air pollution dispersion models.

AERMOD

AERMOD is the USEPA sponsored dispersion model that replaces for ISC3. It is currently the preferred model for regulatory permit modeling. The AERMOD model is applicable to rural and urban areas, flat and complex terrain, surface and elevated releases, and multiple sources (including, point, area and volume sources). AERMOD is a steady-state plume model (Lagrangian).
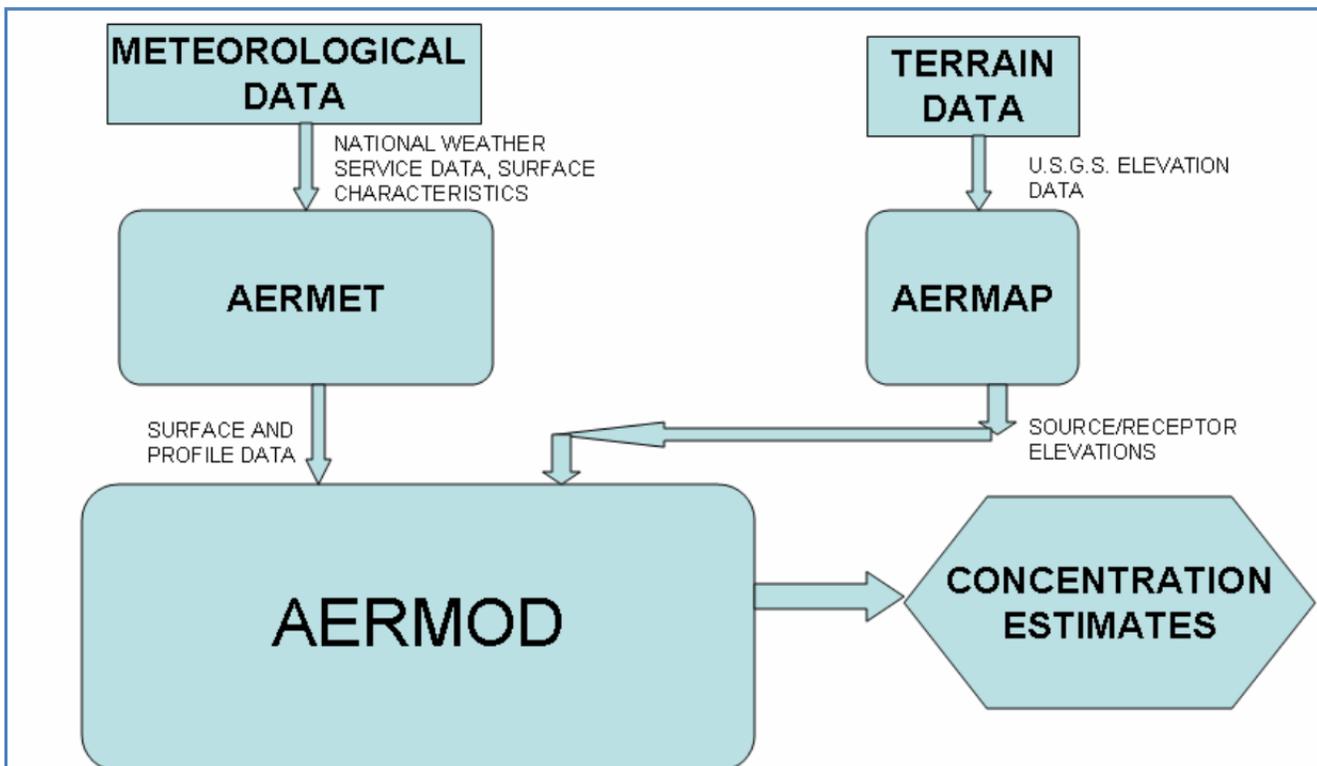

Figure 3 - Flow Diagram of the AERMOD Modeling System

Convective boundary Layer (CBL) - In the stable boundary layer (SBL), it assumes the concentration distribution to be Gaussian in both the vertical and horizontal. In the convective boundary layer (CBL), the horizontal distribution is also assumed to be Gaussian, but the vertical distribution is described with a bi-Gaussian probability density function (pdf). Additionally, in the CBL, AERMOD treats "plume lofting," whereby a portion of plume mass, released from a buoyant source, rises to and remains near the top of the boundary layer before becoming mixed into the CBL. AERMOD also tracks any plume mass that penetrates into the elevated stable layer, and then allows it to re-enter the boundary layer when and if appropriate. For sources in both the CBL and the SBL AERMOD treats the enhancement of lateral dispersion resulting from plume meander.

One of the major improvements in AERMOD as compared to ISC3 is its ability to characterize the PBL through both surface and mixed layer scaling. AERMOD constructs vertical profiles of required meteorological variables based on measurements and extrapolations of those measurements using similarity (scaling) relationships. Vertical profiles of wind speed, wind direction, turbulence, temperature, and temperature gradient are estimated using all available meteorological observations.

Meteorological Data - AERMOD can operate using data that is readily available from National Weather Service (NWS) stations. AERMOD requires only a single surface measurement of wind speed (measured between 7 zo and 100m - where zo is the surface roughness height), wind direction and ambient temperature. Like ISC3, AERMOD also needs observed cloud cover. However, if cloud cover is not available (e.g. from an on-site monitoring program) two vertical measurements of temperature (typically at 2 and 10 meters), and a measurement of solar radiation can be substituted. A full morning upper air sounding (RAWINSONDE) is required in order to calculate the convective mixing height throughout the day. Surface characteristics (surface roughness, Bowen ratio, and albedo) are also needed in order to construct similarity profiles of the relevant PBL parameters.

Complex Terrain - Using a relatively simple approach, AERMOD incorporates current concepts about flow and dispersion in complex terrain. Where appropriate the plume is modeled as either impacting and/or following the terrain. This approach has been designed to be physically realistic and simple to implement while avoiding the need to distinguish among simple, intermediate and complex terrain, as required by other regulatory models. As a result, AERMOD removes the need for defining complex terrain regimes. All terrain is handled in a consistent and continuous manner while considering the dividing streamline concept (Snyder et al. 1985) in stably stratified conditions.

