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# Chapter 2

# The Tool – Mathematical Modeling

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**Abstract:** This chapter addresses modeling background – needs and concepts - and definitions in a brief survey. Topics include uses of models (regulatory compliance and resolution of litigation), categorization of model by general type (Gaussian and grid-based), general governing equations, categories of model inputs, types of solutions of equations, alternative model formulations, spatial and temporal scales addressed and resolutions adopted, types of uncertainty of concern, experience and current and proposed approaches to evaluation of model performance, and data needs.

**Key Words:** Gaussian model, Lagrangian puff model, photochemical models, grid-based models, air quality modeling, simulation models, emissions modeling, dispersion modeling, chemical transformation, regulatory application, resolution, uncertainty, model performance evaluation, data needs.

## 1 Why Air Quality Modeling

Understanding the relationship between primary pollutant emissions and air quality, represented by the ambient concentrations of atmospheric pollutants, is essential to developing emissions control strategies. The better this understanding is achieved, the more effective will be the strategies and the greater the opportunity for minimizing control costs while maintaining an acceptably low risk of exceeding an ambient standard, such as the United States National Ambient Air

[3] Philip M. Roth (deceased) and Steven Reynolds prepared the original Chapter 2 for Vol. I of this book series. This manuscript was subsequently revised to include updated information provided by Robert Paine.

 

Quality Standards (NAAQS). US federal ambient standards exist for 8 pollutants and pollutant groups: CO, $SO_2$, $NO_2$, ozone, fine particles, particles less than 10 microns in diameter ($PM_{10}$), total suspended particles (TSP) and lead. As noted in Chapter 1, many countries have adopted similar air quality standards for these pollutants, although the form and level of the standards may differ from the US NAAQS. In addition, many states in the US and countries throughout the world have adopted acceptable ambient levels for air toxics compounds. In the United States, these ambient levels are documented on state web sites that are accessible from links at www.epa.gov/scram001. In some cases, the emissions-ambient concentration (e/ac) relationship is reasonably straightforward: linear, proportional, and scalable. In others it is extremely complex: nonlinear, controlled either by a number of key chemical reactions or by mixing rates, and necessitating an understanding of a range of dynamic phenomena, such as deposition rates and emissions of biogenic species.

Air quality simulation models (AQSMs) provide a means for relating emissions and air quality. They range in form from quite simple to extremely complex. Many types have been developed during the past three decades. However, three have emerged as the main types in use: (a) the Gaussian model, for use in simulating dynamic plumes in the near field, (b) the Lagrangian puff model (a variant of the Gaussian model applied to puffs) for use in simulating single source transport and simplified chemistry over travel distances of several hundred kilometers, and (c) the grid-based photochemical AQSM, for use originally in simulating ambient ozone concentrations, and more recently for aerosols, $SO_2$ and its reaction products, and other reactive pollutants for a large inventory of sources over long distances. The framework of the grid-based model, omitting chemistry, can also be used to simulate nonreactive pollutant concentration fields.

The main premises in adopting models for use are that:

- They will serve as reasonably accurate estimators of air quality for any selected combinations of emissions
- The time, cost, and staffing requirements that attend their use will be commensurate with the need, and
- If the accuracy of estimates falls short, the model deficiencies will be correctable within the availability of the resources or at least understood and accounted for.

Presuming that a suitable model is available, it may see a number of uses:

- Regulatory planning and analysis, such as the preparation of federal and state implementation plans (FIPs and SIPs)
- Estimation of uncertainties through sensitivity analysis
- Planning for the conduct of field studies, and
- Identification of research and development needs

The most common and most critical use of these techniques in the United States is modeling to support FIP and SIP preparation, as well as for New Source Review.

Generally, planners attempt to ensure that recommendations for emissions controls are consistent with emissions control requirements formulated through modeling that demonstrates compliance with ambient air quality standards. Consequently, participants in the planning process have an interest in models being as accurate as possible. Oftentimes, then, their focus is on improving simulation accuracy, evaluating model performance, conducting sensitivity studies and uncertainty analyses, and simulating alternative emissions control scenarios. If these steps can be conducted with satisfaction, the planner's job is greatly facilitated.

In June 2010, the United States Environmental Protection Agency established[4] a new 1-hour $SO_2$ NAAQS. Part of the implementation of this new standard involves a departure from past practice: dispersion models are to be used to determine compliance with the standard in place of monitors in most cases. This places more importance on the accuracy of models to simulate realistic concentrations, and this issue is discussed at more length later in this chapter.

# 2 Modeling Categorized

## 2.1 Applications of Models

Air quality simulation models are employed in a wide variety of applications, most of which are associated with local, state or federal regulatory requirements in the United States and many other countries.

### 2.1.1 Dispersion Modeling

The principal focus of dispersion modeling, especially for nonreactive pollutants, is estimation of ambient concentrations of primary pollutants that have been dispersed in the atmosphere through turbulent diffusion. Strictly speaking, this modeling category applies to pollutants that do not undergo atmospheric chemical transformation. However, it also applies for pollutants for which simple assumptions are incorporated to mirror mass depletion due to chemical transformation, such as linear decay terms, as well as deposition.

Models in use for modeling nonreactive pollutants include:

- The Gaussian formula in one of its many manifestations. This formula represents the first of the commonly used models, and is applied primarily to plumes, both individual and multiple. If circumstances permit, it may also be applied to groups or aggregations of sources. Also, the Gaussian formula can be written in a form to simulate the dispersion of individual puffs, instead of plumes. In the United States, AERMOD (Cimorelli et al., 2005) is an example of a model in wide use for these types of applications.

[4] http://www.epa.gov/ttnnaaqs/standards/so2/fr/20100622.pdf

CALPUFF (Scire et al., 2000) is a Lagrangian puff model using Gaussian puff formulations that is used for long-range transport modeling of single sources as well as short-range modeling of complex flows.

- The approximate solution of the governing equation of mass conservation, which includes a simplifying assumption that relates turbulent fluxes, <u′c′>, to concentration gradients, $\partial c/\partial x_i$, through the adoption of an eddy diffusivity, $K_i$,

$$\langle u'c' \rangle = -K_i \left( \partial c / \partial x_i \right) \quad (1)$$

  This equation is commonly applied for more widely or uniformly distributed pollutants such as carbon monoxide (CO), where large individual plumes are not dominant.
- An approximate solution of the governing equations of mass conservation in a coordinate system that moves with the average wind velocity – the so-called "trajectory model". The solutions in the fixed and moving coordinate systems are related. They differ in that certain assumptions are made for the trajectory model that do not apply for the "gridded model", notably neglect of horizontal wind shear, horizontal turbulent diffusion, and vertical advective transport (Liu and Seinfeld, 1974). Also, acceptance of the trajectory model implies that parcel integrity is reasonably maintained for the length of time of the model simulation. However, some advanced trajectory models such as HYSPLIT (Air Resources Laboratory, 2009) include dispersion modules to mitigate the limitations of a trajectory model.
- The solution of the governing equation of mass – usually in parallel with the governing equation of momentum – using more rigorous and complex procedures, and thus avoiding the application of K-theory. Such models tend to be research models, in development, computing-intensive, and one-of-a-kind. They are not in common use.

