22

Air Pollution Modeling and Prediction

To build new facilities or to expand existing ones without harming the environment, it is desirable to assess the air pollution impact of a facility prior to its construction, rather than construct and monitor to determine the impact and whether it is necessary to retrofit additional controls. Potential air pollution impact is usually estimated through the use of air quality simulation models. A wide variety of models is available. They are usually distinguished by type of source, pollutant, transformations and removal, distance of transport, and averaging time. No attempt will be made here to list all the models in existence at the time of this writing.

In its simplest form, a model requires two types of data inputs: information on the source or sources including pollutant emission rate, and meteorological data such as wind velocity and turbulence. The model then simulates mathematically the pollutant's transport and dispersion, and perhaps its chemical and physical transformations and removal processes. The model output is air pollutant concentration for a particular time period, usually at specific receptor locations.

Impact estimates by specific models are required to meet some regulatory requirements.

I. PLUME RISE

Gases leaving the tops of stacks rise higher than the stack top when they are either of lower density than the surrounding air (buoyancy rise) or ejected at a velocity high enough to give the exit gases upward kinetic energy (momentum rise). Buoyancy rise is sometimes called *thermal rise* because the most common cause of lower density is higher temperature. Exceptions are emissions of gases of higher density than the surrounding air and stack downwash, discussed next. To estimate effective plume height, the equations of Briggs [1–5] are used. The wind speed u in the following equations is the measured or estimated wind speed at the physical stack top.

A. Stack Downwash

The lowering below the stack top of pieces of the plume by the vortices shed downwind of the stack is simulated by using a value $h\text{¢}$ in place of the physical stack height h. This is somewhat less than the physical height when the stack gas exit velocity v_s is less than 1.5 times the wind speed $u(\text{m s}^{-1})$:

$$h' = h \qquad \text{for } v_s \geq 1.5u \tag{22.1}$$

$$h' = h + 2d[(v_s/u) - 1.5] \qquad \text{for } v_s < 1.5u \tag{22.2}$$

where d is the inside stack-top diameter, m. This $h\text{¢}$ value is used with the buoyancy or momentum plume rise equations that follow. If stack downwash is not considered, h is substituted for $h\text{¢}$ in the equations.

B. Buoyancy Flux Parameter

For most plume rise estimates, the value of the buoyancy flux parameter F in m^4s^{-3} is needed:

$$\begin{aligned} F &= gv_s d^2(T_s - T)/(4T_s) \\ F &= 2.45v_s d^2(T_s - T)/T_s \end{aligned} \tag{22.3}$$

where g is the acceleration due to gravity, about $9.806\,\text{m s}^{-2}$, T_s is the stack gas temperature in K, T is ambient air temperature in K, and the other parameters are as previously defined.

C. Unstable–Neutral Buoyancy Plume Rise

The final effective plume height H, in m, is stack height plus plume rise. Where buoyancy dominates, the horizontal distance x_f from the stack to where the final plume rise occurs is assumed to be at $3.5x^*$, where x^* is the horizontal distance, in km, at which atmospheric turbulence begins to dominate entrainment.

For unstable and neutral stability situations, and for F less than 55, H, in m, and x_f, in km, are

$$H = h' + 21.425F^{3/4}/u \quad x_f = 0.049F^{5/8} \tag{22.4a,b}$$

For F equal to or greater than 55, H and x_f are

$$H = h' + 38.71F^{3/5}/u \quad x_f = 0.119F^{2/5} \tag{22.5a,b}$$

D. Stability Parameter

For stable situations, the stability parameter s is calculated by

$$s = g(\Delta\theta/\Delta z)/T$$

where $\Delta\theta/\Delta z$ is the change in potential temperature with height.

E. Stable Buoyancy Plume Rise

For stable conditions when there is wind, H and x_f are

$$H = h' + 2.6[F/(us)]^{1/3} \quad x_f = 0.00207us^{-1/2} \tag{22.6a,b}$$

For calm conditions (i.e., no wind) the stable buoyancy rise is

$$H = h' + 4F^{1/4}S^{-3/8} \tag{22.7}$$

Under stable conditions, the lowest value of Eq. (22.6a) or (22.7) is usually taken as the effective stack height.

The wind speed that yields the same rise from Eq. (22.6a) as that from Eq. (22.7) for calm conditions is

$$u = 0.2746F^{1/4}S^{1/8} \tag{22.8}$$

F. Gradual Rise: Buoyancy Conditions

Plume rise for distances closer to the source than the distance to the final rise can be estimated from

$$H = h' + 160F^{1/3}x^{2/3}/u \tag{22.9}$$

where x is the source-to-receptor distance, km. If this height exceeds the final effective plume height, that height should be substituted.

G. Unstable–Neutral Momentum Plume Rise

If the stack gas temperature is below or only slightly above the ambient temperature, the plume rise due to momentum will be greater than that due to buoyancy. For unstable and neutral situations,

$$H = h' + 3dv_s/u \tag{22.10}$$

This equation is most applicable when v_s/u exceeds 4. Since momentum plume rise occurs quite close to the source, the horizontal distance to the final plume rise is considered to be zero.

H. Stable Momentum Plume Rise

For low-buoyancy plumes in stable conditions, plume height due to momentum is given by

$$H = h' + 1.5[(v^2_s d^2 T)/(4T_s u)]^{1/3} s^{-1/6} \tag{22.11}$$

Equation (22.10) should also be evaluated and the lower value is used.

I. Momentum–Buoyancy Crossover

There is a specific difference between stack gas temperature and ambient air temperature that gives the same result for buoyancy rise as for momentum rise. For unstable or neutral conditions this is as follows: For F less than 55,

$$(T_s - T)_c = 0.0297 T_s v_s^{1/3}/d^{2/3} \tag{22.12}$$

For F equal to or greater than 55,

$$(T_s - T)_c = 0.00575 T_s v_s^{2/3}/d^{1/3} \tag{22.13}$$

For stable conditions,

$$(T_s - T)_c = 0.01958 T v_s s^{1/2} \tag{22.14}$$

J. Maximum Concentrations as a Function of Wind Speed and Stability

Using the source in the example in Chapter 21 ($Q = 0.37, h = 20, d = 0.537$, $v_s = 20$, and $T_s = 350$), with plume rise calculated using the above equations, maximum ground-level concentrations are shown (Fig. 22.1) as functions of stability class and wind speed calculated using the Gaussian model with

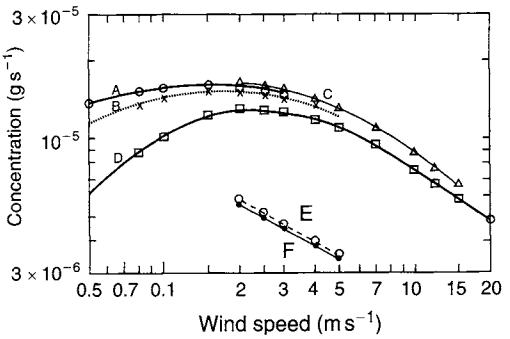

Fig. 22.1. Concentration of an air pollutant at the point of maximum ground-level concentration as a function of wind speed and Pasquill stability category (A–F).

Pasquill–Gifford dispersion parameters. Maximum concentrations are nearly the same for stabilities A, B, and C and occur at wind speeds of 1.5–2.0 $m\,s^{-1}$. The maximum for D stability occurs at around $u = 2.5\,m\,s^{-1}$. Because of the competing effects of dilution by wind and lower effective stack heights with higher wind speeds, concentrations do not change rapidly with wind speed. For E and F stabilities the concentrations are nearly the same (assuming that $\Delta\theta/\Delta z$ is 0.02 $K\,m^{-1}$ for E stability and 0.035 for F stability), but are considerably less than for the unstable and neutral cases.

II. MODELING TECHNIQUES

Gaussian techniques, discussed in Chapter 21, are reasonable for estimates of concentrations of nonreactive pollutants within 20 km of point sources. It is preferable to utilize on-site wind fluctuation measurements to estimate the horizontal and vertical spreading of a pollutant plume released from a point source.

In addition to the Gaussian modeling techniques already discussed, four other methods will be considered.

A. Box Model

Models which assume uniform mixing throughout the volume of a three-dimensional box are useful for estimating concentrations, especially for first approximations. For steady-state emission and atmospheric conditions, with no upwind background concentrations, the concentration is given by

$$\chi = \Delta x q_a/(z_i u) \tag{22.15}$$

where χ is the steady-state concentration, Δx is the distance over which the emissions take place, q_a is the area emission rate, z_i is the mixing height, and u is the mean wind speed through the vertical extent of the box.

When there is an upwind background concentration χ_b and the mixing height is rising with time into a layer aloft having an average concentration of χ_a, the equation of continuity is

$$\delta\chi/\delta t = [\Delta x q_a + u z_i(\chi_b - \chi) + \Delta x(\Delta z_i/\Delta t)(\chi_a - \chi)]/\Delta x z_i \tag{22.16}$$

This forms a basis for an urban photochemical box model (PBM) [6] discussed later in this chapter.

B. Narrow Plume Hypothesis

By assuming that the principal contributors to the concentration at a receptor are the sources directly upwind, especially those nearby, the concentration due to area sources can be calculated using the vertical growth rate rather than uniform vertical mixing and considering the specific area emission rate of each area upwind of the receptor. Area emission rate

changes in the crosswind direction are neglected as being relatively unimportant. The expansion in the vertical is usually considered using the Gaussian vertical growth [7, 8].

C. Gradient Transport Models

The mean turbulent flux of concentration in the vertical direction z is $\overline{w'\chi'}$. Assuming that this turbulent flux is proportional to the gradient of concentration, and in the direction from higher to lower concentrations, an overall diffusivity K can be defined as

$$\overline{w'\chi'} = -K(\delta\chi / \delta z) \tag{22.17}$$

The change in concentration with respect to time can be written as

$$\frac{\delta\chi}{\delta t} + \left(\bar{u}\frac{\delta\chi}{\delta x} + \bar{v}\frac{\delta\chi}{\delta y} + \bar{w}\frac{\delta\chi}{\delta z} \right) = \frac{\delta}{\delta x}K_x\frac{\delta\chi}{\delta x} + \frac{\delta}{\delta y}K_y\frac{\delta\chi}{\delta y} + \frac{\delta}{\delta z}K_z\frac{\delta\chi}{\delta z} + S \tag{22.18}$$

where the term in parentheses on the left accounts for advection. The terms on the right account for diffusivities in three directions, K_x, K_y, and K_z (where K_x is in the direction of the wind, K_y is horizontally crosswind, and K_z is vertically crosswind), and S represents emissions. This equation is the basis for the gradient transport model, which can handle varying wind and diffusivity fields. The vector speeds $\bar{u}$, $\bar{v}$, and $\bar{w}$ (where $\bar{u}$ is in the direction of the wind, $\bar{v}$ is horizontally crosswind, and $\bar{w}$ is vertically crosswind) and concentrations imply both time and space scales. Fluctuations over times and distances less than these scales are considered as turbulence and are included in the diffusivities.

The gradient transport model is most appropriate when the turbulence is confined to scales that are small relative to the pollutant volume. It is therefore most applicable to continuous line and area sources at ground level, such as automobile pollutants in urban areas, and to continuous or instantaneous ground-level area sources. It is not appropriate for elevated point source diffusion until the plume has grown larger than the space scale. Numerical rather than analytical solutions of Eq. (22.18) are used.

Errors in advection may completely overshadow diffusion. The amplification of random errors with each succeeding step causes numerical instability (or distortion). Higher-order differencing techniques are used to avoid this instability, but they may result in sharp gradients, which may cause negative concentrations to appear in the computations. Many of the numerical instability (distortion) problems can be overcome with a second-moment scheme [9] which advects the moments of the distributions instead of the pollutants alone. Six numerical techniques were investigated [10], including the second-moment scheme; three were found that limited numerical distortion: the second-moment, the cubic spline, and the chapeau function.

In the application of gradient transfer methods, horizontal diffusion is frequently ignored, but the variation in vertical diffusivity must be approximated [11–14].

D. Trajectory Models

In its most common form, a trajectory model moves in a vertical column, with a square cross section intersecting the ground, at the mean wind speed, with pollutants added to the bottom of the column as they are generated by each location over which the column passes. Treatment of vertical dispersion varies among models, from those which assume immediate vertical mixing throughout the column to those which assume vertical dispersion using a vertical coefficient K_z with a suitable profile [15].