HYSPLIT

The [4]HYSPLIT (HYbrid Single-Particle Lagrangian Integrated Trajectory) is a dispersion modeling system developed a result of a joint effort between NOAA and Australia's Bureau of Meteorology. The model is a complete system for computing simple air parcel trajectories to complex dispersion and deposition simulations. It is designed to ingest NOAA weather products with very little preprocessing, resulting in relatively easy application.
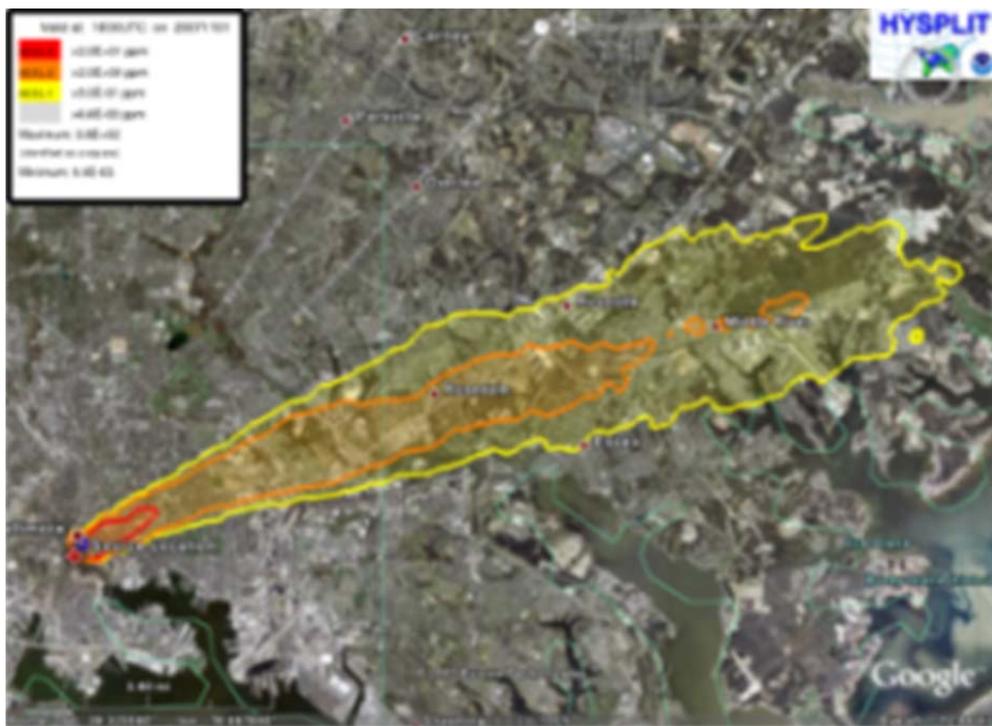
Figure 4 - Typical Dispersion Modeling Output

The dispersion of a pollutant is calculated by assuming either puff or particle dispersion. In the puff model, puffs expand until they exceed the size of the meteorological grid cell (either horizontally or vertically) and then split into several new puffs, each with its share of the pollutant mass. In the particle model, a fixed number of particles are advected about the model domain by the mean wind field and spread by a turbulent component. The model's default configuration assumes a 3-dimensional particle distribution (horizontal and vertical).

The model can be run interactively on the Web through the READY system on the NOAA ARL site or the code executable and meteorological data can be downloaded to a Windows or Mac PC. The web version has been configured with some limitations to avoid computational saturation of our web server. The registered PC version is complete with no computational restrictions, except that user's must obtain their own meteorological data files. The unregistered version is identical to the registered version except that plume concentrations cannot be calculated with with forecast meteorology data files. The trajectory-only model has no restrictions and forecast or archive trajectories may be computed with either version.

Some new features include improved advection algorithms, updated stability and dispersion equations, continued improvements to the graphical user interface, and the option to include modules for chemical transformations. Without the additional dispersion modules, Hysplit computes the advection of a single pollutant particle, or simply its trajectory.

What are the California Models: CALPUFF and CALGRID?

In 1990 California Air Resources Board (ARB) sponsored the development of a suite of models that would work off of the same input files to perform a variety of tasks. A modeling system was designed (Scire et al., 1987) consisting of three components: (1) a meteorological modeling package, (2) a Gaussian puff dispersion model with chemical removal, wet and dry deposition, building downwash, complex terrain algorithms, and other effects, and (3) post processing programs for the output fields of meteorological data, concentrations and deposition fluxes produced by the models. The meteorological model and puff dispersion model were named CALMET and CALPUFF, respectively.

CALPUFF

Since that time, CALPUFF has gained national and international acceptance and it is an accepted model for assessing long range transport of pollutants and their impacts on Federal Class I area. The modeling system consists of three main components and a set of preprocessing and post processing programs.

The main components of the modeling system are CALMET (a diagnostic 3-dimensional meteorological model), CALPUFF (an air quality dispersion model), and CALPOST (a post processing package). Each of these programs has a graphical user interface (GUI).

In addition to these components, there are other processors that may be used to prepare geophysical (land use and terrain) data in many standard formats, meteorological data (surface, upper air, precipitation, and buoy data), and interfaces to other models such as the Penn State/NCAR Mesoscale Model (MM5), the National Centers for Environmental Prediction (NCEP) Eta/NAM and RUC models, the Weather Research and Forecasting (WRF) model and the RAMS model.[5]

CALGRID

CALGRID (California Photochemical Grid Model) is a photochemical grid model and is distributed by the California EPA Air Resources Board (CARB) Modeling and Meteorology Branch. CALGRID has not been fully evaluated and has not been approved for routine regulatory use in California. The model as currently distributed uses the 1990 SAPRC chemical mechanism. CARB will provide revisions at no additional cost as they become available. CALGRID comes with some sample emissions processing routines, and software for chemical mechanism generation. It should be noted that it will be necessary to develop your own emissions pre-processors. While CALGRID does not have a post-processor, the output files from CALGRID are compatible with the CALMET post-processor.

What is Receptor Modeling?

Receptor models are mathematical or statistical procedures for identifying and quantifying the sources of air pollutants at a receptor location. Unlike photochemical and dispersion air quality models, receptor models do not use pollutant emissions, meteorological data and chemical transformation mechanisms to estimate the contribution of sources to receptor concentrations. Instead, receptor models use the chemical and physical characteristics of gases and particles measured at source and receptor to both identify the presence of and to quantify source contributions to receptor concentrations. These models are therefore a natural complement to other air quality models and are used as part of State Implementation Plans (SIPs) for identifying sources contributing to air quality problems.

In recent years more species are being measured in the ambient air. In addition ambient species measurements are stratified by particle size, and shorter durations of sampling. Receptor model algorithms have also improved greatly to take advantage of these higher quality data sets.

The EPA has developed the Chemical Mass Balance (CMB) and UNMIX models as well as the Positive Matrix Factorization (PMF) method for use in air quality management. CMB fully apportions receptor concentrations to chemically distinct source-types depending upon the source profile database, while UNMIX and PMF internally generate source profiles from the ambient data.

Chemical Mass Balance (CMB) Model

The Chemical Mass Balance (CMB) Model EPA-CMBv8.2 calculations are based on an effective-variance least squares method (EVLS). CMB requires speciated profiles of potentially contributing sources and the corresponding ambient data from analyzed samples collected at a single receptor site. CMB is ideal for localized nonattainment problems and has proven to be a useful tool in applications where steady-state Gaussian plume models are inappropriate, as well as for confirming or adjusting emissions inventories. Guidance in their use may be found in Section 5.2.2 of the " Guideline on Air Quality Models".

Positive Matrix Factorization 3.0 (EPA PMF 3.0)

EPA PMF is a receptor model that uses ambient measurements and estimated uncertainties in those measurements to infer emission sources likely impacting a monitor and by how much. The solution is based on a constrained weighted least squares approach. The software has a graphical user interface (GUI) that makes entering data and viewing modeling results easy. The current versions of EPA PMF (versions 1.x) solve the relatively simple bilinear model. The model is being developed and freely distributed by ORD.