### 2.1.2 Modeling of Chemical Transformations[5]

By far, the most common approach for modeling complex chemical transformations is through use of coupled mass balance equations incorporating K-theory, one for each pollutant that is being modeled. In the United States, CMAQ (Byun and Ching, 1999) and CAMx (Morris et al., 2004) are commonly used for these applications. Virtually all models now in use for estimating tropospheric ozone concentrations and the concentrations of secondary fine particles are based on these equations, with differences among models being in the submodels or modules for one or more dynamic processes, such as transport,

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[5] See also: Pun, B.K. et al. 2005. Atmospheric Transformations. Chapter 12 of AIR QUALITY MODELING – Theories, Methodologies, Computational Techniques, and Available Databases and Software. Vol. II – Advanced Topics (P. Zannetti, Editor). Published by The EnviroComp Institute (http://www.envirocomp.org/) and the Air & Waste Management Association (http://www.awma.org/).

chemistry, and deposition, and in the numerical integration procedure. These models are used for SIP and FIP preparation, regional planning, and other regulatory applications.

Trajectory models are also used in special applications. However, each assumption noted earlier still must be considered; in most situations encountered they will not all apply.

### 2.1.3 Modeling of Pollutant Deposition[6]

Generally, the same family of models, based on the governing equation of mass conservation, is used to estimate deposition fluxes as a function of location, and integrated over time, the accumulation of deposited material. Use of the "non-reactive" form of the model, incorporating simplifying assumptions, allows for calculation over longer simulated times at reasonable computational times. Deposition calculations, less common than the calculation of ambient concentrations, are of interest for estimation of:

- Acidic deposition and acid loadings over a seasonal period
- Ecosystem impacts of air pollutants, such as deposition of nitrogen compounds onto sensitive watersheds, and
- Contributions to accumulation of pollutants in lakes and subsequent eutrophication

The sub-models or modules that address deposition can vary greatly in formulation, rigor, and level of detail. In the past, several of the simulation models in use incorporated rather primitive treatments of deposition. More recently, improved algorithms have been developed and included in models. Nevertheless, considerable uncertainty attends deposition estimates due to the lack of evaluation databases and uncertainty in the specification of some of the model input parameters.

### 2.1.4 Modeling of Adverse Impacts

The objective of modeling "impacts", in contrast to ambient concentrations, is to examine more directly certain selected effects. An example mentioned earlier is the estimation of acidic fluxes. Health effects of pollution are, of course, a major issue as far as adverse impacts are concerned.

Visibility degradation also falls under the heading of "impacts", as does ecosystem loading. In the United States, use of a Lagrangian puff model such as CALPUFF for modeling the long-range effects of individual sources with

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[6] See also: San José, R. et al. 2005. Deposition Phenomena. Chapter 13 of AIR QUALITY MODELING - Theories, Methodologies, Computational Techniques, and Available Databases and Software. Vol. II – Advanced Topics (P. Zannetti, Editor). Published by The EnviroComp Institute (http://www.envirocomp.org/) and the Air & Waste Management Association (http://www.awma.org/).

simplified chemistry serves as the most common approach for such analyses, incorporating those modifications or additions needed to address the specific effect. For example, in the case of visibility degradation (an adverse effect of pollution, in the sense that visibility impairment does not allow a full enjoyment of vistas, especially in high sensitive areas, such as National Parks), a post-calculation algorithm is included to convert estimated concentrations into a measure of visibility impairment. This general category of modeling is experiencing increasing use because the range of issues now being examined in the regulatory arena is broadening.

Note that for all modeling applications, spatial extent is a key attribute. Early applications tended to be limited to urban or metropolitan scale. Today, regional scale is of primary concern because of the recognition that pollutant problems are not confined to a local area, but can extend for many hundreds of miles and include a number of emissions centers. Modeling outlined here applies in principle at local to regional – and in some cases – subcontinental scales. Fortunately, substantial advances in computing power and efficient algorithms for numerical computation and display of modeling results have facilitated the expansion of the scope of what is possible for regional modeling.

## 2.2 Estimating Inputs to Air Quality Simulation Models

Three major categories of information are required to formulate inputs to models: air quality, emissions, and meteorology. Consequently, it is appropriate to think in terms of *a modeling system*, as depicted in Figure 1 and not only an air quality model. Emissions and meteorological information, as well as boundary and initial conditions, must be supplied to the air quality model, as shown by the flows in the figure. The output concentrations are often used as input to specialized post-processors that provide graphical displays, source culpability analyses, computation of visibility impacts (as mentioned above), etc.

Boundary and initial conditions are needed to drive models based on conservation of mass. Boundary conditions are generally difficult to estimate, data are sparse, and often no independent means of estimation exists. The two primary approaches to estimation include acquisition of data at the inflow boundaries, both upwind and overhead, and estimation using a model of much broader spatial scale but coarser spatial resolution.

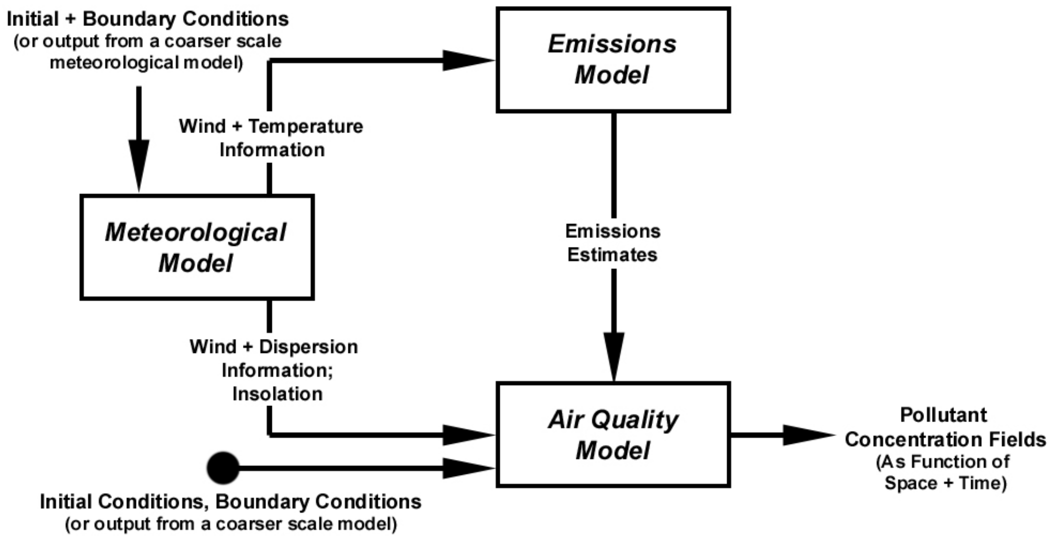


**Figure 1. The Air Quality Modeling System.**

Emissions are estimated using a wide array of options, from hand-counts and bookkeeping to sophisticated modeling. Where possible, computer-based emissions models and management of emissions data are used – to insure uniformity of procedure, reduce error rates, greatly enhance data handling, and increase the rate at which estimation is conducted. Even for a given geographical application, a wide range of approaches to emissions estimation – for the different emissions categories – might be adopted.