Modeling a single parcel of air as it is being moved along allows the chemical reactions in the parcel to be modeled. A further advantage of trajectory models is that only one trajectory is required to estimate the concentration at a given endpoint. This minimizes calculation because concentrations at only a limited number of points are required, such as at stations where air quality is routinely monitored. Since wind speed and direction at the top and the bottom of the column are different, the column is skewed from the vertical. However, for computational purposes, the column is usually assumed to remain vertical and to be moved at the wind speed and direction near the surface. This is acceptable for urban application in the daytime, when winds are relatively uniform throughout the lower atmosphere.

Trajectory models of a different sort are used for long-range transport, because it is necessary to simulate transport throughout a diurnal cycle in which the considerable wind shear at night transports pollutants in different directions. Expanding Gaussian puffs can be used, with the expanded puff breaking, at the time of maximum vertical mixing, into a series of puffs initially arranged vertically but subsequently moving with the appropriate wind speed and direction for each height.

III. MODELING NONREACTIVE POLLUTANTS

A. Seasonal or Annual Concentrations

In estimating seasonal or annual concentrations from point or area sources, shortcuts can generally be taken rather than attempting to integrate over short intervals, such as hour-by-hour simulation. A frequent shortcut consists of arranging the meteorological data by joint frequency of wind direction, wind speed, and atmospheric stability class, referred to as a *STability ARray* (STAR). The ISCLT (Industrial Source Complex Long Term) [16] is a model of this type and is frequently used to satisfy regulatory requirements where concentrations averaged over 1 year (but not shorter averaging times) or longer are required. Further simplification may be achieved by determining a single

effective wind speed for each stability–wind direction sector combination by weighting $1/u$ by the frequency of each wind speed class for each such wind direction–stability combination. Calculations for each sector are made, assuming that the frequency of wind direction is uniform across the sector.

B. Single Sources: Short-Term Impact

Gaussian plume techniques have been quite useful for determining the maximum impact of single sources, which over flat terrain, occurs within 10–20 km of the source. The ISCST model [16] is usually used to satisfy regulatory requirements. Because the combination of conditions that produces multihour high concentrations cannot be readily identified over the large range of source sizes, it has been a common practice to calculate the impact of a source for each hour of the year for a large number of receptors at specific radial distances from the source for 36 directions from the source, e.g., every 10°. Averaging and analysis can proceed as the calculations are made to yield, upon completion of a year's simulation, the highest and second-highest concentrations over suitable averaging times, such as 3 and 24 h. Frequently, airport surface wind data have been utilized as input for such modeling, extrapolating the surface wind speed to stack top using a power law profile, with the exponent dependent on stability class, which is also determined from the surface data. Although the average hourly wind direction at stack top and plume level is likely to be different from that at the surface, this has been ignored because hourly variations in wind direction at plume level closely parallel surface directional variations. Although the true maximum concentration may occur in a somewhat different direction from that calculated, its magnitude will be closely approximated.

Several point source algorithms, Hybrid Plume Dispersion Model (HPDM) [17, 18] and TUPOS [19, 20], incorporate the use of fluctuation statistics (the standard deviations of horizontal and vertical wind directions) and non-Gaussian algorithms for strongly convective conditions. Because during strong convective conditions, thermals with updrafts occupy about 30–35% of the area and slower descending downdrafts occupy 65–70% of the area, the resulting distribution of vertical motions are not Gaussian but have a smaller number of upward motions, but with higher velocity, and a larger number of downward motions, but with lower velocity. These skewed vertical motion distributions then cause non-Gaussian vertical distributions of pollutant concentrations.

C. Multiple Sources and Area Sources

The problem, already noted, of not having the appropriate plume transport direction takes on added importance when one is trying to determine the effects of two or more sources some distance apart, since an accurate estimate of plume transport direction is necessary to identify critical periods when plumes are superimposed, increasing concentrations.

In estimating concentrations from area sources, it is important to know whether there is one source surrounded by areas of no emissions or whether the source is just one element in an area of continuous but varying emissions.

To get an accurate estimate of the concentrations at all receptor positions from an isolated area source, an integration should be done over both the alongwind and crosswind dimensions of the source. This double integration is accomplished in the point, area, and line (PAL) source model [21] by approximating the area source using a number of finite crosswind line sources. The concentration due to the area source is determined using the calculated concentration from each line source and integrating numerically in the alongwind direction.

If the receptor is within an area source, or if emission rates do not vary markedly from one area source to another over most of the simulation area, the narrow plume hypothesis can be used to consider only the variation in emission rates from each area source in the alongwind direction. Calculations are made as if from a series of infinite crosswind line sources whose emission rate is assigned from the area source emission rate directly upwind of the receptor at the distance of the line source. The Atmospheric Turbulence and Diffusion Laboratory (ATDL) model [22] accomplishes this for ground-level area sources. The Regional Air Monitoring (RAM) model [8] does this for ground-level or elevated area sources.

Rather than examining the variation of emissions with distance upwind from the receptor as already described, one can simplify further by using the area emission rate of only the emission square in which the receptor resides [23]. The concentration χ is then given by

$$\chi = Cq_a/u \tag{22.19}$$

where q_a is the area emission rate, u is the mean wind speed over the simulation period, and the constant C is dependent on the stability, the effective height of emission of the sources, and the characteristics of the pollutant. For estimation of annual concentrations with this method, $C = 50$, 200, and 600 for SO_2, particulate matter (PM), and CO, respectively [24].

D. Pollutants that Deposit

The Fugitive Dust Model (FDM) [25] was formulated to estimate air concentrations as well as deposition from releases of airborne dust. It has a greatly improved deposition mechanism compared with that in previous models. It considers the mass removed from the plume through deposition as the plume is moved downwind. Up to 20 particle size fractions are available. The particle emissions caused as material is raised from the surface by stronger winds is built internally into this model. It has the capacity of making calculations for PAL sources. The area source algorithm has two options, simulation of the area source by five finite line sources perpendicular to wind flow, or a converging algorithm which provides greater accuracy. Currently, the model should be used for releases at or below 20 m above ground level.

E. Dispersion from Sources over Water

The Offshore and Coastal Dispersion (OCD) model [26] was developed to simulate plume dispersion and transport from offshore point sources to receptors on land or water. The model estimates the overwater dispersion by use of wind fluctuation statistics in the horizontal and the vertical measured at the overwater point of release. Lacking these measurements, the model can make overwater estimates of dispersion using the temperature difference between water and air. Changes taking place in the dispersion are considered at the shoreline and at any point where elevated terrain is encountered.

F. Dispersion over Complex Terrain

Development efforts in complex terrain by U.S. EPA researchers using physical modeling, both in the wind tunnel and in the towing tank, and field studies at three locations have resulted in the development of CTDMPLUS complex terrain dispersion model plus the calculation of concentrations for unstable conditions [27]. Complex terrain is the situation in which there are receptor locations above stack top. Using the meteorological conditions and the description of the nearby terrain feature, the model calculates the height of a dividing streamline. Releases that take place below the height of this streamline tend to seek a path around the terrain feature; releases above the streamline tend to rise over the terrain feature. Because the dispersion is calculated from fluctuation statistics, the meteorological measurements to provide data input for the model are quite stringent, requiring the use of tall instrumented towers. Evaluations of both the model [28] and a screening technique derived from the model [29] indicate that the model does a better job of estimating concentrations than previous complex terrain models.

IV. MODELING POLLUTANT TRANSFORMATIONS

A. Individual Plumes

Most pollutants react after release. However, many pollutants have such long half-lives in the atmosphere, it is safe to assume for most modeling purposes that they are nonreactive. However, numerous other pollutants undergo degradation within the atmosphere to such an extent that the model needs to consider their transformation to properly predict concentrations of the parent compound. The transformation is affected by numerous factors, including cloud chemistry and other aspects of water vapor, aerosol concentrations, catalysis, and photochemistry. In fact, many of the processes described in Table 6.1 occur in the atmosphere.

An understanding of the transformation of SO_2 and NO_x into other constituents no longer measurable as SO_2 and NO_x is needed to explain mass balance changes from one plume cross section to another. This loss of the

primary pollutant SO_2 has been described as being exponential, and rates up to 1% per hour have been measured [30]. The secondary pollutants generated by transformation are primarily sulfates and nitrates.

The horizontal dispersion of a plume has been modeled by the use of expanding cells well mixed vertically, with the chemistry calculated for each cell [31]. The resulting simulation of transformation of NO to NO_2 in a power plant plume by infusion of atmospheric ozone is a peaked distribution of NO_2 that resembles a plume of the primary pollutants, SO_2 and NO. The ozone distribution shows depletion across the plume, with maximum depletion in the center at 20 min travel time from the source, but relatively uniform ozone concentrations back to initial levels at travel distances 1 h from the source.

B. Urban-Scale Transformations

Approaches used to model ozone formation include box, gradient transfer, and trajectory methods. Another method, the particle-in-cell method, advects centers of mass (that have a specific mass assigned) with an effective velocity that includes both transport and dispersion over each time step. Chemistry is calculated using the total mass within each grid cell at the end of each time step. This method has the advantage of avoiding both the numerical diffusion of some gradient transfer methods and the distortion due to wind shear of some trajectory methods.

It is not feasible to model the reaction of each hydrocarbon species with oxides of nitrogen. Therefore, hydrocarbon species with similar reactivities are lumped together, e.g., into four groups of reactive hydrocarbons: olefins, paraffins, aldehydes, and aromatics [32].

In addition to possible errors due to the steps in the kinetic mechanisms, there may be errors in the rate constants due to the smog chamber databases from which they were derived. A major shortcoming is the limited amount of quality smog chamber data available.

The emission inventory and the initial and boundary conditions of pollutant concentrations have a large impact on the ozone concentrations calculated by photochemical models.

To model a decrease in visibility, the chemical formation of aerosols from sulfur dioxide and oxidants must be simulated.

In a review of ozone air quality models, Seinfeld [33] indicates that the most uncertain part of the emission inventories is the hydrocarbons. The models are especially sensitive to the reactive organic gas levels, speciation, and the concentrations aloft of the various species. He points out the need for improvement in the three-dimensional wind fields and the need for hybrid models that can simulate sub-grid-scale reaction processes to incorporate properly effects of concentrated plumes. Schere [34] points out that we need to improve the way vertical exchange processes are included in the model. Also, although the current models estimate ozone quite well, the

atmospheric chemistry needs improvement to better estimate the concentrations of other photochemical components such as peroxyacyl nitrate (PAN), the hydroxyl radical (OH), and volatile organic compounds (VOCs). In addition to the improvement of databases, including emissions, boundary concentrations, and meteorology, incorporation of the urban ozone with the levels at larger scales is needed.

C. Regional-Scale Transformations

In order to formulate appropriate control strategies for oxidants in urban areas, it is necessary to know the amount of oxidant already formed in the air reaching the upwind side of the urban area under various atmospheric conditions. Numerous physical and chemical processes are involved in modeling transformations [35, 36] on the regional scale (several days, 1000 km): (1) horizontal transport; (2) photochemistry, including very slow reactions; (3) nighttime chemistry of the products and precursors of photochemical reactions; (4) nighttime wind shear, stability stratification, and turbulence episodes associated with the nocturnal jet; (5) cumulus cloud effects—venting pollutants from the mixed layer, perturbing photochemical reaction rates in their shadows, providing sites for liquid-phase reactions, influencing changes in the mixed-layer depth, perturbing horizontal flow; (6) mesoscale vertical motion induced by terrain and horizontal divergence of the large-scale flow; (7) mesoscale eddy effects on urban plume trajectories and growth rates; (8) terrain effects on horizontal flows, removal, and diffusion; (9) sub-grid-scale chemistry processes resulting from emissions from sources smaller than the model's grid can resolve; (10) natural sources of hydrocarbons, NO_x, and stratospheric ozone; and (11) wet and dry removal processes, washout, and deposition.