Unmix 6.0

EPA Unmix is a receptor model that uses ambient measurements to determine the number of source types and their impacts at a monitoring site. The Unmix algorithm is based on defining feasible solution space for the input data. This space is derived using edges or sample groups with relatively low impacts. These edges define source types which account for the majority of variability in the data. The software has a graphical user interface (GUI) that makes entering data and viewing modeling results easy. The model is being developed and freely distributed by ORD.

What is source apportionment within photochemical modeling?

The purpose of source apportionment modeling is to identify culpability for air pollution concentrations to specific upwind sources or regions or source types. Source apportionment is now available within photochemical models, such as CMAQ and CAMX which is an improvement over traditional brute-force (also called "zero-out") modeling, and it has the advantage of being much more computationally efficient. For instance, to estimate the contribution from 20 source regions, a total of 20 individual zero-out simulations would be needed, compared with only one source apportionment simulation. There are multiple source apportionment methodologies. For a particular application, developers can choose a method by deciding the most appropriate balance of computation speed, thoroughness in model formulation, and ease of use.

Ozone, PM2.5, and mercury source apportionment are implemented in photochemical grid models such as CMAQ and CAMx. In CMAQ the particulate and ozone tracking are done by PPTM and OPTM, respectively. In CAMx particulate and ozone tracking are done by The Particulate Source Apportionment Tool (PSAT) and The Ozone Source Apportionment Tool (OSAT) respectively.

Example uses of photochemical model source apportionment include:

- Quantifying the contribution of precursor emissions from source sectors (e.g., points, onroad mobile, non-road, fires) or specific types of facilities (e.g., power plants, pulp and paper mills, chemical manufacturing facilities) to estimated concentrations at selected locations throughout the modeling domain.
- Quantifying the contribution of emissions from selected geographical regions (e.g., one or more states) to regional ozone, mercury, or PM2.5 concentrations.
- Quantifying the contribution from estimated boundary conditions to ozone, mercury, or PM2.5 concentrations at selected locations.
- Tracking the fate of emissions from specific facilities to estimate their range of influence and contribution to ozone or PM2.5 concentrations in nonattainment areas throughout the modeling domain.
- Quantifying the contribution of emissions from selected sources or source categories to visibility impairment in Class I areas (National Parks and Monuments).

An evaluation by USEPA of the CMAQ and CAMx tracking systems found them to be quite similar, although CAMx/PSAT and CAMx/OSAT seem to be more scientifically sound for the following reasons:

- Careful consideration of mass conservation issues,
- Explicit treatment of dry deposition of the tagged (reactive tracers) species, and
- Separation of ozone production scenarios for NOx-limited and VOC-limited conditions.

Ozone source apportionment tracks the contribution to model ozone estimates from precursor emissions of nitrogen oxides (NOx) and volatile organic compounds (VOCs). Particulate source apportionment tracks contributions to particulate species from precursor emissions. Emissions of NOx are tracked through all intermediate nitrogen species to particulate nitrate ion. Sulfur dioxide and sulfuric acid emissions are tracked to particulate sulfate ion. Ammonia emissions are tracked to particulate ammonium ion. Even though ammonium nitrate is chemically coupled, the apportionment schemes typically do not attempt to determine which species is limiting the formation, and directly attributes precursor gases to specific particulate ions. [6]

What is a Modeled Attainment Test including "Relative Reduction Factor" (RRF)?

A *modeled attainment test* is an exercise in which an air quality model is used to simulate current and future air quality. If future estimates of ozone and/or PM2.5 concentrations are less than the NAAQS, then this element of the attainment test is satisfied.

Relative reduction factors (RRF) are used when model estimates are used in a "relative" rather than "absolute" sense. The *relative reduction factors* is the ratio of the model's future to current (baseline) predictions at monitors. Future ozone and/or PM2.5 concentrations are estimated at existing monitoring sites by multiplying a modeled relative response factor at locations "near" each monitor by the observation-based, monitor-specific, "baseline" design value. The resulting predicted "future concentrations" are compared to NAAQS.

The test for ozone is based on the calculation of a single mean ozone RRF for each monitor. The PM2.5 attainment test is more complicated and reflects the fact that PM2.5 is a mixture. In the test, ambient PM2.5 is divided into major components. These are

- mass associated with sulfates
- mass associated with nitrates
- mass associated with ammonium
- mass associated with organic carbon
- mass associated with elemental carbon
- mass associated with particle bound water
- mass associated with "other"primary inorganic particulate matter
- and passively collected mass

A separate RRF is calculated for each of the PM2.5 components (except passive mass). We call each of these site-specific ratios, component-specific RRFs. Future PM2.5 design values are estimated at existing monitoring sites by multiplying modeled relative response factors "near" each monitor times the observed "component specific design value". This latter quantity is estimated using measured site-specific design values for PM2.5 in concert with available measured composition data. Future site-specific PM2.5 design values at a site are estimated by adding the future year values of the seven PM2.5 components. If all future site-specific PM2.5 design values are # the concentration specified in the NAAQS, the test is passed.[7]

Preparing a regional modeling inventory

Select **years** (states)

Gather information from states, EPA, other regions, & Canada (modelers and MARAMA)

Adjust & adapt information

Run **emissions models** for base year (MOVES, NONROAD, CMU Ammonia, ERTAC)

Project the inventory to future years

- Apply growth/control factors for non-EGU point and area (all)
- Run emissions models for on-road, non-road, and EGU (various)
- Adjust base inventory to create "what if" scenarios (various)
- **QA/QC** (all)

Convert files to ORL format and **run SMOKE** to create gridded hourly inventory (modelers and MARAMA)

How many months does all this take?

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
Select Base			Select Future																					
			Gather information for base year								Gather info. for future													
						Adjust & Adapt Information																		
						Run Emission models - base					- future												
											Project to future year													
			QA/QC																					
																			ORL		SMOKE			
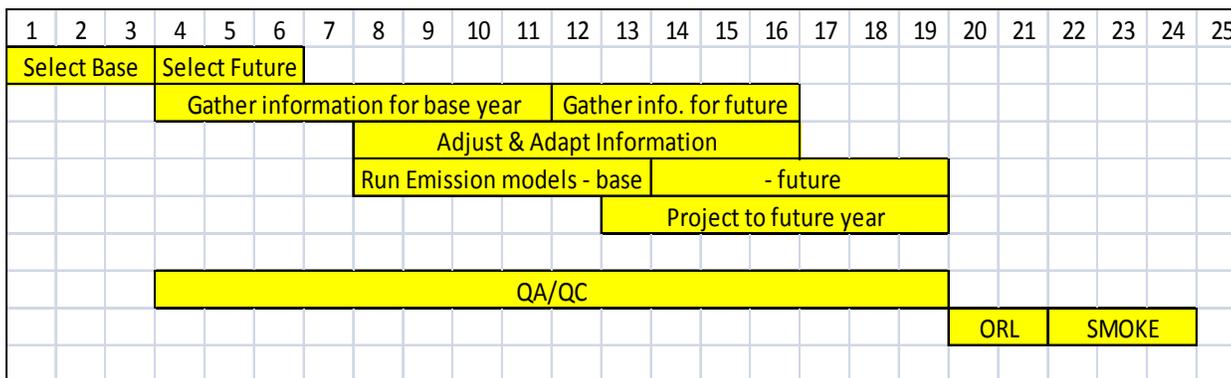
PLUS OR MINUS 6 MONTHS - DEPENDS ON :

- Collaboration by a lot of people…what are their priorities?
- Timing of EPA guidance
- SIP quality or preliminary analysis?
- Time is spent reworking due to errors or change in direction.