In the early stages of air quality modeling, simple approaches to estimation of meteorological variables were prevalent – from hand-prepared wind maps to the use of straightforward diagnostic models, the latter including parameterized treatments of key variables. These models were generally limited to the consideration of meteorological data at a single station, which is most commonly the case for Gaussian models. More recently, prognostic models have been widely accepted for use. These models are based on solving the equations of conservation of mass, energy, and momentum and produce as output 3-dimensional gridded meteorological fields for each hour (or even for sub-hour periods). They have proven to be quite helpful and an excellent complement to the use of air quality models based on the equations of mass conservation.

## 2.3 Categories of Air Quality Models Primarily in Use

The primary models (and modeling systems) in use today are those based on the numerical integration of the equations of conservation of mass and those based on the Gaussian formula, the latter for a range of source configurations and extensions of the basic equation.

### 2.3.1 Numerical Solution of the Equations of Conservation of Mass

The governing equations of conservation of mass are given by:

$$\frac{\partial c_i}{\partial t}+u_x\frac{\partial c_i}{\partial x}+u_y\frac{\partial c_i}{\partial y}+u_z\frac{\partial c_i}{\partial z}=\frac{\partial}{\partial x}\left(K_x\frac{\partial c_i}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial c_i}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial c_i}{\partial z}\right)$$

$$+R_i\left(c_1,c_2,\ldots,c_n\right)+E_i\left(x,y,z,t\right)-S_i\left(x,y,z,t\right) \qquad (2)$$

where:
$u_x$, $u_y$, $u_z$ = velocity
$c_i$ = concentration of i$^{th}$ species
$R_i$ = chemical generation rate of species i
$E_i$ = emissions flux
$S_i$ = removal flux

Emissions, meteorological, and air quality fields are provided as inputs, and the equations are integrated forward numerically in time to produce pollutant concentration fields.

Note that in special circumstances the simpler trajectory solution may apply. However, even advanced trajectory models such as HYSPLIT are not currently accepted for general use for regulatory applications in the USA without a project-specific demonstration. However, these models are useful for computing trajectories, especially with links to archived or predicted databases of gridded meteorological data such as those available to HYSPLIT.

### 2.3.2 Gaussian Models

The basic Gaussian equation,

$$c\left(x,y,z\right)=\frac{q}{2\pi\,\bar{u}\sigma_y\sigma_z}\exp\left(-\frac{y^2}{2\sigma_y^2}\right)\cdot\left[\exp\left(-\frac{\left(z-h\right)^2}{2\sigma_z^2}\right)+\exp\left(-\frac{\left(z+h\right)^2}{2\sigma_z^2}\right)\right] \qquad (3)$$

where:
$q$ = source strength
$h$ = stack height
$\sigma_y$ , $\sigma_z$ = lateral and vertical dispersion coefficients

is a solution to the equation of mass conservation where conditions are steady state ($\partial c/\partial t = 0$), velocity $\bar{u}$ is constant, and diffusion in the x-direction can be neglected. [See Seinfeld and Pandis, 1998, section 18-1 to 18-2, for a full derivation.] Many variants of the Gaussian plume and puff formulas exist; formulas for individual sources are summarized in Seinfeld and Pandis, section

18-3. AERMOD introduces a skewed distribution to the vertical dispersion in convective conditions, for example. These models also have specialized approaches for dealing with source effects such as building downwash (the PRIME model, Schulman et al., 2000). CALPUFF is a widely used Lagrangian puff model that has adapted the Gaussian model to a puff-tracking approach.

These two approaches to modeling dominate applications today and have done so for the past two decades. Consequently, these formulations and supporting emissions and meteorological modeling will receive the preponderance of attention in this book.

# 3 Modeling the Atmosphere

## 3.1 Deterministic Modeling and Stochastic Processes

The atmosphere is stochastic; transport and dispersion exhibit random behavior. Thus, for a given set of parameters – temperature profiles, average wind velocity, solar radiation, and surface roughness – different manifestations might occur in the atmosphere, purely dependent on random events. In addition, Gaussian models rely upon single-station input data for modeling of plume impacts over a large area that is often heterogeneous. Consequently, model outputs should, in principle, be expressed as distributions that display the random character of the variables of interest. In fact, most models in use are deterministic; they display the average behavior of the spectrum of random outcomes that might occur. A few, such as SCIPUFF (Santos et al., 2000) provide estimates of the concentration uncertainty in addition to the expected mean concentration value. In general, those using models or their results should be aware of this aspect of their formulation.

## 3.2 Modeling Representative Conditions vs. A Long-Term Time Record

Typically, modeling is conducted for average conditions or for a limited period of time, sometimes termed "an episode". A great deal can be learned from such an exercise, and the results themselves are generally useful. However, atmospheric and man-made conditions, such as wind fields and traffic intensity, vary, and can vary in many ways and combinations.

Modeling longer periods of time provides a means for examining a range of outcomes, but does so at additional cost, use of staff time, and level of detail. In the past modeling was largely confined to shorter intervals – from one day to a few days. More recently, especially with advances in computational power, parallel processing, and numerical algorithm efficiencies; investigators have demonstrated the use of models – even the more complex models - for one or more annual periods. With attention being given to longer averaging periods in the formulation of new ambient air quality standards, the application of models for longer periods is critical.

### 3.3 Using Models Instead of Monitors to Demonstrate Compliance with Ambient Standards

Ambient monitoring data has been the traditional, long-established benchmark used by the USEPA to determine compliance with the NAAQS and dispersion modeling has been used primarily to evaluate the impact of proposed sources. However, the USEPA has concerns with relying only upon monitoring data to evaluate current air quality in terms of compliance with the 1-hour $SO_2$ NAAQS, and instead favors the use of dispersion modeling. The following reasons are identified in their final rule[7] that establishes the 1-hour $SO_2$ NAAQS:

- It would take considerable time to design and implement new monitoring networks.
- Ambient monitoring is resource-intensive, and even with many more monitors; the coverage around each major $SO_2$ source may not be adequate to determine the peak impacts.
- A reliance upon modeling rather than monitoring is a "technically appropriate, efficient, and readily available method for assessing short-term ambient $SO_2$ concentrations in areas with large point sources."
- Due to the generally localized impacts of $SO_2$, USEPA has not historically considered monitoring alone to be an adequate, nor the most appropriate, tool to identify all maximum concentrations of $SO_2$. In the case of $SO_2$, USEPA further believes that monitoring is not the most cost-efficient method for identifying all areas of maximum concentrations.

The use of modeling in past compliance assessments has been very limited. Modeling practices such as those described in USEPA's guidance for modeling the peak emissions for all hours and using peak regional background concentrations are mostly suited to future sources, rather than existing sources. These modeling procedures could lead to large overestimates in the actual concentrations, which are what monitors would provide. The use of modeling rather than monitoring should focus upon the "gold standard" of matching the actual concentrations that a monitor would measure at each model receptor point. This means modeling realistic source and background conditions.