Approaches to long-term (monthly, seasonal, annual) regional exchanges are EURMAP [37] for Europe and ENAMAP [38] for eastern North America. These two models can calculate SO_2 and sulfate air concentrations as well as dry and wet deposition rates for these constituents. The geographic region of interest (for Europe, about 2100 km N–S by 2250 km E–W) is divided into an emissions grid having approximately 50 by 50 km resolution. Calculations are performed by releasing a 12-h average emission increment or "puff" from each cell of the grid and tracking the trajectories of each puff by 3-h time steps according to the 850-mb winds interpolated objectively for the puff position from upper-air data.

Uniform mixing in the vertical to 1000 m and uniform concentrations across each puff as it expands with the square root of travel time are assumed. A $0.01\,h^{-1}$ transformation rate from SO_2 to sulfate and 0.029 and $0.007\,h^{-1}$ dry deposition rates for SO_2 and sulfate, respectively, are used. Wet deposition is dependent on the rainfall rate determined from the surface observation network every 6 h, with the rate assumed to be uniform over each 6-h period. Concentrations for each cell are determined by averaging the concentrations

of each time step for the cell, and deposition is determined by totaling all depositions over the period.

The EURMAP model has been useful in estimating the contribution to the concentrations and deposition on every European nation from every other European nation. Contributions of a nation to itself range as follows: SO_2 wet deposition, 25–91%; SO_2 dry deposition, 31–91%; sulfate wet deposition, 2–46%; sulfate dry deposition, 4–57%.

In the application of the model to eastern North America, the mixing height is varied seasonally, and hourly precipitation data are used.

V. MODELING AIR POLLUTANTS

A. The Need for Models

Models provide a means for representing a real system in an understandable way.[1] They take many forms, beginning with "conceptual models" that explain the way a system works, such as delineation of all the factors and parameters of how a particle moves in the atmosphere after its release from a power plant. Conceptual models help to identify the major influences on where a chemical is likely to be found in the environment, and as such, need to be developed to help target sources of data needed to assess an environmental problem.

In general, developing an air pollution model requires two main steps. First, a model of the domain and the processes being studied must be defined. Then, at the model boundaries, a model of the boundary conditions is especially needed to represent the influential environment surrounding the study domain. The quality of the model study is related to the accuracy and representativeness to the actual study.

B. Physical Models

Research scientists often develop "physical" or "dynamic" models to estimate the location where a contaminant would be expected to move under controlled conditions, only on a much smaller scale. For example, the US Environmental Protection Agency's (EPA) wind tunnel facility in Research Triangle Part is sometimes used to support studies when local buildings and terrain have significant influences. For example, the wind tunnel housed a scaled model of the town of East Liverpool, Ohio and its surrounding terrain to estimate the movement of the plume from an incinerator. The plume could be observed under varying conditions, including wind direction and height of release. Like all models, the dynamic models' accuracy is dictated by the

[1] See Leete, J., Groundwater modeling in health risk assessment, in *A Practical Guide to Understanding, Managing and Reviewing Environmental Risk Assessment Reports* (Benjamin, S., and Belluck, D., eds.), Chapter 17. Lewis Publishers, Boca Raton, FL, 2001.

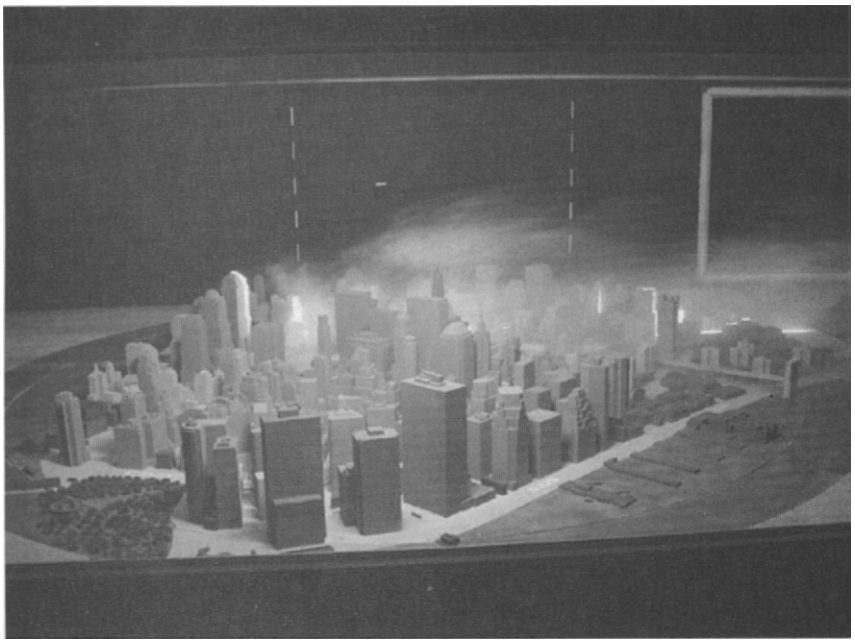

Fig. 22.2. Example of neutrally buoyant smoke released from the WTC physical model, showing flow from left to right is displayed; natural light is illuminating the smoke and a vertical laser sheet is additionally illuminating the plume near the centerline of source. *Source*: US Environmental Protection Agency. Perry, S., and Heath, D., *Fluid Modeling Facility*. Research Triangle Park, NC, 2006.

degree to which the actual conditions can be simulated and the quality of the information that is used. More recently, the wind tunnel was used to simulate pollutant transport and dispersion in Lower Manhattan to simulate possible plumes of pollutants from the collapse of the World Trade Center (WTC) towers on September 11, 2001. The 1:600 scale model was constructed on a turntable to test different wind directions (see Fig. 22.2). In addition to the building of Lower Manhattan and the rubble pile as it appeared approximately 1 week after the collapse, smoke for visualization and tracer gas for measurement dispersion patterns were released from positions throughout the simulated 16 acre site.

The study design includes smoke visualization for a qualitative examination of dispersion in this very complex urban landscape, known as an "urban street canyon." Detailed measurements were taken of flow velocities and turbulence, as well as concentration distribution, which suggested a number of flow phenomena that are not possible to consider using simple Gaussian dispersion algorithms (see Fig. 22.3). These include vertical venting behind large/tall buildings, channeling down street canyons, and both horizontal and vertical re-circulations associated with individual structures

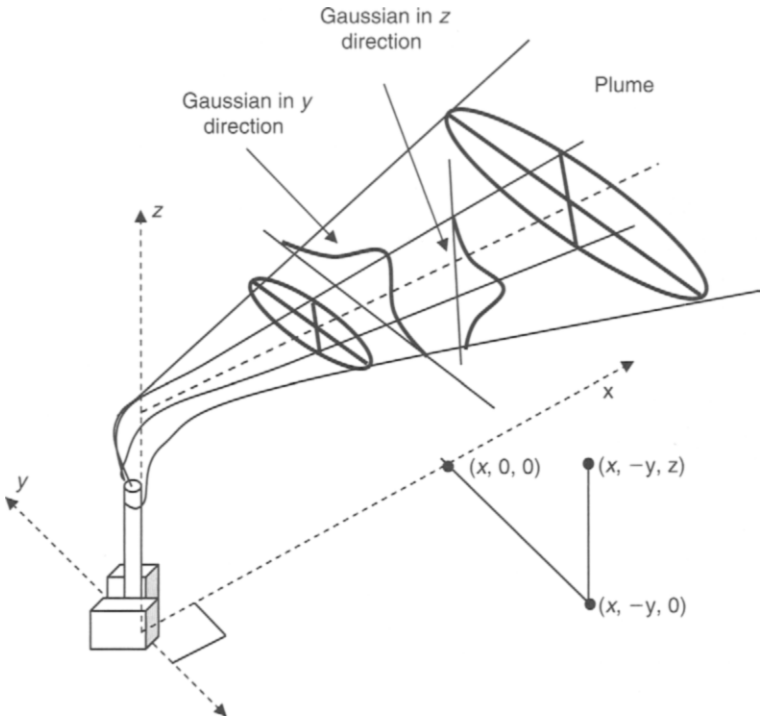

Fig. 22.3. Atmospheric plume model based on random distributions in the horizontal and vertical directions. *Source*: Turner, D., *Workbook of Atmospheric Dispersion Estimates*. Office of Air Programs Publication No. AP-26 (NTIS PB 191 482). US Environmental Protection Agency, Research Triangle Park, NC, 1970.

and groups of tall and tightly compacted buildings (such as the Wall Street area in the southeast edge of Manhattan, New York).

C. Numerical Simulation Models[2]

Numerical models apply mathematical expressions to approximate a system. System is a thermodynamic concept. Recall that we deal with three basic types of systems in air pollution sciences:

1. Isolated systems, in which no matter or energy crosses the boundaries of the system (i.e. no work can be done on the system).
2. Closed systems, in which energy can exchange with surroundings, but no matter crosses the boundary.
3. Open systems, in which both matter and energy freely exchange across system boundaries.

[2] Alan H. Huber contributed substantially to this discussion. The author appreciates these insights from one of the pioneers in the application of CFD to air pollutant transport phenomena.

Isolated systems are usually only encountered in highly controlled reactors, so are not pertinent to this discussion. In fact, most air pollution systems are open, but with simplifying assumptions, some subsystems can be treated as closed.

Rapid advances in high performance computing hardware and software are leading to increasing applications of numerical simulation models that characterize an atmospheric plume as a system. These methods simulate spatially and temporally resolved details of the pathways of air pollutants from source emissions to pollutant concentrations within the local "virtual" microenvironment. This approach to air pollution modeling applies numerical representation of fluid flow in a fluid continuum. Such an approach is known as computational fluid dynamics (CFD), which determines a numerical solution to the governing equations of fluid flow while advancing the solution through space or time to obtain a numerical description of the complete flow field of interest. CFD models are based on the first principles of physics; in particular, they start with single-phase flow based on Navier–Stokes equations.

The Navier–Stokes equations are deterministic. They consider simultaneously the conservation of energy, momentum, and mass. Practical CFD solutions require a sub-grid-scale model for turbulence. As computing capacities advance, the scale where turbulence is modeled can be reduced and the application of higher-order numerical methods can support increasingly representative and accurate turbulence models. The transport and dispersion of air pollutants is part of the fluid flow solution. CFD methods have been developed and routinely applied to aerospace and automotive industrial applications and are now being extended to environmental applications.

High-fidelity fine-scale CFD simulation of pollutant concentrations within microenvironments (e.g. near roadways or around buildings) is feasible now that high performance computing has become more accessible. Fine-scale CFD simulations have the added advantage of being able to account rigorously for topographical details such as terrain variations and building structures in urban areas as well as their local aerodynamics and turbulence. Thermal heat fluxes may be added to terrain and building surfaces to simulate the thermal atmospheric boundary layer, their influences on pollution transport and dispersion. The physics of particle flow and chemistry can be included in CFD simulations. The results of CFD simulations can be directly used to better understand specific case studies as well as to support the development of better-simplified algorithms for adoption into other modeling systems. For example, CFD simulations with fine-scale physics and chemistry can enhance and complement photochemical modeling with Community Multiscale Air Quality (CMAQ). Also, detailed CFD simulation for a complex site study can be used to develop reliable parameterizations to support simplified and rapid application air pollution model.