Keys to Success:

- Engaged state inventory staff / Coordination by MARAMA / Competent contractor support
- An early and organized start can help.
- Uncertain direction from USEPA – changing target on NAAQS deadline
- Extra burden imposed on state staff when selecting a non-NEI inventory year. Develop strategies to minimize the effort.
- Substantial review time needed for state & stakeholder feedback
- Significant delays due to MOVES and ERTAC EGU – still ongoing

What are emissions models?

Several emissions models are available for use in SIPs. While no single model has been specifically created for all situations of SIP development, each model is generally capable of performing the temporal, chemical, and spatial allocation steps as well as various other steps. The models each have different capabilities, limitations, and nuances. Examples of emissions models include MOVES, IPM, NMIM, BEIS and the Residential Wood Calculation Tool. These are discussed further as follows:

What is MOVES?

MOVES (MOtor Vehicle Emissions Simulator) is a computer program designed by the US Environmental Protection Agency (EPA) to estimate air pollution emissions from mobile sources covering a broad range of pollutants and allows multiple scale analysis.   MOVES currently estimates emissions from cars, trucks & motorcycles. EPA plans to add the capability to model non-highway mobile sources in future releases.

MOVES is designed to allow users to analyze motor vehicle emissions at multiple scales, from national to county level to project level, using different levels of input data.[8]

Why did EPA develop MOVES?

The Clean Air Act requires EPA to develop and regularly update emission factors for all emission sources. Pursuant to this charge, EPA.s Office of Transportation and Air Quality (OTAQ) has developed a number of emission and emission factor estimation tools for mobile sources, including MOBILE (for highway vehicles) and NONROAD (for off-road mobile source pollutants). EPA is proposing to update these tools with the Multi-scale mOtor Vehicle and equipment Emission System (MOVES), which is intended to include and improve upon the capability of these tools and, eventually, to replace them with a single, comprehensive modeling system.

The National Research Council (NRC) published a thorough review of EPA's mobile source modeling program in 2000. The NRC provided several recommendations for improving EPA's mobile source modeling tools, including: (a) the development of a modeling system more capable of supporting smaller-scale analyses; (b) improved characterization of emissions from high-emitting vehicles, heavy-duty vehicles, and off-road sources; (c) improved characterization of particulate matter and toxic emissions; (d) improved model evaluation and uncertainty assessments; and (e) a long-term planning effort coordinated with other governmental entities engaged in emissions modeling.[9]

What types of input data are needed for MOVES?

The County Data Manager (CDM) requires certain inputs in order to reflect local conditions.

Age Distribution - Age distribution is the input that describes the average age of the local fleet. In the CDM, the user must supply the age distribution for each source use type defined in MOVES.

Average Speed Distribution - Average speed distributions describe the range of driving behavior on local roads. In the CDM the user must supply the fraction of activity for each of the average speed bins for each source use type on each road type for each hour of each day type in MOVES.

Road Type Distribution - Road type distributions describe the fraction of vehicle activity that occurs on each road type. In the CDM the user must supply the fraction of activity for each source use type on each road type in MOVES.

Meteorology Data - Meteorology data are the ambient atmospheric parameters that affect emissions. The CDM requires the user to supply the hourly temperature and relative humidity for the county (zone). More detailed meteorological data is provided through the MetforMOVES model for use with the look up table mode.

Ramp Fraction - Ramp fraction indicates the amount of ramp activity associated with road type.

Fuel Supply - Fuel supply indicates the properties of the fuels used in a county at a particular time. In the CDM the user must supply the market share for each fuel formulation for each month. To reduce the resources needed to run MOVES, OTC used only two "fuel months" rather than having a different value for each of 12 months.

Vehicle Type VMT - Vehicle type vehicle miles traveled (VMT) indicates vehicle operation in the county. The CDM requires users to supply annual VMT for each of six Highway Performance Monitoring System (HPMS) vehicle classifications.

I/M - Inspection and maintenance (I/M) programs are mandatory periodic vehicle inspections that require repairs to emission control systems on vehicles. [10]

What is the difference between the inventory mode and the look-up table mode in MOVES?

The inventory mode of MOVES is used to calculate county-wide or project level emissions. In this mode average monthly temperatures are used to estimate emissions.

The look-up table mode uses actual hourly temperatures to estimate emissions. To simplify this process the program first generates a large table of emission rates for every possible temperature and emission sources. The table is then used in conjunction with SMOKE-MOVES to create hourly, gridded inventories for use in regional air quality models.

What is SMOKE-MOVES?

The SMOKE-MOVES interface is a set of programs that use the MOVES emission rate tables to create data for use in the SMOKE model. SMOKE processes the output of these models and creates gridded hourly mobile source emissions data files for use in regional air quality models. A diagram follows that shows the relationships between the various models.

Where can I find guidance for using MOVES in SIP planning?

1. "Policy Guidance on the Use of MOVES2010 for State Implementation Plan Development, Transportation Conformity, and Other Purposes" EPA-420-B-09-046December 2009 is posted on the internet at http://www.epa.gov/otaq/models/moves/420b09046.pdf
2. "MOVES2010 User Guide": This guide provides detailed instructions for setting up and running MOVES2010. Available at http://www.epa.gov/otaq/models/moves/index.htm.
3. "Technical Guidance on the Use of MOVES2010 for Emission Inventory Preparation in State Implementation Plans and Transportation Conformity": This document provides guidance on appropriate input assumptions and sources of data for the use of MOVES2010 in SIP submissions and regional emissions analyses for transportation conformity determinations. Available at http://www.epa.gov/otaq/stateresources/transconf/policy.htm.
4. "Transportation Conformity Guidance for Quantitative Hot-spot Analyses in PM2.5 and PM10 Nonattainment and Maintenance Areas": This document explains how to use MOVES2010 to complete hot-spot analyses required for projects of local air quality concern in PM2.5 and PM10 nonattainment

and maintenance areas. This guidance is presently under development and will be posted on the EPA's transportation conformity policy guidance website (http://www.epa.gov/otaq/stateresources/transconf/policy.htm) when available.3

5. Additional training materials, examples, and MOVES2010 technical information are available at the MOVES website: http://www.epa.gov/otaq/models/moves/index.htm.