Although refined models such as AERMOD have shown good performance for predicting short-term concentrations, this performance is subject to the following best practices if monitored compliance is replaced with modeled compliance:

- Actual hourly emissions concurrent with meteorological data used in the modeling analysis should be used. Use of peak emission rates for all hours of the analysis will likely result in indications of false violations of the NAAQS.

[7] http://www.epa.gov/ttnnaaqs/standards/so2/fr/20100622.pdf

- Actual stack heights should be used as input to the models.
- Modeling of background sources should follow the same approach – use of actual hourly emissions should be used.
- Inclusion of regional monitoring concentrations should be done on an hourly basis concurrent with the hourly emissions for sources being modeled and the hourly meteorology used in the modeling. Use of multiple monitors with the highest value for each hour not included in the hourly average is one approach to prevent double counting of modeled and monitored concentrations.

## 4 Modeling Alternatives

While grid models and Gaussian models provide a means for simulating a broad range of atmospheric processes, alternative modeling approaches may prove as or more useful in supporting particular avenues of research and analysis. For example, box models play a central role in air chemistry research studies. Receptor models provide direct *emissions-air quality* relationships using basic source information and measured ambient pollutant concentrations. In recognition of the stochastic character of the atmosphere, limited efforts have been devoted to developing suitable statistical models. Although each of these approaches has a limited range of applicability, they provide insight into certain aspects of air pollution phenomena and in some cases may serve to corroborate or place in question the results obtained from comprehensive simulation models.

### 4.1 Box Models

A box model is a mathematical representation of pollutant dynamics that take place in a well-mixed volume of air. In general, these models provide very limited representations of atmospheric transport phenomena. However, they are well suited to supporting atmospheric chemistry research studies. For example, a smog chamber is a stirred vessel that employs natural light or ultraviolet lamps to study the chemical transformations of precursors in forming ozone and other photochemical reaction products under controlled laboratory conditions. Fresh precursors may be added to the chamber to simulate basic characteristics of actual diurnal emissions patterns that occur in urban or rural areas. Since chamber-specific wall effects may be important, they need to be characterized and simulated in the box model. Typically, the governing equations of a box model are a set of coupled, nonlinear, stiff ordinary differential equations derived from a chemical kinetics mechanism that are solved using suitable numerical solution procedures.

## 4.2 Receptor Models[8]

Receptor models are based on statistical analyses of ambient pollutant measurements and pertinent emissions information. They are of particular value in situations where detailed knowledge of actual emissions rates is subject to significant uncertainties. For example, receptor models provide an important means for apportioning measured values of certain types of primary particulates. Establishing such relationships using a source-oriented model is much more problematic given the large uncertainties in emissions estimates for fugitive sources of particulates.

Receptor models can be grouped into three major categories (Seigneur, 2001): (1) models that apportion primary PM using source information, (2) models that apportion primary PM without using source information, and (3) models that apportion primary and secondary PM. In each of these categories, there exist some well-established techniques as well as some recent emerging techniques. For example, the chemical mass balance approach has been applied to $PM_{10}$ problems throughout the western U.S. with generally good success ($PM_{10}$ is defined as particulate matter – PM – made of particles less than 10 $\mu$m in diameter). New methods of factor analysis can also be employed in areas where source profiles are not available. The reliability of receptor models for $PM_{2.5}$ is quite different since the majority of the fine particle mass is due to secondary particle formation ($PM_{2.5}$ is defined as particulate matter – PM – made of particles less than 2.5 $\mu$m in diameter). The ability of these models to provide quantitative apportionment of the measured aerosol mass to the pertinent sources is more uncertain. In regulatory applications, a key issue is the ability of these models to adequately represent source-receptor relationships associated with nonlinear chemical reaction phenomena that lead to secondary fine particle formation.

## 4.3 Statistical Models[9]

Statistical models provide estimates of concentration levels as a function of some combination of space, time, meteorological, emissions and other pertinent variables. These relationships are derived using various regressions, statistical and analysis techniques. Since these relationships are derived from available measurements, their range of applicability is limited to the conditions under which the data were collected. Nonlinear relationships between reactive precursors and

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[8] See also: Watson, J.G. and J.C. Chow 2005. *Receptor Models.* Chapter 16B of *AIR QUALITY MODELING - Theories, Methodologies, Computational Techniques, and Available Databases and Software. Vol. II – Advanced Topics* (P. Zannetti, Editor). Published by The EnviroComp Institute (http://www.envirocomp.org/) and the Air & Waste Management Association (http://www.awma.org/).

[9] See also: Finzi, G. and G. Nunnari 2005. Air Quality Forecast and Alarm Systems. Chapter 16A of AIR QUALITY MODELING - Theories, Methodologies, Computational Techniques, and Available Databases and Software. Vol. II – Advanced Topics (P. Zannetti, Editor). Published by The EnviroComp Institute (http://www.envirocomp.org/) and the Air & Waste Management Association (http://www.awma.org/).

secondary pollutants are particularly difficult to accurately represent in such models. To date, limited effort is being devoted to the development of statistical models largely because of their constrained range of applicability, the lack of physical characterizations in the model, and, often, a limited database. Models using "fuzzy logic" that depend upon a study of past events are sometimes used in ozone forecasting (see, for example, Sen et al., 2009).

### 4.4 Lagrangian Particle Models[10]

Lagrangian particle models – often referred to as Monte Carlo models – simulate atmospheric diffusion by tracking the movement of thousands of fictitious particles representing air pollution. Particles move according to average wind and turbulence parameters and include semi-random pseudo-velocities calculated using a computer-based random-number generator. These models apply well for unreactive pollutants, but revert to a gridded formulation for reactive systems, with various imposed limitations. Their use is becoming more common, particularly for unreactive species, though regulatory applications are still rare.

### 4.5 Other Specialized Models

Other modeling approaches are used for specialized applications. One of these is a set of dispersion models for heavy gas releases, as described in Chapter 1. Other such specialized models include computational fluid dynamics models and wind tunnel models. These two types of models are used to simulate complex flows, often around complicated structures for situations that are not well accommodated by larger-scale routine models.

## 5 Spatial and Temporal Scales

Models are typically applied to study impacts of individual sources, multiple-source industrial facilities, metropolitan areas, or larger regional areas up to subcontinental scale. The spatial scales of concern can range from up to a few tens of kilometers for large industrial point sources, to a few hundred kilometers for individual urban areas, to a few thousand kilometers for larger regional areas comprised of several metropolitan areas. When applying models to regional-scale domains, consideration must be given to the spatial scale of important atmospheric phenomena that ultimately contributes to regional air quality problems. Nested grid capabilities, an important feature of contemporary regional models, allow them to resolve important phenomena and concentration gradients in areas of the domain where significant sources are present.

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[10] See also: Anfossi, D. and W. Physick 2005. Lagrangian Particle Models. Chapter 11 of AIR QUALITY MODELING – Theories, Methodologies, Computational Techniques, and Available Databases and Software. Vol. II – Advanced Topics (P. Zannetti, Editor). Published by The EnviroComp Institute (http://www.envirocomp.org/) and the Air & Waste Management Association (http://www.awma.org/).