A few examples illustrate the utility of CFD modeling. Currently the main features of CFD application are the inclusion of site-specific geometry and dynamic processes affecting air pollution transport and dispersion. The

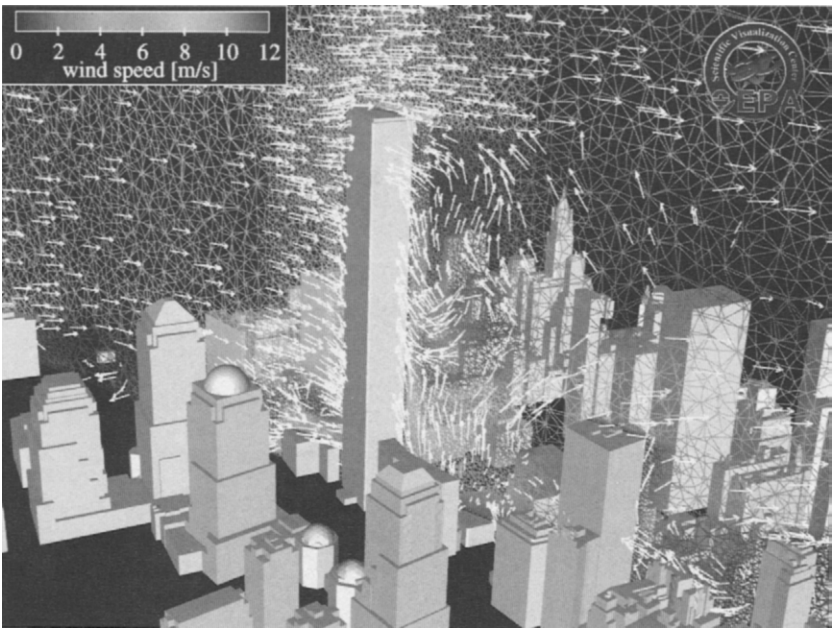

Fig. 22.4. A vertical slice of the resolved grid and sample (10%) of wind vectors in a CFD model of New York City. *Courtesy*: Huber, A. H., US Environmental Protection Agency, Research Triangle Park, NC (unpublished work, used with permission).

future will bring more refined spatial and temporal details, along with particle physics and chemistry. A vertical slice of the domain cells and a 10% sample of calculated wind vectors for these cells are shown in Fig. 22.4. The figure demonstrates a tendency for downward airflow on the windward faces of buildings and upward airflow on the leeward building faces. Figure 22.4 shows two different looking plume depictions for ground-level point emissions. In one case the emissions plume is caught in the leeward building updraft leading to significant vertical mixing, whereas the other case shows emissions remaining close to the ground as they move through the street canyons. Figure 22.5 shows vertical slices of concentration for roadway emissions represented as a box along the streets. There are significant differences for the case with a building on only one side of the roadway (a) relative to the street canyon (b), which induces a region of circulation (c).

CFD models have also found much use in estimating indoor and personal exposure to air pollutants. CFD modeling can also be used to simulate indoor air movement and pollution dispersion. For example, Furtaw[3] presents an example of this in a room where air movement vectors and pollutant concentration isopleths are around an emission source (represented by the small

[3] Furtaw., E. J., An overview of human exposure modeling activities at the USEPA's National Exposure Research Laboratory, *Toxicol. Ind. Health* **17** (5–10), 302–314 (2001).

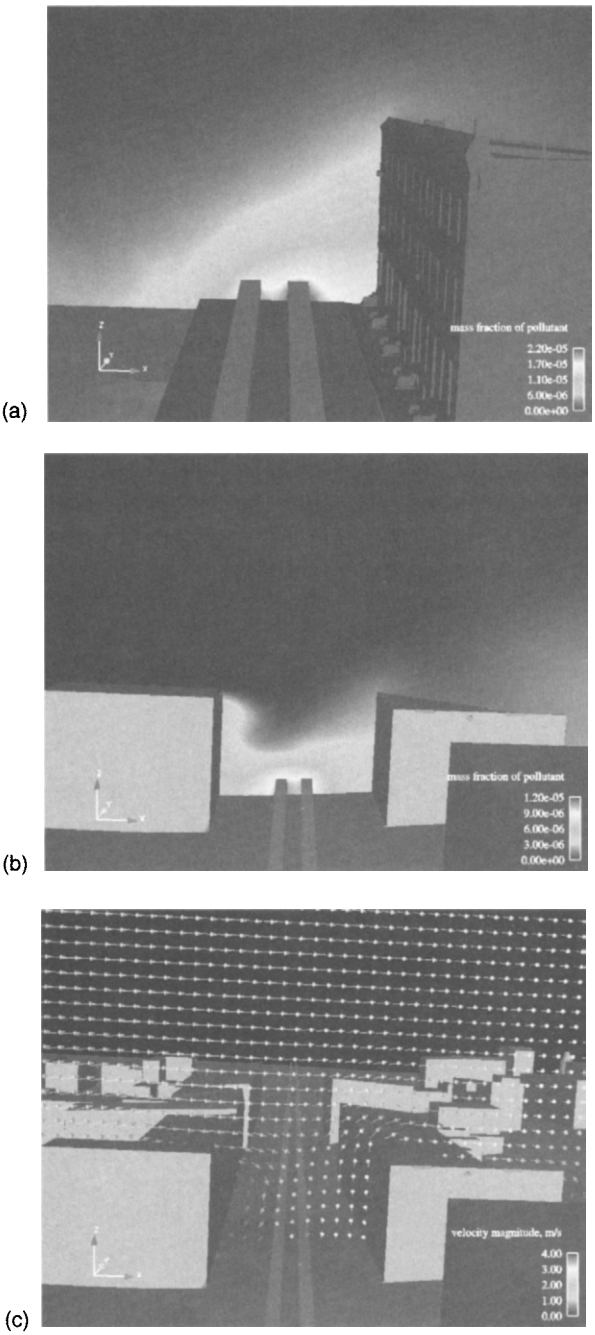

Fig. 22.5. Vertical slice view of a CFD model of roadway emissions represented as a source box along the roadway: (a) concentrations for street bounded by building on one side; (b) concentrations for street canyon; and (c) wind vectors for street canyon. *Courtesy*: Unpublished work by Huber, A. H., US Environmental Protection Agency, Research Triangle Park, NC.

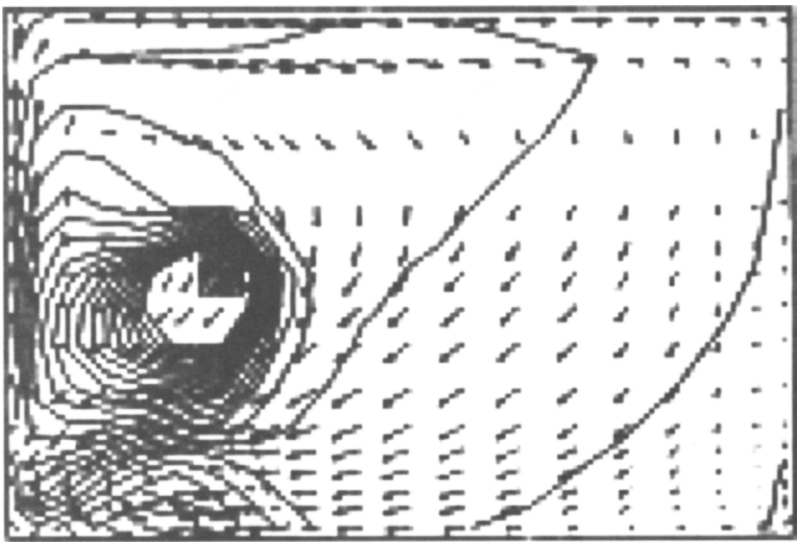

Fig. 22.6. CFD model simulation of indoor air in a room. *Source*: Furtaw, E. J., An overview of human exposure modeling activities at the USEPA's National Exposure Research Laboratory. *Toxicol.Ind. Health* **17** (5–10), 302–314 (2001).

square in Fig. 22.6). While CFD model simulation of every room in many buildings may not be a feasible, example case studies are possible for very critical situations or generic situations leading to the development of exposure factors for typical indoor room environments. Similarly, Settles[4] provides an excellent perspective on the increasing role for CFD model simulations for both ambient and indoor air concentrations as are critical to many homeland security issues involving potential human exposures. Figure 22.7 illustrates an application of CFD model simulations of trace concentrations behind a walking human. CFD model simulations at the human exposure scales can be very detailed and particularly useful in developing human exposure factors applicable for more general population-based human exposure models.

Some of atmospheric concentrations of pollutants consist of a regional background concentration due to long-range transport and regional-scale mixing as well as specific local microenvironmental concentrations. Concentrations within the local microenvironment often dominate a profile of total human exposure to the pollutant. Regional air quality applications are normally applied at grid resolutions larger than 10 km. Urban applications are applied at smaller grid scales but there is a meaningful limit due to the sub-grid-scale process models. In other words, there is no value in applying the model at fine scales without supporting details on the finer resolution. For example, the present framework of the CMAQ modeling system well supports environmental

[4] Settles, G. S., Fluid mechanics and homeland security. *Annu. Rev. Fluid Mech.* **38**, 87–110 (2006).

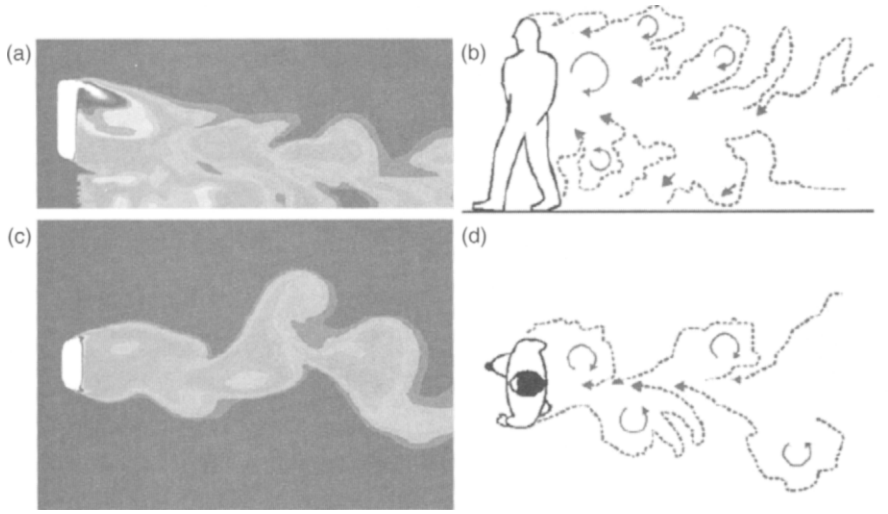

Fig. 22.7. The instantaneous trace contaminant concentration in the wake of a walking person, from Edge *et al.* (2005). Frames (a) and (c) are RANS solutions using a blended k–ϖ/k–ϵ 2-equation turbulence model and a simplified representation of the human body. Frames (b) and (d) are drawn from flow visualization experiments of an actual walking person. A side view is depicted in frames (a) and (b); frames (c) and (d) show the top view. *Source*: Settles, G. S., Fluid mechanics and homeland security. *Annu. Rev. Fluid Mech.* **38**, 87–110 (2006).

issues where large-sized grid-averaged concentrations are applicable. For example, regional emission control strategies are especially applicable while specific profiles of human exposure concentrations are not.

The large grid-sized modeling system may be used for estimating profiles of human exposure for pollutants having course temporal and spatial distributions. Human exposure concentrations on the sub-grid scales need to apply a sub-grid-scale model including human exposure factors to estimate exposed populations (such as that shown in Fig. 22.8). Such constraints related to local-scale air pollution and human exposure will be further discussed in the modeling sections below. Advances in numerical simulations models will continue to supplement and to improve the more simplified models presented in the following sections, particularly for simulations where building environments and complex terrain are significant.

Transport and fate models can be statistical and/or "deterministic." Statistical models include the pollutant dispersion models, such as the Lagrangian models, which assume Gaussian distributions of pollutants from a point of release (see Fig. 22.3). That is, the pollutant concentrations are normally distributed in both the vertical and horizontal directions from the source. The Lagrangian approach is common for atmospheric releases. "Stochastic" models are statistical models that assume that the events affecting the behavior of a chemical in the environment are random, so such models are based on probabilities.

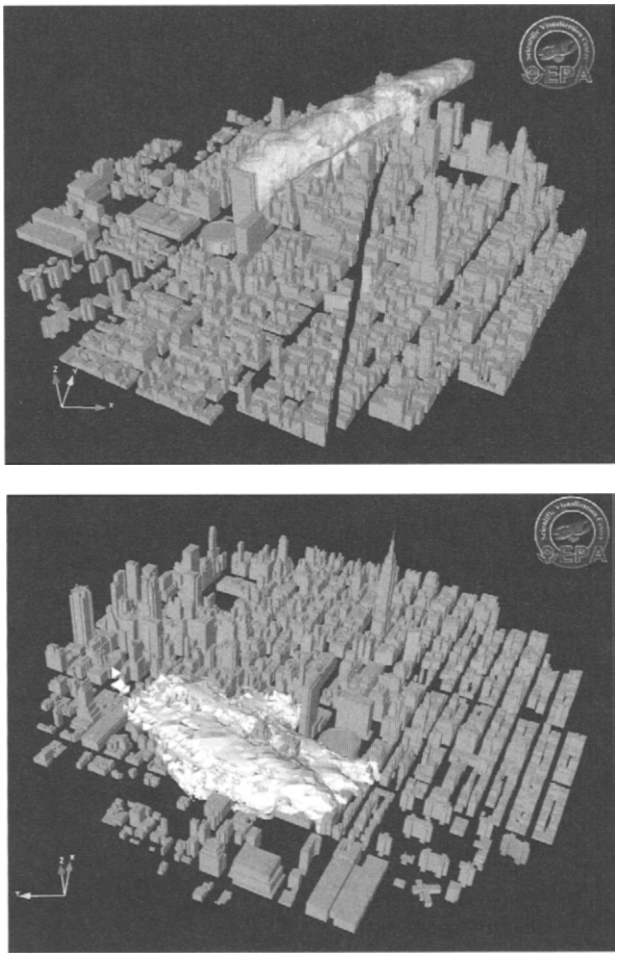

Fig. 22.8. Plumes from ground-level point source emissions in a CFD model of New York City (midtown area). *Courtesy*: Huber, A. H., US Environmental Protection Agency, Research Triangle Park, NC (unpublished work, used with permission).