6. The following contacts are available at EPA's Office of Transportation and Air Quality regarding this guidance:
   - for general questions about the MOVES model, email mobile@epa.gov;
   - for SIP questions, contact Rudy Kapichak at (734) 214-4574;
   - for transportation conformity questions, contact Meg Patulski at (734) 214-4842; and
   - for questions about the National Emissions Inventory, contact Laurel Driver at EPA's Office of Air Quality Planning and Standards at (919) 541-2859.
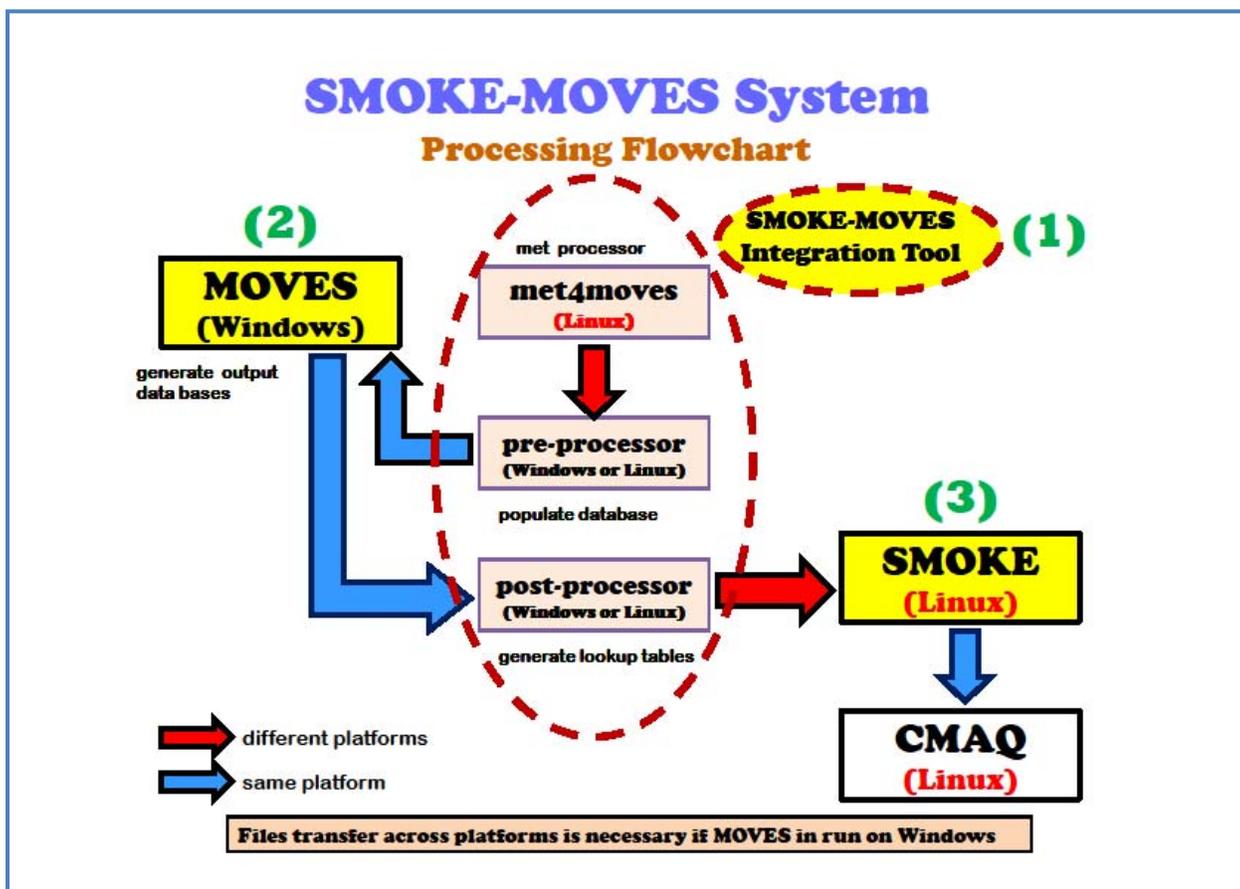
Figure 5 - SMOKE - MOVES System

What is NMIM?

The **National Mobile Inventory Model** (NMIM) is a free, desktop computer application developed by EPA to develop estimates of current and future emission inventories for on-road motor vehicles and nonroad equipment. NMIM uses current versions of MOBILE6 and NONROAD to calculate emission inventories. However, MOBILE6, used in NMIM, has been replaced by MOVES as EPA's official model for

estimating emissions from cars, trucks and motorcycles. Thus, NMIM cannot be used for official modeling of onroad emissions.

What is the NONROAD Model?

The NONROAD model calculates past, present, and future emission inventories (i.e., tons of pollutant) for all nonroad equipment categories except commercial marine, locomotives, and aircraft. Fuel types included in the model are: gasoline, diesel, compressed natural gas, and liquefied petroleum gas. The model estimates exhaust and evaporative hydrocarbons (HC), carbon monoxide (CO), oxides of nitrogen (NOx), particulate matter (PM), sulfur dioxide (SO2), and carbon dioxide (CO2). The user may select a specific geographic area (i.e., national, state, or county) and time period (i.e., annual, monthly, seasonal, or daily) for analysis.

NONROAD2008 updated NONROAD2005 to include new nonroad emission standards promulgated in 2008 related to small gasoline engines and pleasure craft. NONROAD2008 accounts for the emission reductions associated with two rules finalized in 2008:

- Diesel recreational marine standards in the Locomotive/Marine final rule, (Federal Register Vol 73, No. 88, page 25098, May 6, 2008).
- Small SI and SI Recreational Marine final rule (Federal Register Vol 73, No. 196, page 59034, October 8, 2008). [11]

What is IPM?

The Integrated Planning Model (IPM) is a proprietary, multi-regional, dynamic, deterministic linear programming model of the U.S. electric power sector. It provides forecasts of least-cost capacity expansion, electricity dispatch, and emission control strategies for meeting energy demand and environmental, transmission, dispatch, and reliability constraints. It can be used to evaluate the cost and emissions impacts of proposed policies to limit emissions of SO2, NOx, carbon dioxide (CO2), and Hg from the electric power sector. The IPM model was a key analytical tool used by EPA in developing the Clean Air Interstate Rule (CAIR) and the Clean Air Mercury Rule (CAMR).

IPM was developed by ICF Consulting, Inc. (ICF) and used to support public and private sector clients.

IPM is particularly well suited to model multi-emissions environmental policies like CAIR and CAMR because it[12]:

- Captures complex interactions among the electric power, fuel, and environmental markets;
- Detail-rich representation of emission control options encompassing a broad array of retrofit technologies along with emission reductions through fuel switching, changes in capacity mix and electricity dispatch strategies; and
- Can model a variety of environmental market mechanisms, such as emissions caps, allowances, trading, and banking.

What quality assurance checks are needed for emissions modeling?

The purpose of QA for emissions modeling is to ensure that the inventories are correctly processed using the information the modeler intended. (It is assumed here that the inventory itself has already been QA'd through inventory QA procedures, as referenced in Section 17.3.) Emissions modeling QA includes such activities as reviewing log files for errors and warnings and addressing problems; comparing emissions between each of the processing stages (e.g., data import, speciation, temporal allocation) to ensure mass is conserved; checking that the correct speciation, temporal allocation, and spatial allocation factors were

applied; ensuring that emissions going into the air quality model are consistent with expected results; and checking modeling-specific parameters such as stack parameters. In addition, the process of running emission inventories through emissions models and air quality models often provides insights into the emission inventories. These insights can lead to inventory changes that improve the quality of inventories for additional modeling iterations.