The time scales of concern are related to ambient air quality standards, which have averaging times ranging from one hour to one year. In Gaussian model regulatory applications in the US, simulations using up to five years of meteorological data may be carried out to develop estimates of peak concentrations with averaging times ranging from one hour to one year. In photochemical model regulatory applications in the US, simulations of annual periods have become more common with computational and numerical algorithm advances.

Models are formulated to represent key phenomena on the spatial and temporal scales of interest. For example, localized urban models typically do not provide sufficient treatment of upper air dynamics and, therefore, are generally not applicable to regions of the order of several hundreds of kilometers where vertical transport in the free troposphere, up to several kilometers above ground, may be important. Air quality models that include a detailed treatment of chemistry may be limited in their applications sub-annual periods because of the computational costs associated with the numerical integration of the chemical kinetic equations. Models that use a simplified treatment of atmospheric chemistry can be applied to longer time periods (e.g., one year or more) without prohibitive computational costs. The ability to simulate long time periods is generally obtained at the expense of some accuracy (since the treatment of chemistry is less accurate in long-term models). Another approach for estimating annual-average concentrations is to apply an episodic model for several typical meteorological scenarios and to reconstruct a full year by combining these scenarios with appropriate weighting factors. This approach involves making approximations with the representativeness of the meteorology, whereas the use of a long-term model involves making approximations with the chemistry.

## 6 Spatial and Temporal Resolution

Short-term Gaussian plume models are typically applied using hourly meteorological data spanning a period of up to five years. However, recent versions of CALPUFF have allowed the input of sub-hourly meteorological and emissions data to characterize better temporal resolution for these input parameters. However, most models provide hourly concentration estimates at any user-specified point downwind of the source. However, because these models are based on steady-state assumptions, they cannot truly resolve concentration fluctuations and their applicability is effectively limited to a 1-hour travel distance.

Grid-based models provide concentration estimates that are spatially averaged over the volume of a grid cell, whose size may range from 1 to 40 km or more in the horizontal directions and from ten meters to several hundred meters in the vertical direction. Contemporary grid models employ nested grids with relatively fine spatial resolution in dense and/or heterogeneous source areas (such as cities where significant spatial gradients may exist in the concentration field) and relatively coarse resolution in rural areas (where spatial gradients are much smaller). Use of nested grids is largely motivated by a desire to optimize the computational time required to perform a simulation.

The ability to provide variable vertical resolution can also be important. In general, relatively fine vertical resolution is used near the ground where large vertical gradients in the concentration field are likely to occur because of the near proximity of most sources. Concentration gradients aloft are often much smaller, allowing the use of coarser vertical grid resolution. In establishing the vertical grid structure, careful consideration must be given to the spatial features of elevated stable layers aloft and the possible need to adequately resolve elevated plumes from large point sources. If such plumes are not adequately resolved, they may be subject to significant averaging errors. In addition, the timing and location of plume fumigation to the ground may be in error. For nitrogen oxides ($NO_x$) plumes, this can have a significant effect on VOC/$NO_x$ in the areas where plume fumigation is predicted to occur (or not occur) and can also have a profound influence on the relative effectiveness of VOC versus $NO_x$ controls on ozone formation in such areas. (VOC stands for volatile organic compounds, for example, reactive, non-methane hydrocarbons)

# 7 Uncertainty: Bias, Imprecision, and Variability

Uncertainty attends all elements of the modeling enterprise: accuracy and precision of the supporting and test data bases, the model-generated emissions and meteorological fields, initial and boundary conditions, and at the end of the sequence, air quality modeling and the results of interest. Variability also accompanies meteorological and biogenic emissions variables (natural variability) and activities that derive from human behavior, such as traffic loading (man-derived variability). As should be apparent, the contributions of uncertainty to modeling results are broadly-based, and the results of modeling are quite susceptible to errors. Modelers, of course, attempt to reduce error levels as effectively as possible, but uncertainties will persist, as many sources of uncertainty are outside the modeler's range of influence. Notable among these are errors in inputs, particularly emissions-related, and variability of all types. Model outputs may range widely in their sensitivity to uncertainties. Where they are insensitive, errors or variability may be of only casual concern; where sensitivity is high, errors particularly may be a major issue. See Morgan and Henrion (1990) and Hanna (1993) for detailed introduction to and treatment of uncertainty in air quality modeling.

Typically, little attempt is made to estimate quantitatively the bias or error in model output. While it may be important to know model bias and error, and it may be of particular interest to the decision-maker, it may be quite difficult or impossible to calculate. In these circumstances, modelers sometimes use "best judgment" to estimate errors; however, this cannot be expected to be reliable.

An example of how the uncertainty of several input model variables can be evaluated at once is illustrated by Irwin and Hanna (2005). In this study, a Monte Carlo (MC) probabilistic uncertainty analysis was applied to releases from 26 field study experiments. In the MC probabilistic uncertainty procedure, the modeling system was run to simulate 100 years of hourly concentrations that were altered for random choices of variations in the input parameters. The resulting geometric standard deviations in the reported predicted concentrations were then analyzed.

As noted by Irwin and Hanna, the Gaussian dispersion model provides a smoothed viewed of reality. Irwin and Lee (1996) analyzed the Prairie Grass data, as well as additional tracer data from the Kincaid power plant, which had a 183-m stack with a typical buoyant plume rise on the order of 200 m. They concluded that the scatter in the concentration values about the ensemble average Gaussian lateral profile could be characterized for both experimental data sets as having a log-normal distribution with a geometric standard deviation on the order of 2.

The SCIPUFF model (Santos et al., 2000) explicitly solves for the fluctuations in concentration internal to the plume. Typically, the relative fluctuation (standard deviation divided by the mean) is simulated to be about 2 on the plume centerline, and is larger towards the edges of the plume.

In the absence of such studies, sensitivities of the model results to uncertainties in the model inputs are often estimated. They generally provide information on the response of the output to uncertainties in inputs, under the assumption that the model is basically correctly formulated and the inputs are sound. If there is error in the model or inputs, the results of sensitivity analyses may be derivatively tainted.

Efforts are being made to introduce more sophisticated approaches to uncertainty analysis into modeling. For example, Yang, Wilkinson, and Russell (1997) have developed techniques for facilitating the conduct of sensitivity analysis through use of the direct decoupled method. However, if there is an unknown error in the model or inputs, no sensitivity analysis will properly address its presence. Rather, an attempt must be made to detect its presence, determine the cause or causes and the importance of the error (if feasible) and, as appropriate, correct, mitigate, or eliminate the problem and repeat the modeling and sensitivity analysis.

# 8 Evaluation of Model Performance[11]

Model performance evaluation (MPE) is the process of testing a model's ability to estimate accurately observed measures of air quality over a range of meteorological, emissions, and air quality conditions. When conducted thoughtfully and thoroughly, the process focuses and directs the continuing cycle of model development, data collection, model testing, diagnostic analysis, refinement, and retesting. Far too often in the past this process has been foreshortened in order to "validate" the model with readily available data so that its use in regulatory decision-making could be justified. Obviously, serious inquiry into the model's adequacy or reliability is difficult if not impossible in such a situation.