Deterministic models are used when the physical, chemical, and other processes are sufficiently understood so as to be incorporated to reflect the movement and fate of chemicals. These are very difficult models to develop because each process must be represented by a set of algorithms in the model. Also, the relationship between and among the systems, such as the kinetics and mass balances, must also be represented.

Thus, the modeler must "parameterize" every important event following a chemical's release to the environment. Often, hybrid models using both statistical and deterministic approaches are used, for example, when one part of a system tends to be more random, while another has a very strong basis is physical principals. Numerous models are available to address the

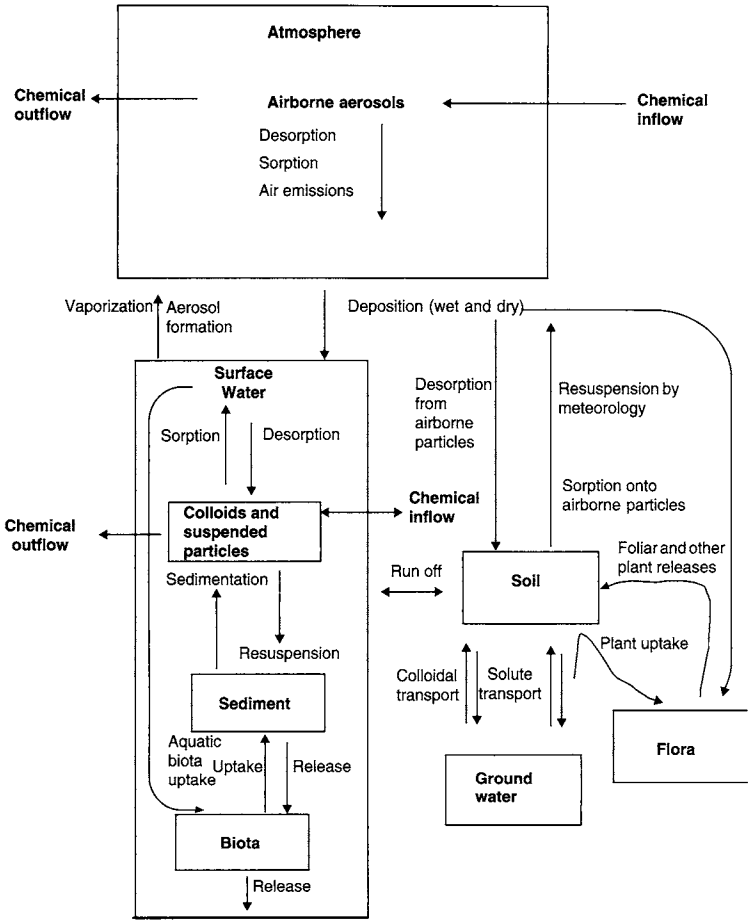

Fig. 22.9. Example framework and flow of a multimedia, compartmental chemical transport, and transformation model. Algorithms and quantities must be provided for each box. Equilibrium constants (e.g. partitioning coefficients) must be developed for each arrow and, steady-state conditions may not be assumed, reaction rates and other chemical kinetics must be developed for each arrow and box.

movement of chemicals through a single environmental media, but increasingly, environmental scientists and engineers have begun to develop "multimedia models," such as compartmental models that help to predict the behavior and changes to chemicals as they move within and among the soil, water, air, sediment, and biota (see Fig. 22.9).[5] Such models will likely see increased use in all environmental science and engineering.

[5] The compartmental or box models such as the one in Fig. 3.29 are being enhanced by environmental scientists and chemical engineers. Much of the information in this figure can be attributed to discussions with Yoram Cohen, a chemical engineering professor at UCLA, and Ellen Cooter, a National Oceanic and Atmospheric Administration modeler on assignment to the US EPA's National Exposure Research Laboratory in Research Triangle Park, NC.

Environmental chemodynamics describe the movement and change of chemicals in the environment (see Chapter 6). From an air pollution modeling perspective, the air is among one compartment among many. Most air pollution modeling is conducted as if the troposphere were the only compartment. This is usually a reasonable approach. However, we must keep in mind that the influences shown in Fig. 22.9 are always present. The air is a medium by which pollutants are transported. It is also the location of chemical reactions and physical changes, such as the agglomeration of smaller particles and the formation of particles from gas-phase pollutants. Fluid properties have a great bearing on the movement and distribution of contaminants. However, specific partitioning relationships that control the "leaving" and "gaining" of pollutants among particle, soil, and sediment surfaces, the atmosphere, organic tissues, and water can also be applied to model where a chemical ends up and the chemical form it assumes. This is known as environmental fate. These relationships are sorption, solubility, volatilization, and organic carbon–water partitioning, which are respectively expressed by coefficients of sorption (distribution coefficient (K_D) or solid–water partition coefficient (K_p)), dissolution or solubility coefficients, air–water partitioning (and the Henry's law (K_H) constant), and organic carbon–water (K_{oc}). These equilibrium coefficients are discussed in detail in Chapter 6.

D. Using Models to Predict Air Pollution

Air quality models mathematically simulate the physical and chemical processes that affect air pollutants as they disperse and react in the atmosphere. Meteorological data and source information (e.g. emission rates and stack height) are put into models to characterize pollutants that are emitted directly into the atmosphere. Air quality modelers generally refer to these as primary pollutants. Secondary pollutants, those that form as a result of complex chemical reactions within the atmosphere, can also be modeled. Models are a key component of air quality management at all scales. They are widely used by local, state and federal agencies charged with addressing air pollution, especially to identify source contributions to air quality problems and to help to design effective strategies aimed at reducing air pollutants. Models can be used to verify that before issuing a permit, a new source will not exceed ambient air quality standards or, if appropriate, to agree on appropriate additional control requirements. Models are useful as prediction tools, for example, to estimate the future pollutant concentrations from multiple sources after a new regulatory program is in place. This gives a measure of the expected effectiveness of various options in reducing harmful exposures to humans and the environment.

E. Dispersion Modeling

Dispersion modeling is used to predict concentrations at selected downwind receptor locations. According to the EPA, these air quality models help

to determine compliance with National Ambient Air Quality Standards (NAAQS), and other regulatory requirements such as New Source Review (NSR) and Prevention of Significant Deterioration (PSD) regulations.[6] These guidelines are periodically revised to ensure that new model developments or expanded regulatory requirements are incorporated. The EPA recommends the AERMOD modeling system be used by states and local regulators to determine their progress in reducing criteria air pollutants under the Clean Air Act (CAA). AERMOD is a steady-state plume model that incorporates air dispersion based on planetary boundary-layer turbulence structure and scaling concepts, including treatment of both surface and elevated sources, and both simple and complex terrain.

AERMOD is better able to characterize plume dispersion than the model it replaced, the Industrial Source Complex (ISC3), which had been EPA's preferred model since 1980. In particular, AERMOD can simulate elevated air pollution sources as well as those at the surface, and can assimilate both simple and complex terrain (see Fig. 22.10). A substantial advance is that AERMOD makes use of updated physics algorithms. Thus, since November 9, 2006, AERMOD replaced ISC3 as the EPA's preferred general-purpose model. Regulators now use it to estimate local levels of ozone, VOCs, carbon monoxide, NO_2, SO_2, PM, and lead. Areas that have been unable to attain CAA standards for these criteria pollutants are required to use AERMOD to revise their State Implementation Plans (SIPs) for existing air pollution sources. States must also use AERMOD for their NSR and PSD determinations.

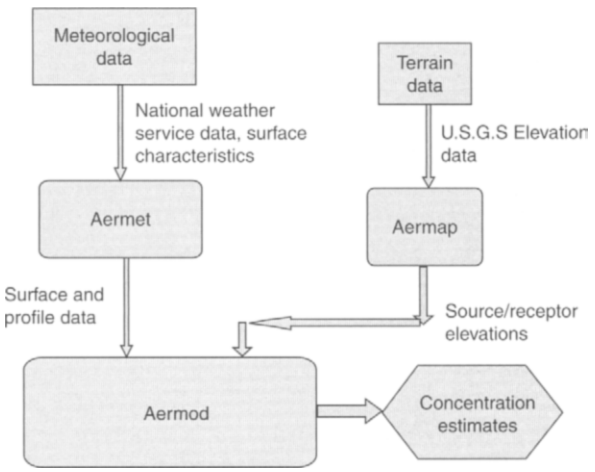

Fig. 22.10. Flow and processing of the complete AERMOD modeling system, which consists of the AERMOD dispersion model and two pre-processors. *Source*: US Environmental Protection Agency.

[6] These models are addressed in Appendix A of EPA's *Guideline on Air Quality Models* (also published as *Appendix W* of 40 CFR Part 51), which was originally published in April 1978 to provide consistency and equity in the use of modeling within the US air quality management system.

AERMOD modeling can be used to extrapolate from a limited number of data points. For example, it was recently used by the EPA in its regulatory impact analysis of the new standard for particulates by comparing a number of regulatory scenarios in terms of the costs and human health and welfare benefits. In this case, the comparison was among scenarios associated with attaining both the selected and one alternative standard for annual and daily $PM_{2.5}$ concentrations:

Combination of annual and daily values (annual/daily in $\mu g\,m^{-3}$)	Scenario
15/65	1997 Standards
15/35	New Standard
14/35	Alternative

One of the urban areas compared in analysis was the Detroit, Michigan. The primary $PM_{2.5}$ impacts at monitor locations in Wayne County, Michigan; the model shows locations where the annual ($15\,\mu g\,m^{-3}$) and daily ($35\,\mu g\,m^{-3}$) standards may well be exceeded.[7] Figure 22.11 provides the spatial gradient

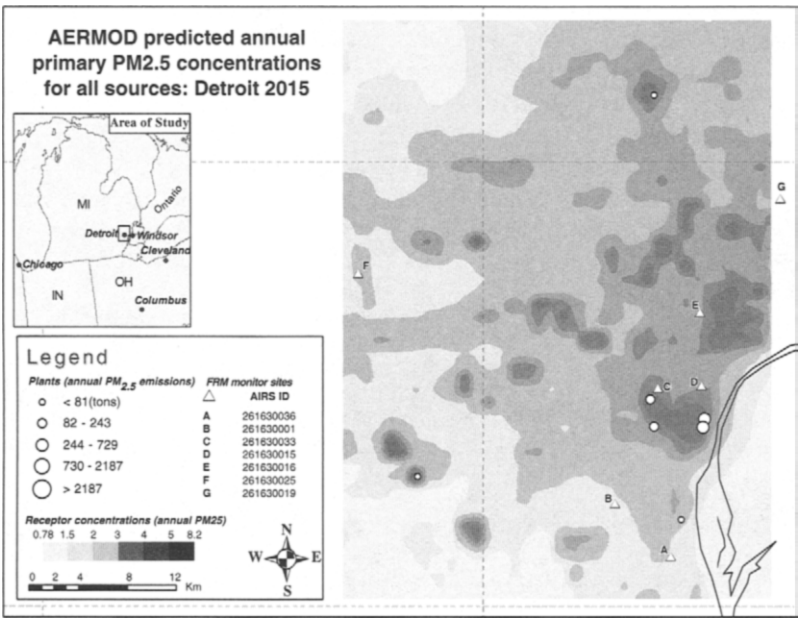

Fig. 22.11. Spatial gradient in Detroit, MI of AERMOD predicted annual primary $PM_{2.5}$ concentrations ($\mu g\,m^{-3}$) for all sources: 2015. *Note*: Dashed line reflect the 36-km grid cells from regional-scale modeling with CMAQ model.