In general, this guidance also encourages the use of graphical analysis and Geographic Information Systems (GIS) for improved QA of emissions data and processing. A commonly used analysis tool for model-ready emissions data is the **Package for Analysis and Visualization of Environmental Data (PAVE)**, available at http://www.cep.unc.edu/empd/EDSS/pave_doc/index.shtml.

Lastly, at the time this document was written, the EPA is developing the **Emissions Modeling Framework (EMF)**, which includes extensive data management and quality assurance features intended to assist emissions modelers with the enhanced quality of their data. This tool will be available for use in 2007 for support of ozone, PM2.5, and regional haze SIPs .[13]

A brief synopsis of appropriate quality assurance (QA) approaches for emissions modeling is available in Section 2.19 of the SMOKE manual (http://cf.unc.edu/cep/empd/products/smoke/version2.1/html/ch02s19.html).[14]

What models are used for biogenic emissions?

Biogenic emission sources are emissions that come from natural sources, and need to be accounted for in photochemical grid models, as most types are widespread and ubiquitous contributors to background air chemistry. Often only the emissions from vegetation and soils are included, but other relevant sources include volcanic emissions, lightning, and sea salt.

Biogenic emissions are typically computed using a model which utilizes spatial information on vegetation and land use and environmental conditions of temperature and solar radiation. The model inputs are typically horizontally allocated (gridded) data, and the outputs are gridded biogenic emissions which can then be speciated and utilized as input to photochemical grid models.[15]

What is BEIS?

EPA's biogenic emissions model is called the Biogenic Emission Inventory System (BEIS),[16]. The current version of BEIS estimates volatile organic compound (VOC) emissions from vegetation and nitric oxide (NO) and carbon monoxide (CO) emissions from soils. The current version of BEIS, the BEIS3.12 model, requires a land use database known as the Biogenic Emissions Land use Database, version 3 (BELD3). BELD3 data provides distributions of 230 vegetation classes at 1km resolution over most of North America.

Recent BEIS development has been incorporated into the Sparse Matrix Operational Kernel Emissions (SMOKE) system, so that the native version of BEIS is built within the SMOKE architecture.

What is MEGAN?

The Model of Emissions of Gases and Aerosols from Nature (MEGAN) is a modeling system for estimating the net emission of gases and aerosols from terrestrial ecosystems into the atmosphere. Driving variables include land cover, weather, and atmospheric chemical composition. MEGAN is a global model with a base resolution of ~ 1 km and so is suitable for regional and global models. A FORTRAN code is available for generating emission estimates for the CMAQ regional air quality model. The algorithms have also been incorporated as an on-line component in several regional and global chemistry and transport models. Global distributions of land cover variables (Emission Factors, Leaf Area Index, and Plant Functional Types) are available for spatial resolutions ranging from ~ 1 to 100 km and in several formats (ARCGIS, netcdf).

The MEGAN model was developed by the National Center for Atmospheric Research (NCAR).

What biogenic model is OTC using?

OTC modelers are using the MEGAN model.

What are Meteorological Models?

For air quality modeling purposes, meteorological grid models are used in conjunction with chemical interaction models to provide gridded output of chemical species or pollutant data. Meteorological grid models use mathematical formulations that simulate atmospheric processes such as the change of winds and temperature in time. These meteorological parameters are calculated at distinct spatially equidistant points over an area of interest which is called a grid. When these models are applied in a retrospective mode (i.e. modeling a past event) they are able to blend ambient data with model predictions via four-dimensional data assimilation, thereby yielding temporal and spatially complete data sets that are grounded by actual observations.

There are several commonly-used meteorological grid models that can develop inputs for air quality models. These grid models differ in their simulation of atmospheric processes but each produce gridded meteorological parameters. There are also several post-processors which are needed to convert the raw meteorological modeling output to suitable air quality model input. A few of the most commonly used meteorological models and post-processors are briefly described below.[17]

What is WRF?

The Weather Research and Forecasting (WRF) Model is a next-generation mesoscale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs. It features multiple dynamical cores, a 3-dimensional variational (3DVAR) data assimilation system, and a software architecture allowing for computational parallelism and system extensibility. WRF is suitable for a broad spectrum of applications across scales ranging from meters to thousands of kilometers.

The effort to develop WRF has been a collaborative partnership, principally among the National Center for Atmospheric Research (NCAR), the National Oceanic and Atmospheric Administration (the National Centers for Environmental Prediction (NCEP) and the Forecast Systems Laboratory (FSL), the Air Force Weather Agency (AFWA), the Naval Research Laboratory, the University of Oklahoma, and the Federal Aviation Administration (FAA). WRF allows researchers the ability to conduct simulations reflecting either real data or idealized configurations. WRF provides operational forecasting a model that is flexible and efficient computationally, while offering the advances in physics, numerics, and data assimilation contributed by the research community.[18]

What is MM5?

The PSU/NCAR mesoscale model (known as MM5) is a limited-area, nonhydrostatic, terrain-following sigma-coordinate model designed to simulate or predict mesoscale atmospheric circulation. The model is supported by several pre- and post-processing programs, which are referred to collectively as the MM5 modeling system. The MM5 modeling system software is mostly written in Fortran, and was developed at Penn State and NCAR as a community mesoscale model with contributions from users worldwide.[19]

Which model is OTC using?

The NY DEQ modelers for OTC chose to use WRF. It is newer than MM5 and has replaced MM5 for regional modeling.

What are emissions preprocessors like SMOKE?

Currently there are four emissions models used to process emissions for input into photochemical grid models. They are:

- Sparse Matrix Operator Kernel Emissions (SMOKE);
- Emissions Modeling System (EMS-2001);
- Emissions Preprocessor System - Version 2.5 (EPS 2.5) and version 3.0 (EPS-3); and
- Consolidated Community Emissions Processing Tool (CONCEPT).

The **Sparse Matrix Operator Kernel Emissions (SMOKE)**, SMOKE supports processing of criteria, mercury, and toxics inventories for stationary point, stationary area, mobile, and biogenic emissions.

It can create input files for the CMAQ, CAMX, UAM-V, and REMSAD air quality models. SMOKE was the basis for development of the BEIS3 system, so BEIS3 in its original form can be used easily with SMOKE. SMOKE is available for UNIX and Linux operating systems and is not recommended for use on a PC. It does not require third party software. It does not include utilities for creating speciation profiles, biogenic land use, or spatial surrogates, though the latter two datasets can be built using the Multimedia Integrated Modeling System (MIMS) Spatial Allocator Tool (http://www.cep.unc.edu/empd/projects/mims/spatial/).

Support for the SMOKE system is available through the Community Modeling and Analysis System (CMAS) help desk (http://www.cmascenter.org/html/help.html). The software and User's Guide are available through the University of North Carolina, Carolina Environmental Program (http://www.cep.unc.edu/empd/products/smoke).

The **Emissions Modeling System, (EMS 2001**), http://www.ladco.org/tech/emis/ems_2001/) is a later version of EMS-95, which was used in the modeling underlying the U.S. EPA NOx SIP call rule to reduce regional NOx emissions (U.S. EPA 1998b), as well as in other applications of nested regional air quality models. It can create inputs for the CAMX and UAM-V models. It includes the BIOME3 model, which provides access to similar calculations of biogenic emissions as are available in the BEIS3 system. EMS-2001 can be run on either Linux or Windows NT, and users must purchase a license for the SAS® software to use it. It includes utilities for creating speciation profiles, biogenic land use, and spatial surrogates. An updated version has new spatial processors, which limit the need for GIS software.