The performance of Gaussian models has been the subject of numerous studies. Typically, an inert tracer gas is released from a source and measured at various downwind locations. Assessments of model performance rely on comparisons of calculated and measured concentration levels. Routine application of these models in a regulatory setting generally does not involve any performance evaluation due to the time and expense involved, and because approved models are considered by reviewing agencies to be generally applicable (although this is typically considered on a case-by-case basis). At best, the models are applied using site-specific meteorological data.

In contrast, there is a long history of MPE for photochemical models involving the comparison of observed and estimated concentrations of ozone and, to a lesser extent, other pollutant species. The principal comparisons included temporal comparisons of differences between observation and estimation for individual monitoring sites, spatial comparisons of differences, as shown through deficit-enhancement maps, and a range of statistics, including regional and subregional average bias, gross error, and differences in area-wide maximum ozone concentrations, independent of time and location.

The focus of all these types of comparisons has been on ozone. Although $NO_x$ and VOC comparisons have been carried out for some time, no requirement or informal rule was ever developed stipulating that $NO_x$ or VOC estimates correspond at any prescribed level. Furthermore, no standard practice for judging model performance has evolved. Traditionally, the EPA guideline model (Urban Airshed Model) (EPA, 1990) was accepted for use in control strategy assessment when average discrepancies (e.g., gross errors) for ozone were of the order of 35% or less, and inaccuracy or bias is "not large" (i.e., $\pm$ 5-15% according to EPA's definition) (EPA, 1991). Often, however, it was determined that models

[11] See also: Canepa, E. and J. Irwin 2005. Evaluation of Air Pollution Models. Chapter 17 of AIR QUALITY MODELING - Theories, Methodologies, Computational Techniques, and Available Databases and Software. Vol. II – Advanced Topics (P. Zannetti, Editor). Published by The EnviroComp Institute (http://www.envirocomp.org/) and the Air & Waste Management Association (http://www.awma.org/).

passing these arbitrary performance criteria contained significant flaws, commonly in the form of internal, compensating errors that compromised the overall reliability of the entire modeling demonstration. To accommodate inevitable modeling errors, photochemical models are often used to determine the *relative change* in the levels of ozone or fine particulate matter rather than the absolute value. For example, in order to determine the effect of emission controls, photochemical models will be run for the controlled (future) and uncontrolled (current) cases, and the ratio of the results are applied to the current ozone concentrations to estimate the future concentrations. The United States EPA has provided guidance for conducting regional and photochemical modeling simulations in a 2007 guidance document, "Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze".

While in many scientific disciplines "hands-off" testing of models is required, a different tradition evolved in the evaluation of grid-based photochemical models. The improvement of model performance is an integral part of MPE. In cases in which differences between observations and estimates are unacceptably large, the modeler is expected (allowed) to carry out a diagnostic analysis, identify the potential causes of the discrepancies, suggest and make changes in model formulation or processing of input data, and repeat model testing. Thus, evaluation and improvement make up an iterative sequence and, in fact, they are inextricably coupled. Evolving from this philosophy is the common practice of undertaking model performance improvement activities with each modeling episode separately.

A key limitation in MPE to date has been the generally inadequate level of stressfulness to which models have been subjected in testing. Three main outcomes of testing are possible: A model performs inadequately and is so judged, a model performs well and is so judged, or a model appears to perform adequately but is, in fact, significantly flawed. To ensure during testing that a model reveals its flaw(s), it must be adequately "stressed," that is, subjected to testing that is designed to reveal and even highlight or amplify inherent inadequacies.

Because testing has not been properly implemented, flawed models containing compensatory errors internally have been historically accepted for use. A notable instance is the long-standing use of underestimates of VOC emissions as input to the Urban Airshed Model (UAM), previously used in the United States for photochemical modeling. Modelers had either directly or inadvertently compensated for these underestimates by introducing offsetting bias into the model. In one instance, modelers compensated for suspected underestimation of the emissions inventory by artificially elevating the boundary conditions (on the top and sides). In another study, a "lid" was placed on the vertical velocity in the UAM to prevent or reduce the loss of surface ozone to layers aloft and thus improve model performance. In a third case, meteorological inputs were "beneficially altered" to advect the high ozone cloud directly toward the peak ozone monitoring station. These types of input modifications no doubt changed the source-receptor emissions characteristics of the air basins and had unknown effects on the reliability of the emissions control strategies. In these and other situations, the changes were asserted to be "within the range of experimental or scientific uncertainty."

Several scientists, motivated by a number of objectives, have proffered recommendations for improvements to the MPE process. They include improving the process, adequately stressing models, improving the quality of available databases, standardizing the practice, and demystifying the practice through clearer communication. Indeed, guidelines have been developed (Reynolds, Roth, and Tesche, 1994; ASTM, 2000; Chang and Hanna, 2004) for providing a sound context for performance evaluation, establishing a common understanding of the process, and ensuring that evaluation efforts are properly formulated and reasonably complete. Elements of such a comprehensive and satisfactory model evaluation process include:

(a) Evaluating the scientific formulation of the model through a thorough review process
(b) Assessing the fidelity of the computer code to the scientific formulation, governing equations, and numerical solution process
(c) Evaluating the predictive performance of individual process modules and preprocessor models (e.g., emissions and meteorological)
(d) Evaluating the predictive performance of the full model
(e) Conducting sensitivity analyses
(f) Carrying out corroborative analyses
(g) Carrying out comparative modeling, and
(h) Implementing a quality assurance activity.

All of these activities should be carried out in accordance with the procedures prescribed in an application-specific MPE protocol.

Obviously, the effort suggested above is considerably greater than that customarily devoted to MPE. However, air quality models are being viewed as essential tools in the development of emissions control plans. The costs of controls are sufficiently high that society will wish assurance that imposed controls would be effective in reducing air pollution levels. It is thus vital that the overall planning process includes sufficient time and resources for conducting thorough evaluations of model performance. In addition, there is likely to be a significantly increased demand for the collection of suitable emissions, meteorological, and air quality data to support MPE. The comprehensive evaluation of model performance should be considered essential to the overall air quality management program for an area.

# 9 Data Needs

AQSMs require various types of emissions, meteorological, air quality, and geophysical data. Model inputs may be assembled directly from suitable data sources or may be generated through use of other preprocessor models (e.g., emissions or prognostic meteorological modeling systems). The availability of appropriate data to derive model inputs, to evaluate model performance, and to diagnose and rectify model performance problems is crucial to the successful application of an air quality model.

## 9.1 Gaussian Models

Gaussian models are typically applied using one to five years of on-site surface meteorological data, including wind speed and direction, temperature, relative humidity, standard deviation of the horizontal wind direction, and rainfall. Upper air meteorological data are employed to estimate hourly mixing height estimates. Some models require estimates of other boundary layer parameters. Geophysical data include estimates of terrain height at source and receptor locations as well as land use. Tracer release experiments with suitable downwind measurements might be carried out to provide a database for evaluating model performance, although this is typically not carried out in routine applications of Gaussian models.

Lagrangian puff models require more extensive input data such as three-dimensional meteorological fields with accompanying two-dimensional databases for land use and terrain.