[7] US Environmental Protection Agency, *Regulatory Impact Analysis for the Revised Particulate Matter*, National Ambient Air Quality Standards, 2006.

of primary $PM_{2.5}$ for the urban area associated with emissions from all sources. The model shows that this particular Wayne County monitor is expected to exceed $15\,\mu g\,m^{-3}$ by $2.4\,\mu g\,m^{-3}$ in the year 2015. This indicates that local sources of primary $PM_{2.5}$ contribute $3.3\,\mu g\,m^{-3}$ to this monitor location and that the application of controls for the 15/65 scenario would yield a $0.56\,\mu g\,m^{-3}$ reduction in $PM_{2.5}$ concentrations. The modeling results indicate little additional reductions at this monitor for the 15/35 scenario but an additional $0.46\,\mu g\,m^{-3}$ reduction in $PM_{2.5}$ concentrations for the 14/35 scenario. The AERMOD simulations of annual and daily exceedences are shown in Tables 22.1 and 22.2, respectively.

For non-steady-state conditions, the EPA recommends the CALPUFF modeling system, which is a non-steady-state puff dispersion model that simulates the effects of time- and space-varying meteorological conditions on pollution transport, transformation, and removal. CALPUFF is a multi-layer, multi-species non-steady-state puff dispersion model that simulates the effects of time- and space-varying meteorological conditions on pollution transport, transformation and removal. It can be applied at scales of tens to hundreds of kilometers. It includes algorithms for sub-grid-scale effects (such as terrain impingement), as well as, longer-range effects (such as pollutant removal due to wet scavenging and dry deposition, chemical transformation, and visibility effects of PM concentrations). Thus, CALPUFF is particularly useful for long-range pollutant transport and for complex terrain.

CALPUFF is one of the models used to characterize the plume from Ground Zero at WTC in New York City. The predicted plumes provided general insights into the likely pathway for pollutant emissions released from the collapse and the fire at the WTC site, both temporally and spatially (see Fig. 22.12). Huber *et al.*[8] give some perspective about the use of CALPUFF:

> A CALMET–CALPUFF type modeling system cannot provide as precise an estimate of pollution levels as fuller physics models might, is considered to be adequate for many applications. Even without the precise concentrations, knowing generally where the plume may have been can still help determine where to conduct more refined modeling of human exposures and where to study the population exposure in epidemiological studies. Having such results rapidly as a forecast or screening model could be very valuable to decision-makers.

Other models used by regulatory agencies include:

- BLP—A Gaussian plume dispersion model designed to handle unique modeling problems associated with aluminum reduction plants, and other industrial sources where plume rise and downwash effects from stationary line sources are important.

[8] Huber, A., Georgopoulos, P., Gilliam, R., Stenchikov, G., Wang, S-W., Kelly, B., and Feingersh, H., Modeling air pollution from the collapse of the World Trade Center and assessing the potential impacts on human exposures. *Environ. Manage.* 23–26 (February 2004).

TABLE 22.1

Summary of Modeled Source Contributions of Primary $PM_{2.5}$ to Monitors with Potential Annual Exceedences in Detroit, Michigan for the Year 2015

Source sectors	Primary $PM_{2.5}$ emissions (ton $year^{-1}$)	Model predicted annual concentrations ($\mu g\, m^{-3}$)[a] Primary $PM_{2.5}$ contribution	15/65 Control scenario	15/35 Control scenario	14/35 Control scenario
Wayne County Monitor #261630033, Annual DV = 17.4					
Other industrial sources	1375	0.712	0.171	0.000	0.222
CMV, aircraft, locomotive	638	0.540	0.191	0.000	0.000
Metal processing	852	0.484	0.037	0.000	0.000
Onroad (gasoline and diesel)	1187	0.336	0.000	0.025	0.025
Commercial cooking	984	0.271	0.050	0.000	0.000
Area fugitive dust	10270	0.237	0.000	0.000	0.000
Power sector	18016	0.233	0.059	0.000	0.014
Other area	888	0.210	0.000	0.000	0.168
Nonroad (gasoline and diesel)	1603	0.197	0.033	0.019	0.019
Natural gas combustion	119	0.034	0.000	0.000	0.000
Residential wood burning	703	0.026	0.005	0.000	0.000
Residential waste burning	1741	0.015	0.000	0.000	0.007
Glass manufacturing	334	0.010	0.000	0.000	0.000
Cement manufacturing	700	0.009	0.009	0.000	0.000
Auto industry	413	0.005	0.000	0.000	0.000
Prescribed/open burning	444	0.004	0.000	0.000	0.003
Point fugitive dust	15	0.001	0.000	0.000	0.000
Wildfires	51	0.001	0.000	0.000	0.000
Total (all sources)	40333	3.324	0.556	0.043	0.459
Wayne County Monitor #261630015, Annual DV = 15.69					
CMV, aircraft, locomotive	638	0.727	0.257	0.000	0.000
Metal processing	852	0.399	0.031	0.000	0.000
Other industrial sources	1375	0.395	0.094	0.000	0.125
Commercial cooking	984	0.365	0.068	0.000	0.000
Power sector	18016	0.311	0.064	0.000	0.031
Onroad (gasoline and diesel)	1187	0.214	0.000	0.016	0.016
Area fugitive dust	10270	0.183	0.000	0.000	0.000
Other area	888	0.154	0.000	0.000	0.123
Nonroad (gasoline and diesel)	1603	0.147	0.025	0.014	0.014
Residential wood burning	703	0.024	0.005	0.000	0.000
Residential waste burning	1741	0.013	0.000	0.000	0.007
Glass manufacturing	334	0.009	0.000	0.000	0.000
Cement manufacturing	700	0.008	0.008	0.000	0.000
Auto industry	413	0.005	0.000	0.000	0.000
Prescribed/open burning	444	0.003	0.000	0.000	0.003
Natural gas combustion	119	0.002	0.000	0.000	0.000
Point fugitive dust	15	0.001	0.000	0.000	0.000
Wildfires	51	0.000	0.000	0.000	0.000
Total (all sources)	40333	2.962	0.550	0.030	0.319

[a] Natural gas combustion source category results are adjusted to reflect new emissions factor (94% reduction).

Source: US Environmental Protection Agency, Regulatory Impact Analysis for the Revised Particulate Matter National Ambient Air Quality Standards, 2006.

TABLE 22.2

Summary of Modeled Source Contributions of Primary $PM_{2.5}$ to Monitors with Potential Daily Exceedences in Detroit, Michigan for the Year 2015

Source sectors	Primary $PM_{2.5}$ emissions (ton $year^{-1}$)	Primary $PM_{2.5}$ contribution	15/65 Control scenario	15/35 Control scenario	14/35 Control scenario
	Model predicted annual concentrations ($\mu g\, m^{-3}$)[a]				
Wayne County Monitor #261630033, Daily DV = 39.06[b]					
Power sector	18 016	0.896	0.344	0.000	0.021
Metal processing	852	0.623	0.048	0.000	0.000
Cement manufacturing	700	0.024	0.024	0.000	0.000
Glass manufacturing	334	0.025	0.000	0.000	0.000
Auto industry	413	0.014	0.000	0.000	0.000
Other industrial sources	1375	1.691	0.378	0.000	0.579
CMV, aircraft, locomotive	638	0.833	0.297	0.000	0.000
Nonroad (gasoline and diesel)	1603	0.296	0.041	0.030	0.030
Onroad (gasoline and diesel)	1187	0.475	0.000	0.035	0.035
Residential waste burning	1741	0.022	0.000	0.000	0.011
Residential wood burning	703	0.038	0.008	0.000	0.000
Commercial cooking	984	0.587	0.109	0.000	0.000
Prescribed/open burning	444	0.006	0.000	0.000	0.005
Wildfires	51	0.000	0.000	0.000	0.000
Area fugitive dust	10270	0.522	0.000	0.000	0.000
Point fugitive dust	15	0.002	0.000	0.000	0.000
Other area	888	0.362	0.000	0.000	0.289
Natural gas combustion	119	0.003	0.000	0.000	0.000
Total (all sources)	40333	6.418	1.250	0.065	0.970
Wayne County Monitor #261630015, Daily DV = 38.6[b]					
Power sector	18 016	0.730	0.149	0.000	0.083
Metal processing	852	1.604	0.123	0.000	0.000
Cement manufacturing	700	0.003	0.003	0.000	0.000
Glass manufacturing	334	0.008	0.000	0.000	0.000
Auto industry	413	0.003	0.000	0.000	0.000
Other industrial sources	1375	0.844	0.264	0.000	0.153
CMV, aircraft, locomotive	638	2.082	0.725	0.000	0.000
Nonroad (gasoline and diesel)	1603	0.118	0.017	0.012	0.012
Onroad (gasoline and diesel)	1187	0.189	0.000	0.014	0.014
Residential waste burning	1741	0.021	0.000	0.000	0.011
Commercial cooking	984	0.534	0.099	0.000	0.000
Prescribed/open burning	444	0.005	0.000	0.000	0.004
Wildfires	51	0.000	0.000	0.000	0.000
Area fugitive dust	10270	0.159	0.000	0.000	0.000
Point fugitive dust	15	0.003	0.000	0.000	0.000
Other area	888	0.160	0.000	0.000	0.128
Natural gas combustion	119	0.024	0.000	0.000	0.000
Total (all sources)	40333	6.502	1.383	0.026	0.406

[a] Natural gas combustion source category results are adjusted to reflect new emissions factor (94% reduction).

[b] Each daily results reflects the 98th percentile day or the 3rd highest day modeled with AERMOD so for monitor #261630015, that day is November 18 and for monitor #261630033, that day is January 1.

Source: US Environmental Protection Agency, Regulatory Impact Analysis for the Revised Particulate Matter National Ambient Air Quality Standards, 2006.

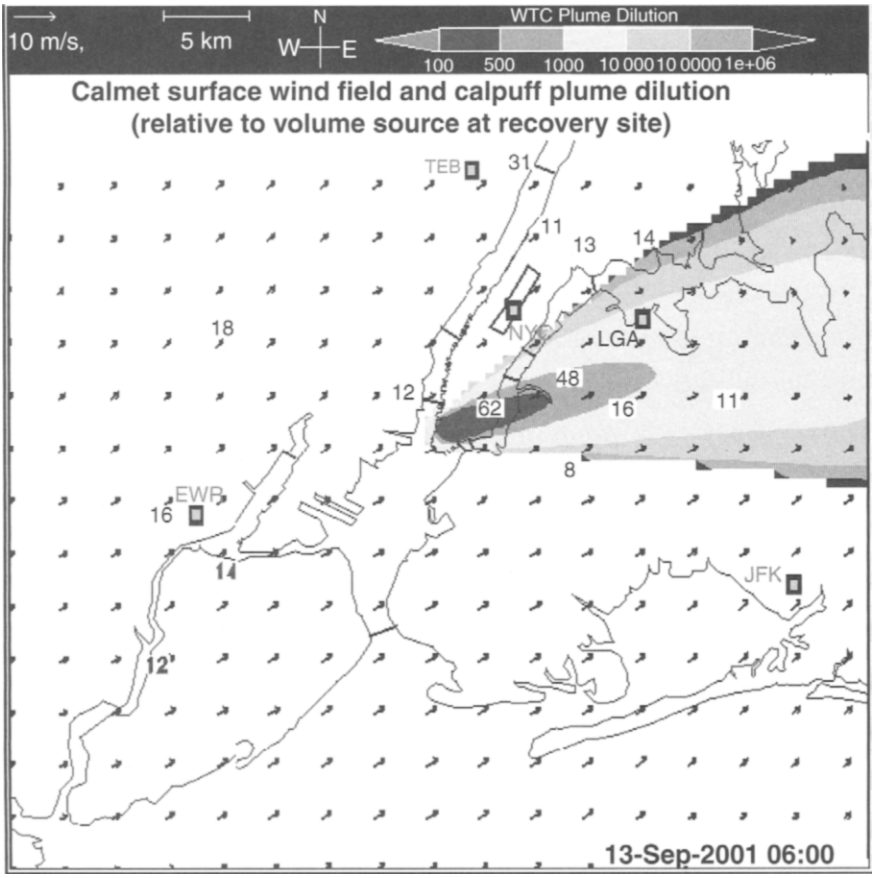

Fig. 22.12. Plume simulated with CALPUFF showing the averaged hourly $PM_{2.5}$ dilution of a volume source at the World Trade Center, New York City. *Source*: Huber, A., US Environmental Protection Agency.