The **Emissions Preprocessor System - Version 2.5 (EPS-2.5)**, software and User's Guide are available through Systems Applications International/ICF Consulting (www.uamv.com). EPS-2.5 is a comprehensive emissions processing system that supports processing of stationary point, stationary area, and mobile emissions for the development of base and future-year modeling inventories for input to the CAMX, UAM-V, and REMSAD models. EPS-2.5 consists of a set of stand-alone FORTRAN programs that do not require third-party software. The system is capable of preparing local, regional, and continental-scale emission inventories for ozone, particulate matter, mercury, and air toxics modeling applications. EPS 2.5 is available for UNIX and Linux operating systems. It includes utilities for creating source-specific temporal and chemical speciation profiles based on locally provided detailed information for episode specific emission inventories. It also includes utilities for preparing spatial surrogates. In addition, EPS-2.5 has the capability of creating modeling inventories required for the application of source apportionment techniques such as UAM-V's Ozone and Precursor Tagging Methodology (OPTM). A newer version of EPS is also available, called EPS-3.

The **Consolidated Community Emissions Processing Tool (CONCEPT)** is an open source model written primarily in PostgreSQL. The database structure of the model makes the system easy to

understand, and the modeling codes themselves are documented to encourage user participation in customizing the system for specific modeling requirements. The CONCEPT model structure and implementation allows for multiple levels of QA analysis during every step of the emissions calculation process. Using the database structures, an emissions modeler can easily trace a process or facility and review the calculation procedures and assumptions for any emissions value. CONCEPT includes modules for the major emissions source categories: area source, point source, on-road motor vehicles, non-road motor vehicles and biogenic emissions, as well as a number of supporting modules, including spatial allocation factor development, speciation profile development, growth and control for point and area sources, and CEM point source emissions handling. Additional work by the emissions modeling community has begun development of CEM preprocessing software, graphical QA tools, and an interface to the traffic demand models for on-road motor vehicle emissions estimation.[20]

How does the modeling all fit together?

Selecting the modeling domain

The modeling domain will be selected based on the scale of the project. For source permitting, screening modeling is used to identify the area of impact. For NAAQS attainment modeling, the OTC domain is the eastern half of the United States because sources as far away as the Mississippi affect ozone and fine particulate air quality. Areas outside the modeling domain are represented as boundary conditions. This means the concentration of emissions flowing into the modeling domain across the boundary.

What is "Pre-processing" and "Post-Processing"? What is done? Why? What impact does it have?

Pre and Post processing means adjusting or converting the raw data to meet the requirements of the model and end user, respectively.

Pre - processing is done for a variety of reasons. Data used in models comes from a variety of sources. The groups that developed the data we use generally did not have air quality modeling in mind when it is collected, reported and stored. So, the data must be adjusted to meet the requirements of the model. In some cases this is pretty simple, like format changes, unit conversions (lb -> kg) or selecting out just a portion of a larger dataset for input to the model. In other cases it can be pretty complicated. For example: much of the meteorological data is pretty spotty. For whatever reason, it is just missing for many hours. The model cannot deal with gaps so the data must be preprocessed to fill those gaps using some statistical techniques to interpolate between complete data records.

Post-processing is also done for many different reasons. In MOVES, for example, the SMOKE-MOVES output is not reported by SCC – which is the format that we use in inventories. So, some rules have been developed to squeeze the MOVES output into the SCC categories that match the rest of our inventory.

The impact of the process is to make the input and output usable, but it has the down side that it is an opportunity for errors to creep into the work.

What is sensitivity modeling as opposed to "real" modeling?

Sensitivity modeling is done to understand how important a particular parameter is to the final result. In a sensitivity run a single parameter is varied and the resulting change in the modeled outcome is compared. Often times the term "sensitivity" is used interchangeably with "draft" or non-SIP quality runs. It these runs estimates or old data are used for certain parameters and sectors that are not yet fully calculated or available for use. For example, we do not yet have future year emissions calculated for 2020 EGUs so an estimate is being used for the draft model runs that have been performed to date. This is not a particularly appropriate use of the term sensitivity, but it is common so you should be aware of it.

A SIP-quality run will be run for entire year and will include final input files including emissions, and meteorology.

Summary

Type	Uses	Characteristics	Current Models		Associated or component programs	Developer	Status	Date
Photochemical Models	Used to estimate ozone and reactive particulate matter. Designed to predict long range transport and atmospheric chemical transformations over hundreds and even thousands of miles.	Coarse grid. Incorporates meteorological conditions and atmospheric chemical transformation of pollutants. For example: VOC + NOX -> Ozone. Usually Eularian construction.	CAMx		SMOKE, GEOS Chem, CBO5	Environ	Current	2006
			CMAQ		SMOKE, GEOS Chem, CBO5	U.S. EPA	Current	1998
			UAM-V		SMOKE, GEOS Chem, CBO5	SAIC	Current	1996
			CALGRID		CALMET, CALPOST	Scire, et al.	Other	1989
			MAQSIP			MCNC	Other	1996
			MAQSIP			Odman	Other	1996
			SAQM			Chang	Other	1997
			SAQM			CARB	Other	1996
			URM			Kumar	Other	1996
			REMSAD				Superceded	
Dispersion Models	Used to estimate the effect of local sources on the local atmosphere of pollutants that are not affected by chemical transformation.	Trajectory/Lagrangian modeling. Fine grid. Incorporates meterological conditions, local and regional topography and site characteristics. No chemical transfomation of pollutants. Usually Lagrangian construction.	AERMOD		AERMET, AERMAP	U.S. EPA	Current	2004
			Screen3	Screening		U.S. EPA	Current	
			CALPUFF		CALMET	Scire	Current	2000
			HYSPLIT			NOAA	Current (Fires)	1998
			ISC3			U.S. EPA	Superceded	1995
Receptor Models	Used to identify the primary sources of individual pollutants measured at a given location.	Uses a variety of means to estimate the source of elevated pollutant concentrations at a given location: including source measurements, statistical analysis and back trajectory meteorology.	PMF			Eberly	Current	2005
			PMF			Hopke	Current	2001
			UNMIX			Lewis	Current	2003
			CMB			U.S. EPA	Current	2004
Emissions Models	Used to calculate emissions for particular sectors of the inventory.	Combines information from a variety of sources including source measurements, economic models, the census, and GIS to estimate emissions from source sectors.	MOVES	Mobile	CDM	U.S. EPA	Current	2009
			SMOKE-MOVES	Mobile				
			MOBILE6	Mobile		U.S. EPA	Superceded	
			CAL3QHC /QHCR	Mobile (CO at intersections)	CALINE-3	California & USEPA	Other	Various
			ERTAC EGU	EGU		ERTAC	Under Development	2011
			IPM	EGU		ICF	Current	
			NMIM	Nonroad		U.S. EPA	Current	?
			BIOME3	Biogenic				
			BEIS	Biogenic	BELD3		Current	
			MEGAN	Biogenic			Current	
			Res Wood Tool.	Residential wood Comb.		ERTAC	Current	2010
Meteorological Models	Used to describe the meteorology for the modeled area.	Uses meterological observations and typical atmospheric patterns to estimate meterological conditions throughout the modeling domain.	WRF					
			CALMET					
			MM5					

Status:

- Current = USEPA considers this to be a default model. Acceptable for use in the described setting without justification.
- Other = A model that can be used in special circumstances if properly justified.
- Superceded = No longer an accepted model.