## 9.2 Photochemical Grid Models

Photochemical grid models are mostly used for ozone simulations and require several data sets for input preparation and model evaluation: air quality, meteorological, emissions, and geophysical. Such models require a complete specification of the spatial and temporal variations of key atmospheric phenomena. Unfortunately, the available data needed to derive such estimates fall far short of what is desired.

A typical air quality data set with which to evaluate model performance consists of hourly surface measurements of ozone and oxides of nitrogen ($NO_x$) derived from monitoring stations operated by air regulatory agencies, usually located in or immediately downwind of urban areas. Those monitoring sites located in rural are often in the general proximity of commercial or industrial sources. Very little routine $NO/NO_x$ monitoring is conducted at true rural sites, nor is there routine collection of total or speciated volatile organic compounds (VOC) data. No routine monitoring of ozone or precursors aloft is conducted. Data are rarely available for direct specification of pollutant concentrations on upwind boundaries of the modeling domain.

Photochemical grid models require a complete specification of the temporal and spatial variations of key meteorological variables, such as wind velocity, temperature, and cloud cover. The National Weather Service collects surface weather data supplemented by twice-daily radiosonde soundings at various locations throughout the country. These data supplemented with the surface meteorological data gathered at the air monitoring stations constitute the typical meteorological database available for developing meteorological inputs to photochemical grid models.

Photochemical grid models also require a complete specification of gridded, temporally resolved emissions estimates for all chemical species. Emissions data are normally assembled by air regulatory agencies with varying quality, representativeness, and reliability, often influenced by the ozone National Ambient Air Quality standards - NAAQS - attainment status of the particular area. (A region in the US is defined as an attainment region if air pollution measurements indicate the NAAQS are not exceeded). An emission modeling system may be needed to provide an effective means to organize, manipulate, and process emissions data for a large modeling domain.

Geophysical data are needed for specifying gridded terrain and land use inputs. Various federal agencies maintain geophysical data bases for topography, land use/land cover, population, employment, and so on that are used in various ways to develop the inputs needed by photochemical modeling systems.

In a few nonattainment areas, such as the northeast US, special field measurement studies have been performed to provide a better characterization and understanding of meteorological and air quality conditions than is otherwise provided by routine surface monitoring. Typically, these programs are carried out over a limited time period and consist of intensive monitoring of aloft meteorological and air quality conditions via instrument aircraft and remote sounding devices, enhanced surface monitoring of ozone and precursor species (sometimes including VOCs) in urban and rural sites, tracer-diffusion studies for model evaluation, and intensive, focused collection of emissions data from key source categories such as power plants, on-road motor vehicles, and targeted area sources. Though useful, these studies are very costly, capture a fraction of aerometric conditions associated with ozone exceedances, and have decreasing utility to support modeling as time passes.

Occasionally, major field studies are designed and implemented in parallel with integrated model development, testing and refinement activities. The SARMAP (Demassa, 1996) study in central California was a noteworthy example. Here, models were used to assist in the design of an intensive emissions, air quality, and meteorological data collection activity, supplemented with many research-grade investigations into specific processes: dry deposition and turbulence, biogenic emissions from various plant species, on-road motor vehicle driving patterns, boundary layer transport dynamics, and so on. Though very costly, these programs provide a solid basis for further model development as well as the opportunity for testing of individual process modules in the overall modeling system.

# 10 Uses of Models

Several uses of models have been listed earlier, ranging from the practical to the research-oriented. In this section we discuss two practical arenas of application: regulatory compliance and resolution of litigation.

## 10.1 Regulatory Compliance

Today models are commonly used in planning to estimate if a geographical area:

- That now exceeds a specified standard will attain the standard if certain prescribed emissions reductions are implemented
- Now in attainment will remain so due to the favorable offsetting effects of growth and emissions controls, and
- Now in attainment is likely to exceed a standard due to the effects of growth and insufficient emissions control

As noted, these modeling activities are often included under the general umbrella of SIP and FIP preparation. A comprehensive process might include:

- Detailed planning and protocol preparation
- Conduct of a field program to obtain data needed for many purposes, including the preparation of model inputs and the evaluation of model performance
- Independent programs for quality assurance and control
- Archiving and error-checking for the complete data base, including emissions
- Adaptation and testing of a model system selected for use, including air quality, emissions, and meteorological models
- Iterative improvement of model performance consistent with good scientific practice until a specified standard of performance is met
- Conduct of sensitivity studies, to better understand the system being modeled
- Control strategy analysis, and
- Estimation and analysis of uncertainties and risks

Funding needed for such efforts may range from a $2-5M to $25M or more. If a comprehensive field program is included, that component alone may cost from $3M to $15M or more. The total elapsed time required ranges from 4 to 6 years or more. Clearly, such commitments are substantial.

While grid-based photochemical modeling offers the best opportunity for long range planning for the attainment and maintenance of secondary air pollutant standards, its potential may be limited in one or more of the following ways:

- Components of an ambient air quality and meteorological data base may be sparse, inaccurate, or lacking
- Funding to conduct a comprehensive study may be inadequate
- Staff to conduct the work may be available for only a portion of the time needed, or may be unacceptably inexperienced in modeling
- The calendar time available may be inadequate, and/or
- Model performance may be inadequate and not easily correctable

See Roth, Tesche and Reynolds (1998), for an evaluation of regulatory modeling efforts conducted during the 1990-95 period. In recent years, the USEPA has held annual modeling workshops and has posted the presentations made at these workshops to keep the modeling user community updated on current modeling guidance and performance. Ongoing updates to USEPA modeling guidance are available at www.epa.gov/scram001.

Section 3.3 has a discussion of how models can be applied to replace monitors to demonstrate compliance with ambient standards. As noted in the discussion, it is important to supply models with realistic (hourly) emissions input data in order to replicate what would be measured at a monitor. If such modeling is done on a widespread basis (there are about 2000 major $SO_2$ sources in the United States), then there would be a substantial effort involved in the preparation of the emissions data, which would involve compiling hourly data for many stacks.

## 10.2 Resolution of Litigation[12]

Environmental litigation has been steadily increasing over the last four decades, especially in relation to accidental releases of chemicals into the environment. This phenomenon is particularly noticeable in the United States (US). However, this trend is also affecting European countries and courts that deal with international issues. The parties and their attorneys involved in litigation need expert witnesses such as scientists, engineers, medical doctors, etc., in order to comprehend various cases and help define litigation strategy, producing accurate and convincing written reports as well as providing expert testimony to judges and juries.

In the past, experts hired for litigation cases were required to provide opinions and subsequently support them with published citations, professional experience, and simple "pen-and-paper" calculations. Today computer simulations are used in virtually all-technical fields. For example, in air pollution, computer simulation models have been used in the US since the early 1970s as "regulatory tools", i.e.,

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official tools recommended by regulatory agencies to simulate the concentration impact of emissions of chemicals into the atmosphere. But the same "regulatory" models, or similar tools, can also be used to simulate the past, e.g., to simulate an accidental release from an industrial facility. Accidental releases in the US are often litigated in court, whereas experts are hired in order to perform a reconstruction of the incidents. Today, these experts commonly use simulation models to estimate the concentration impact in the neighboring areas downwind from the release. The use of computer simulation models is clearly necessary in accidental release cases (as well as in many other environmental litigation cases, e.g., groundwater contamination). The formidable task for attorneys on both sides is to understand as much as possible about modeling techniques and be able to present or criticize the results of those models in court.