- *CALINE3*: A steady-state Gaussian dispersion model esigned to determine air pollution concentrations at receptor locations downwind of roadways located in relatively uncomplicated terrain.
- *CAL3QHC*: A CALINE3-based CO model with queuing and hot spot calculations and with a traffic model to calculate delays and queues that occur at signalized intersections.
- *CAL3QHCR*: This is a more refined version based on CAL3QHC that requires local meteorological data.
- *Complex Terrain Dispersion Model Plus Algorithms for Unstable Situations (CTDMPLUS)*: A refined point source Gaussian air quality model for use in all stability conditions for complex terrain. The model contains, in its entirety, the technology of CTDM for stable and neutral conditions.

- *OCD Model Version 5*: A straight line Gaussian model developed to determine the impact of offshore emissions from point, area, or line sources on the air quality of coastal regions. OCD incorporates overwater plume transport and dispersion as well as changes that occur as the plume crosses the shoreline. Hourly meteorological data are needed from both offshore and onshore locations.

Documentation and access to these models are available at the EPA Technology Transfer Network website: http://www.epa.gov/scram001/dispersion_prefrec.htm#blp.

F. Photochemical Models

Photochemical air quality models have become widely recognized and routinely utilized tools for regulatory analysis and attainment demonstrations by assessing the effectiveness of control strategies. These 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. They are applied at multiple spatial scales from local, regional, national, and global.

Photochemical models structure the atmosphere as a modeled volume with a three-dimensional grid with thousands of grid cells. Each grid cell can be envisioned as a box. The boxes are stacked one atop another and differ in height. Shorter boxes represent the parcels of air nearest to the ground surface. The photochemical calculates concentrations of pollutants, such as ozone, in each cell by simulating the movement of air into and out of cells by advection and dispersion. The model also includes algorithms to simulate mixing of pollutants vertically among layers, introduction of emissions from sources into each cell, as well as sets of chemical reactions, equations of pollution precursors and meteorology, especially incoming solar radiation (i.e. insolation) in each cell.

Photochemical air quality models are of two basic mathematical types: 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. Early modeling efforts often used Lagrangian methods to simulate the formation of pollutants because of its computational simplicity. Describing physical processes, however, is incomplete, which is the major disadvantage of the Lagrangian method. Thus, most photochemical air quality models in operation today use three-dimensional Eulerian grid mathematics that allow for improved and more complete characterization of the physical processes in the atmosphere. This allows chemical-species concentrations to be predicted throughout the entire model domain.

Arguably, the principal photochemical model in use is the CMAQ modeling system, which has been developed to improve the environmental management community's ability to evaluate the impact of air quality

management practices for multiple pollutants at multiple scales and enhance the scientist's ability to probe, to understand, and to simulate chemical and physical interactions in the atmosphere. The most recent CMAQ version is available for download from the Community Modeling and Analysis System website at: http://www.cmascenter.org/.

Several other photochemical models have been developed and are applied to various pollutants. These include:

- Comprehensive Air Quality Model with Extensions (CAMx)—simulates air quality over different geographic scales; treats a wide variety of inert and chemically active pollutants, including ozone, PM, inorganic and organic $PM_{2.5}/PM_{10}$, and mercury and other toxics; and has plume-in-grid and source apportionment capabilities.
- Regional Modeling System for Aerosols and Deposition (REMSAD)—calculates 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; and includes processes relevant to regional haze, PM, and other airborne pollutants, including soluble acidic components and mercury.
- Urban Airshed Variable Grid (UAM-V) Photochemical Modeling System—pioneering effort in photochemical air quality modeling in the early 1970s that 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. It is typically applied to model air quality episodes, i.e. periods during which adverse meteorological conditions result in elevated ozone pollutant concentrations.

G. Receptor Models

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 SIPs for identifying sources contributing to air quality problems. 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.

The CMB fully apportions receptor concentrations to chemically distinct source types depending on the source profile database, while UNMIX and

PMF internally generate source profiles from the ambient data. It is one of several receptor models that have been applied to air quality problems since the 1980s. Based on an effective-variance least-squares method (EVLS), it has supported numerous SIPs, when they include a source apportionment component. 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.

The EPA UNMIX model, as the name implies, disaggregates ("unmixes") the concentrations of chemical species measured in the ambient air to identify the contributing sources. Chemical profiles of the sources are not required, but instead are generated internally from the ambient data by UNMIX, using a mathematical formulation based on a form of factor analysis. For a given selection of chemical species, UNMIX estimates the number of sources, the source compositions, and source contributions to each sample.

The PMF technique is a form of factor analysis where the underlying covariability of many variables (e.g. sample to sample variation in PM species) is described by a smaller set of factors (e.g. PM sources) to which the original variables are related. The structure of PMF permits maximum use of available data and better treatment of missing and below-detection-limit values.

When the results of air pollution measurements are interpreted, one of the first questions asked by scientists, engineers, and policy makers is where did it come from? Sorting out the various sources of pollution is known as *source apportionment*. A number of tools are used to try to locate the sources of pollutants. A widely used approach is the "source–receptor model" or as it is more commonly known, the *receptor model*.

The distinction between receptor and dispersion models has to do with the direction of the prediction. Dispersion models start from the source and estimate where the plume and its contaminants are heading. Conversely, receptor models are based on measurements taken in the ambient environment and from these observations, make use of algorithms and functions to determine pollution sources. One common approach is the mathematical "back trajectory" model. Often, chemical co-occurrences are applied. So, it may be that a certain fuel is frequently contaminated with a conservative and, hopefully, unique element. Some fuel oils, for example, contain trace amounts of the element vanadium. Since there are few other sources of vanadium in most ambient atmospheric environments, its presence is a strong indication that the burning of fuel oil is a most likely source of the plume. The model, if constructed properly, can even quantify the contribution. So, if measurements show that sulfur dioxide (SO_2) concentrations are found to be $10\,\mu g\,m^{-3}$ in an urban area, and vanadium is also found at sufficient levels to indicate that home heating systems are contributing a certain amount of the SO_2 to the atmosphere, the model will correlate the amount of SO_2 coming

from home heating systems. If other combustion sources, e.g. cars and power plants, also have unique trace elements associated with their SO_2 emissions, further SO_2 source apportionment can occur, so that the total may look something like Table 7.2.

For a discussion of source–receptor relationships and modeling, see Discussion Box: Source Apportionment, Receptor Models, and Carbon Dating in Chapter 7.

H. Personal Exposure Models

The actual exposures that people receive can also be modeled (see Fig. 22.13). According to the EPA, there are three techniques to estimate pollutant exposures quantitatively:

> Sometimes the approaches to assessing exposure are described in terms of "direct measures" and "indirect measures" of exposure (e.g. NRC, 1994). Measurements that actually involve sampling on or within a person, for example, use of personal monitors and biomarkers, are termed as "direct measures" of exposure. Use of models, microenvironmental measurements, and questionnaires, where measurements do not actually involve personal measurements, are termed as "indirect measures" of exposure. The direct/indirect nomenclature focuses on the type of measurements being made; the scenario evaluation/point-of-contact/reconstruction nomenclature focuses on how the data are used to develop the dose estimate. The three-term nomenclature is used in these guidelines to highlight the point that three independent estimates of dose can be developed.

There is seldom a sufficient amount of direct information from measurements to estimate and to predict exposures for a population. Thus, indirect

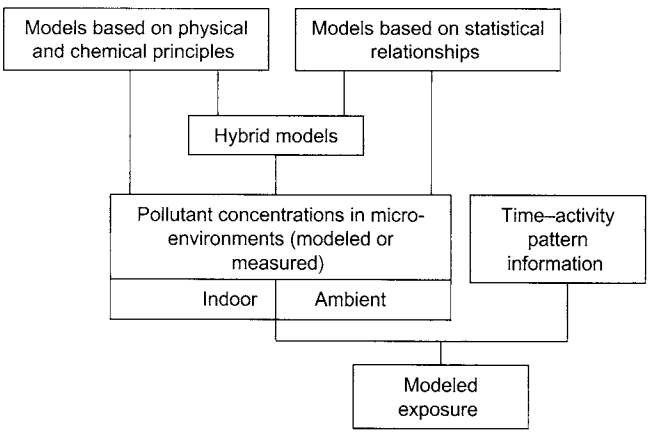

Fig. 22.13. Schematic of human exposure modeling. Adapted from: US National Research Council, Chapter 6: Models, in *Human Exposure Assessment for Airborne Pollutants: Advances and Applications*. Committee on Advances in Assessing Human Exposure to Airborne Pollutants and Committee on Geosciences, Environment, and Resources. National Academy Press, Washington, DC, 1990.

methods must be used. Personal exposure[9] can be expressed mathematically as a composite of the time in a microenvironment (e.g. in a garage, indoors at home, or in a car) and the concentration of the pollutant in that microenvironment:

$$E_i = \sum_{j=1}^{m} T_{ij} C_{ij} \tag{22.20}$$

where T_{ij} is the time spent in microenvironment j by person i with typical units of minutes, C_{ij} is the air pollutant concentration person i experiences in microenvironment j with typical units of $\mu g\, m^{-3}$, E_i represents the exposure for person i integrated T_{ij}, and m is the number of different microenvironments. Thus, the units of exposure are mass per volume-time ($\mu g\, m^{-3} min^{-1}$). Note, then, that exposure is the concentration per unit time. The calculation amounts to a weighted sum of concentrations with the weights being equal to the time spent experiencing a given concentration.

What people are doing is crucial to modeling their exposure to air pollutants. To support exposure, intake dose, and risk assessments, the EPA developed the Consolidated Human Activity Database (CHAD). CHAD is a relational database with a graphical user interface that facilitates queries and report generation.[10] It contains databases from previously existing human activity pattern studies, which were incorporated in two forms: (1) as the original raw data and (2) as data modified according to predefined format requirements. CHAD contains data obtained from pre-existing human activity studies that were collected at city, state, and national levels. People's diary information is input in CHAD. Figure 22.14 and Tables 22.3 and 22.4 provide the structure and data elements of CHAD. Most of the fields are answers from the questionnaire. Some fields vary from day to day for an individual and fields based on the diary entries will most likely be different for each day. The CHAD_DIARY table contains one record for each activity during a 24-h period. No record represents more than an hour or crosses the hour boundary. The minimal information in the diary data is the CHADID which links to the CHAD_DATA, a sequence number, which indicates the

[9] The principal reference for this discussion is: Klepeis, N. E., Modeling human exposure to air pollution, in *Exposure Analysis* (Ott, W. R., Wallace, L. A., and Steinemann, A., eds.). CRC Press, Boca Raton, 2006; and Klepeis, N. E., and Nazaroff, W. W., Modeling residential exposure to secondhand tobacco smoke. *Atmos. Environ.* **40** (23), 4393–4407 (2006). Other resources for all discussions about human exposure science have benefited from ongoing discussions with Wayne Ott and Lance Wallace, as well as the insights of Gerry Alkand, Larry Purdue, Judy Graham, Jerry Blancato, Paul Lioy, Tom McCurdy, Alan Huber, Alan Vette, Linda Sheldon, Dave Mage, Dale Pahl, Tom McKone, Edo Pellizzari, Ron Williams, and Curt Dary.

[10] The source of this discussion is: Stallings, C., Tippett, J. A., Glen, G., and Smith, L., *CHAD Users Guide: Extracting Human Activity Information from CHAD on the PC*. ManTech Environmental Services, modified by Systems Development Center Science Applications International Corporation, Research Triangle Park, NC, 2002.