Resources for Learning about Air Quality Modeling

Some resources for learning more about air quality modeling

- EPA Technology Transfer Network
- Support Center for Regulatory Atmospheric Modeling http://www.epa.gov/scram001/guidanceindex.htm
- Materials from the EPA 2012 Modeling Conference http://www.epa.gov/ttn/scram/10thmodconf.htm

Some sources of EPA Guidance include:

Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze. (1,072KB,pdf) - Final version of the Ozone, PM2.5, and Regional Haze modeling guidance document.

Receptor Models – Information Online

Chemical Mass Balance (CMB Model)

Download the model and documentation:

http://www.epa.gov/ttn/scram/

Positive Matrix Factorization (PMF Model)

Download the model and documentation:

ftp://rock.helsinki.fi/pub/misc/pmf/

Get selected IMPROVE data in PMF format:

http://www.clarkson.edu/chemistry/pmf/

HySPLIT Trajectory Model

Run the Model Online

http://www.arl.noaa.gov/ready/traj.html

Download the Model

http://www.arl.noaa.gov/ss/models/gethysplit.html

Download Upper Air Data

EDAS: ftp://www.arl.noaa.gov/pub/archives/edas/

FNL: ftp://www.arl.noaa.gov/pub/arch/fnl/

NGM: ftp://www.arl.noaa.gov/pub/archives/ngm/

Raw Sounding Data: http://raob.fsl.noaa.gov/

UNMIX

Online Tutorial

http://capita.wustl.edu/PMFine/Workbook/PMTopics_PPT/WB_SourceAttr/Version2/tsld028.htm

IMPROVE Data and Information

Main Page: http://vista.cira.colostate.edu/improve/

Download Aerosol Data:
http://vista.cira.colostate.edu/improve/Data/DataQuery/IMP_Aer_Data_Access.asp

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Gebhart, Kristi A., Sonia A. Kreidenweiss, and William C. Malm (2001) "Back-Trajectory Analyses of Fine Particulate Matter Measured at Big Bend National Park in the Historical Database and the 1996 Scoping Study" *Science of the Total Environment*, **276**, 185-204. (A very recent paper in which back-trajectory techniques are used to examine source regions by season.)

Gebhart, Kristi A. and William C. Malm (2000) "A Preliminary Look at Source-Receptor Relationships in the Texas-Mexico Border Area," *Journal of the Air & Waste Management Association*, **50**, 858-868. (Another recent paper in which a variety of receptor techniques were used to examine source-receptor relationships at Big Bend National Park.)

Green, Mark C. and Ivar Tombach (2000) "Use of Project MOHAVE Perfluorocarbon Tracer Data to Evaluate Source and Receptor Models," *Journal of the Air & Waste Management Association*, **50**, 717-723. (A discussion of the ability of several source-apportionment techniques to predict measured tracer concentrations in a recent special study.)

Henry, Ronald C., Yi-Jin Wang, and Kristi A. Gebhart (1991) "The Relationship Between Empirical Orthogonal Functions and Sources of Air Pollution," *Atmospheric Environment*, **25A**, 503-509. (A discussion of the theory of how and why EOFs are related to airborne pollutant concentrations.)

Henry, Ronald C. (1987) "Current Factor Analysis Receptor Models are Ill-Posed," *Atmospheric Environment*, **21**, 1815-1820. (An easily understandable discussion of singular value decomposition and factor analysis, why results are sometimes un-physical, why additional constraints are needed, why rotation sometime gives more reasonable answers.)

Malm, William C., Kristi A. Gebhart, and Ronald C. Henry (1990) "An Investigation of the Dominant Source Regions of Fine Sulfur in the Western United States and their Areas of Influence," *Atmospheric Environment*, **24A**, 3047-3060. (An interesting comparison between the results of a back-trajectory technique and EOF analysis.)

Malm, William C. and Kristi A. Gebhart (1997) "Source apportionment of sulfur and light extinction using receptor modeling techniques, " *Journal of the Air & Waste Management Association*, **47**, 250-258. (Use of a combination of different receptor techniques to apportion primary and secondary particulate matter.)

Miller, M.S., S.K. Friedlander, and G.M. Hidy (1972) "A Chemical Element Balance for the Pasadena Aerosol," *J. Colloid Interface Sci.*, **39**, 165-176. (The original paper on what evolved into the CMB model.)

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Poirot, Richard L. and Paul R. Wishinski (1986) "Visibility, Sulfate and Air Mass History Associated with the Summertime Aerosol in Northern Vermont,"*Atmospheric Environment*, **20**, 1457-1469. (Like Ashbaugh et al., this is an early back-trajectory residence time paper. It came out about the same time, but describes the theory and derives the equations a bit differently.)

Richman, Michael B. "Rotation of Principal Components" (1986) *Journal of Climatology*, **6**, 293-335. (An excellent understandable discussion of principal components, empirical orthogonal functions (EOFs), rotation of factors, etc., written by a meteorologist rather than a mathematician or statistician.)

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Watson, John G., John A. Cooper, and James J. Huntzicker (1984) "The Effective Variance Weighting for Least Squares Calculations Applied to the Mass Balance Receptor Model," *Atmospheric Environment*, **18**, 1347-1355. (An often-referenced paper on the inclusion of uncertainties in the regressions for the CMB model.)

White, Warren H., Edward R. Macias, Jonathan D. Kahl, Perry J. Samson, John V. Molenar, and William C. Malm (1994) "On the Potential of Regional-Scale Emissions Zoning as an Air Quality Management Tool for the Grand Canyon," *Atmospheric Environment*, **28**, 1035-1045. (Back-trajectory modeling and the clean air corridor concept.)

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3 UPDATES TO THE CARBON BOND CHEMICAL MECHANISM: CB05, by Greg Yarwook and Sunja Rao, ENVIRON, and Mark Yocke, Yocke & Company and Gary Z. Whitten, Smog Reyes, for EPA, December 8, 2005. Downloaded from http://www.camx.com/publ/pdfs/CB05_Final_Report_120805.pdf on 3/5/2012.

4 HYSPLIT - NOAA Air Resources Laboratory website downloaded 3/5/2012 at http://www.arl.noaa.gov/HYSPLIT_info.php

5   TRC Atmospheric Studies Group website at http://www.src.com/calpuff/calpuff1.htm downloaded 3/5/2012

6 http://www.epa.gov/scram001/reports/SourceApportionmentPeerReview.pdf

7 -- Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze, EPA-454/B-07-002, April 2007, posted at http://www.epa.gov/ttn/scram/guidance/guide/final-03-pm-rh-guidance.pdf pages 15-16.

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