If modeling is to be used in a litigation case, the expert witness must make several important choices. First of all, does the case warrant the use of a complex computer model? Should perhaps a simple model be chosen? Which model will be easier to explain to a jury? In one case, for example, the expert may use a computer model developed and recommended by the US Environmental Protection Agency (EPA). In another scenario, the expert might use a "research prototype" code developed at a university or a national laboratory. In yet another case, the expert might utilize a model recently developed, or even a model (or a set of calculations) expressly developed for the case at hand. The expert should bear in mind that each choice has advantages and disadvantages. Clearly, models that are widely used by other scientists and recommended by regulatory agencies can be perceived as more reliable than others. However, in litigation, an expert witness has ample latitude in selecting the tools that are most appropriate for the case. Whatever tool is chosen, the expert witness must be able to persuasively present it as reliable, peer-reviewed science whose results can be trusted. In all cases, the expert witness must feel comfortable in the ability to justify results and opinions to a non-technical audience under an often-hostile cross-examination. For additional information on the subject of the use of air pollution models in litigation cases, see Zannetti (2001).

**References**

Air Resources Laboratory, 2009, HYSPLIT - Hybrid Single Particle Lagrangian Integrated Trajectory Model. http://ready.arl.noaa.gov/HYSPLIT.php.

American Society for Testing and Materials, 2000, Standard Guide for Statistical Evaluation of Atmospheric Dispersion Model Performance (D 6589), (Available at http://www.astm.org), 100 Barr Harbor Drive, PO Box C700, West Conshohocken, PA 19428, 17 pages.

Byun, D.W. and J.K.S. Ching, 1999, Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modelling System, U.S. Environmental Protection Agency, Research Triangle Park, NC. EPA/600/R-99/030.

Chang, J.C. and S.R. Hanna, 2004, Air Quality Model Performance Evaluation, *Meteorol. Atmos. Phys. 87*, 167–196.

Cimorelli, A.J., S.G. Perry, A. Venkatram, J.C. Weil, R.J. Paine, R.B. Wilson, R.F. Lee, W.D. Peters, and R.W. Brode, 2005, AERMOD: A Dispersion Model for Industrial Source Applications. Part I: General Model Formulation and Boundary Layer Characterization'. *Journal of Applied Meteorology*, 44**,** 682-693. American Meteorological Society, Boston, MA.

DeMassa, J. et al., 1996, "Performance Evaluation of SAQM in Central California and Attainment Demonstration for the 3-6 August 1990 Ozone Episode." California Air Resources Board, Sacramento, CA, 1996.

Hanna, S.R., 1993. Uncertainties in Air Quality Model Prediction. *Boundary-Layer Meteorology, 62*: 3-20.

Irwin, J. S. and R. F. Lee, 1996. Comparative evaluation of two air quality models: Within-regime evaluation statistic. *Int. J. Environ. Pollut.,* 8: 346–355.

Irwin, J. S. and S. R. Hanna, 2005. Characterizing uncertainty in plume dispersion models. *Int. J. Environ. Pollut*., 25: 6–24.

Liu, M. K., and Seinfeld, J. H., 1974, On the Validity of Grid and Trajectory Models of Urban Air Pollution. *Atmos. Environ., 9*, pp. 555-574.

Morgan, M. G., and Henrion, M., 1990, Uncertainty: A Guide to Dealing with Uncertainty in Quantitative Risk and Policy Analysis. Cambridge Univ. Press.

Morris, R., G. Yarwood, C. Emery, and B. Koo, 2004, Development and Application of the CAMx Regional One-Atmospheric Model to Treat Ozone, Particulate and Visibility, Air Toxics, and Mercury. Presented at the 97$^{th}$ Annual Meeting and Exhibition of the Air & Waste Management Association, Indianapolis, IN USA.

Reynolds, S. D., Roth, P. M. and Tesche, T. W., 1994, A Process for Stressful Evaluation of Photochemical Model Performance. Envair, San Rafael, CA.

Roth, P. M., Tesche, T. W. and Reynolds, S. D., 1998, A Critical Review of Regulatory Air Quality Modeling for Tropospheric Ozone. North American Research Strategy for Tropospheric Ozone (NARSTO), Research Triangle Park, NC.

Santos, L., R. I. Sykes, P. Karamchandani, C. Seigneur, F. Lurmann, R. Arndt, and N. Kumar, 2000, Second-Order closure integrated puff (SCIPUFF) model with gas and aqueous phase chemistry and aerosols - Paper 6.8. Preprints, *11$^{th}$ Joint Conference on the Applications of Air Pollution Meteorology with the A&WMA,* American Meteorological Society, Boston, MA.

Schulman, L. L., D. G. Strimaitis, and J. S. Scire, 2000, Development and evaluation of the PRIME plume rise and building downwash model. *J. Air Waste Manage. Assoc.,* 50, 378–390.

Scire, J.S., D.G. Strimaitis, and R.J. Yamartino, 2000, A User's Guide for the CALPUFF Dispersion Model (Version 5). Available through http://www.epa.gov/scram001.

Seigneur, C., 2001, Current Status of Air Quality Models for Particulate Matter. *Journal of the Air & Waste Management Association, 51*, pp. 1508-1521.

Seinfeld, J. H, and Pandis, S. N., 1998, Atmospheric Chemistry and Physics. Wiley-Interscience.

Sen, Z, A. Altunkaynak, and, K. Alp, 2009, Contour diagram fuzzy model for maximum surface ozone prediction, Expert Systems with Applications, Volume 36, Issue 3, Part 2, April 2009, Pages 6389-6402, ISSN 0957-4174, DOI: 10.1016/j.eswa.2008.07.050. (http://www.sciencedirect.com/science/article/B6V03-4T1Y3PX9/2/3983d721634c65015e7746ea557d9bdf).

U.S. Environmental Protection Agency, 1990, "User's Guide for the Urban Airshed Model-Volume I: User's Manual for UAM (CBIV)." U.S. Environmental Protection Agency, EPA-450/4-90-007a, Research Triangle Park, NC.

U.S. Environmental Protection Agency, 1991, "Guideline for Regulatory Application of the Urban Airshed Model," EPA-450/4-91-013, Office of Air Quality Planning and Standards, Research Triangle Park, NC.

U. S. Environmental Protection Agency, 2007, Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze. April 2007. EPA - 454/B-07-002.

Yang, Y.J., Wilkinson, J.G., and Russell, A.G., 1997, Fast Direct Sensitivity Analysis of Multidimensional Photochemical Models. *Environ. Sci. Technol., 31*, 2859-2868.

Zannetti, P., 2001, Environmental Litigation – Air Pollution Models and Modelers in Court (Invited Paper). Air Pollution 2001, Ninth International Conference on Modeling, Monitoring, and Management of Air Pollution, 12-14 Sept 2001, Ancona, Italy, Wessex Institute of Technology, Ashurst, Southampton, U.K.