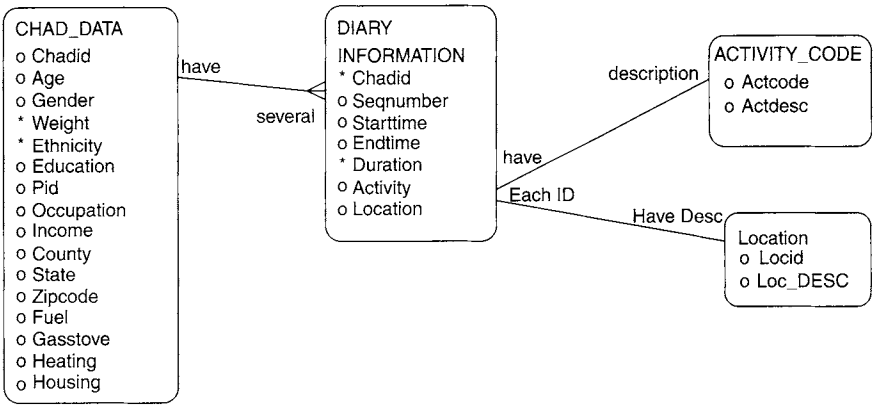

Fig. 22.14. Schematic of the tables and relationships among the tables in the combined CHAD. *Source*: Stallings, C., Tippett, J. A., Glen, G., and Smith, L., *CHAD Users Guide: Extracting Human Activity Information from CHAD on the PC*. ManTech Environmental Services, modified by Systems Development Center Science Applications International Corporation, Research Triangle Park, NC, 2002.

TABLE 22.3

CHAD Diary Location Codes

30000 Residence, general	31300 Waiting
30010 Your residence	31310 Wait for bus, train, ride (at stop)
30020 Other's residence	31320 Wait for travel, indoors
30100 Residence, indoor	31900 Other travel
30120 Your residence, indoor	31910 Travel by other vehicle
30121 Kitchen	32000 Other, indoor general
30122 Living room/family room	32100 Office building/bank/post office
30123 Dining room	32200 Industrial plant/factory/warehouse
30124 Bathroom	32300 Grocery store/convenience store
30125 Bedroom	32400 Shopping mall/non-grocery store
30126 Study/office	32500 Bar/night club/bowling alley
30127 Basement	32510 Bar/night Club
30128 Utility room/laundry room	32520 Bowling alley
30129 Other indoor	32600 Repair shop
30130 Other's residence, indoor	32610 Auto repair shop/gas station
30131 Other's kitchen	32620 Other repair shop
30132 Other's living room/family room	32700 Indoor gym/sports or health club
30133 Other's dining room	32800 Child care facility
30134 Other's bathroom	32810 Child care facility, house
30135 Other's bedroom	32820 Child care facility, commercial
30136 Other's study/office	32900 Public building/library/museum/theater
30137 Other's basement	32910 Auditorium, sport's arena/concert hall
30138 Other's utility room/laundry room	32920 Library/courtroom/museum/theater
30139 Other indoor	33100 Laundromat
30200 Residence, outdoor	33200 Hospital/health care facility/doctor's office
30210 Your residence, outdoor	33300 Beauty parlor/barber shop/hairdresser's

(*continued*)

TABLE 22.3 (*Continued*)

CHAD Diary Location Codes

30211 Your residence—pool, spa
30219 Your residence—other outdoor
30220 Other's residence, outdoor
30221 Other's residence—pool, spa
30229 Other's residence—other outdoor
30300 Garage
30310 Indoor garage
30320 Outdoor garage
30330 Your garage
30331 Your indoor garage
30332 Your outdoor garage
30340 Other's garage
30341 Other's indoor garage
30342 Other's outdoor garage
30400 Other, residence
31000 Travel, general
31100 Motorized travel
31110 Travel by car
31120 Travel by truck
31121 Travel by truck (pick-up van)
31122 Travel by Truck (other than pick-up or van)
31130 Travel by Motorcycle/moped/ motorized scooter
31140 Travel by bus
31150 Travel by train/subway/rapid transit
31160 Travel by airplane
31170 Travel by boat
31171 Travel by motorized boat
31172 Travel by unmotorized boat
31200 Non-motorized travel
31210 Travel by walk
31220 Travel by bicycle/skateboard/roller-skates
31230 Travel in a stroller or carried by an adult
33400 At work: no specific location, moving among locations
33500 At school
33600 At restaurant
33700 At church
33800 At hotel/motel
33900 At dry cleaners
34100 Parking garage
34200 Laboratory
34300 Other, indoor
35000 Other outdoor, general
35100 Sidewalk/street/neighborhood
35110 Within 10 yards of street
35200 Public garage/parking lot
35210 Public garage
35220 Parking lot
35300 Service station/gas station
35400 Construction site
35500 Amusement park
35600 School grounds/playgrounds
35610 School grounds
35620 Playground
35700 Sports stadium and amphitheater
35800 Park/golf course
35810 Park
35820 Golf course
35900 Pool, river, lake
36100 Restaurant, picnic
36200 Farm
36300 Other outdoor
U Uncertain
X Missing

Source: Stallings, C., Tippett, J. A., Glen, G., and Smith, L., *CHAD Users Guide: Extracting Human Activity Information from CHAD on the PC*. ManTech Environmental Services, modified by Systems Development Center Science Applications International Corporation, Research Triangle Park, NC, 2002.

order of the records in a day, start, end, and duration times, and an activity and location.

Thus, if we measure concentrations with personal and indoor air pollution monitors and we apply activity patterns, such as those in CHAD, we can estimate and predict personal exposures to numerous pollutants.

Obviously the mean personal exposure can be expressed in concentration units ($\mu g\, m^{-3}$) by dividing E_i by the total time spent in each microenvironment and summing these exposures. Further, this can also be seen as a

TABLE 22.4

CHAD Diary Activity Code Descriptions

10000 Work and other income-producing activities, general
10100 Work, general
10110 Work, general, for organizational activities
10111 Work for professional/union organizations
10112 Work for special interest identity organizations
10113 Work for political party and civic participation
10114 Work for volunteer/ helping organizations
10115 Work of/for religious groups
10116 Work for fraternal organizations
10117 Work for child/youth/family organizations
10118 Work for other organizations
10120 Work, income-related only
10130 Work, secondary (income-related)
10200 Unemployment
10300 Breaks
11000 General household activities
11100 Prepare food
11110 Prepare and clean-up food
11200 Indoor chores
11210 Clean-up food
11220 Clean house
11300 Outdoor chores
11310 Clean outdoors
11400 Care of clothes
11410 Wash clothes
11500 Build a fire
11600 Repair, general
11610 Repair of boat
11620 Paint home/room
11630 Repair/maintain car
11640 Home repairs
11650 Other repairs
11700 Care of plants
11800 Care for pets/animals
11900 Other household

12000 Child care, general
12100 Care of baby
12200 Care of child
12300 Help/teach
12400 Talk/read
15200 Attend other classes

15300 Do homework
15400 Use library

15500 Other education

16000 General entertainment/social activities

16100 Attend sports events

16200 Participate in social, political, or religious activities
16210 Practice religion
16300 Watch movie
16400 Attend theater

16500 Visit museums
16600 Visit
16700 Attend a party
16800 Go to bar/lounge
16900 Other entertainment/social events
17000 Leisure, general
17100 Participate in sports and active leisure
17110 Participate in sports
17111 Hunting, fishing, hiking
17112 Golf
17113 Bowling/pool/ping pong/pinball
17114 Yoga
17120 Participate in outdoor leisure
17121 Play, unspecified
17122 Passive, sitting
17130 Exercise
17131 Walk, bike, or jog (not in transit)
17140 Create art, music, participate in hobbies
17141 Participate in hobbies
17142 Create domestic crafts
17143 Create art
17144 Perform music/drama/dance
17150 Play games
17160 Use of computers
17170 Participate in recess and physical education
17180 Other sports and active leisure
17200 Participate in passive leisure
17210 Watch
17211 Watch adult at work
17212 Watch someone provide child care

(*continued*)

TABLE 22.4 (*Continued*)

CHAD Diary Activity Code Descriptions

12500 Play indoors	17213 Watch personal care
12600 Play outdoors	17214 Watch education
12700 Medical care—child	17215 Watch organizational activities
12800 Other child care	17216 Watch recreation
13000 Obtain goods and services, general	17220 Listen to radio/listen to recorded music/watch TV
13100 Dry clean	17221 Listen to radio
13200 Shop/run errands	17222 Listen to recorded music
13210 Shop for food	17223 Watch TV
13220 Shop for clothes or household goods	17230 Read, general
13230 Run errands	17231 Read books
13300 Obtain personal care service	17232 Read magazines/not ascertained
13400 Obtain medical service	17233 Read newspaper
13500 Obtain government/financial services	17240 Converse/write
13600 Obtain car services	17241 Converse
13700 Other repairs	17242 Write for leisure/pleasure/paperwork
13800 Other services	17250 Think and relax
14000 Personal needs and care, general	17260 Other passive leisure
14100 Shower, bathe, personal hygiene	17300 Other leisure
14110 Shower, bathe	18000 Travel, general
14120 Personal hygiene	18100 Travel during work
14200 Medical care	18200 Travel to/from work
14300 Help and care	18300 Travel for child care
14400 Eat	18400 Travel for goods and services
14500 Sleep or nap	18500 Travel for personal care
14600 Dress, groom	18600 Travel for education
14700 Other personal needs	18700 Travel for organizational activity
15000 General education and professional training	18800 Travel for event/social activity
15100 Attend full-time school	18900 Travel for leisure
15110 Attend day-care	18910 Travel for active leisure
15120 Attend K-12	18920 Travel for passive leisure
15130 Attend college or trade school	U Unknown
15140 Attend adult education and special training	X Missing

Source: Stallings, C., Tippett, J. A., Glen, G., and Smith, L., *CHAD Users Guide: Extracting Human Activity Information from CHAD on the PC*. ManTech Environmental Services, modified by Systems Development Center Science Applications International Corporation, Research Triangle Park, NC, 2002.

continuum in which the personal exposure is assumed to be constant during each time comprising T_{ij}:

$$E_i = \int_1^2 C_{ij}(t;x;y;z)dt \tag{22.21}$$

where $C_i(t, x, y, z)$ is the concentration occurring at a specific point occupied by person i at time t and spatial coordinates (x, y, z), and t_1 and t_2 are the

respective starting and ending times of a given exposure episode. The concentrations can be measured using a real-time personal monitoring device. These data are not actually continuous, but can be quite frequent (e.g. every few seconds).

Other times, fully continuous space is not assumed, which means that discrete microenvionments are used. If this is the case the equation appears as

$$E_i = \left(\sum_{j=1}^{m} \int_{j1}^{j2} C_{ij}(t)dt \right) \tag{22.22}$$

where $C_{ij}(t)$ is the concentration to which the person is exposed in the discrete microenvironment j at a specific point in time t over the time interval defined by $[t_{j1}, t_{j2}]$, where t_{j1} is the starting time for the microenvironment and t_{j2} is the ending time. If we assume that every person in a population is exposed to the same microenvironment concentrations, a simplified population exposure can be derived to show the total time spent by all receptors in each microenvironment:

$$\tilde{E} = \sum_{j=1}^{m} C_j \tilde{T}_j \tag{22.23}$$

where m is the number of microenvironments encountered, C_j is the average pollutant concentration in microenvironment j assigned to every person i, $\tilde{E}$ is the integrated exposure over all members of the population. The total time spent by all persons in microenvironment j is

$$\tilde{T}_i = \sum_{i=1}^{n} T_{ij} \tag{22.24}$$

where n is the total number of people in the population being modeled. This can be further simplified if we assume that each person spends the same total amount of time across all microenvironments:

$$T = T_i = \sum_{j=1}^{m} T_{ij} \tag{22.25}$$

Further, if the time spent by certain individuals in particular microenvironments is zero, then the average personal exposure for the population would be

$$\bar{E}_c \frac{1}{nT} \sum_{j=1}^{m} C_j \tilde{T}_j \tag{22.26}$$

Therefore, time–activity relationships and concentrations can be used to model expected exposures to air pollutants. Indoor and personal exposures

can dominate exposures to many pollutants. For example, Fig. 22.15 shows the modeled results of expected exposures to particulates ($PM_{2.5}$) for a simulated population based on available measurements of ambient, indoor, and personal measurements, combined with information about microenvironments (e.g. types and time in each) and activities. Note that ambient contribution is quite small compared to personal and indoor exposures.[11]

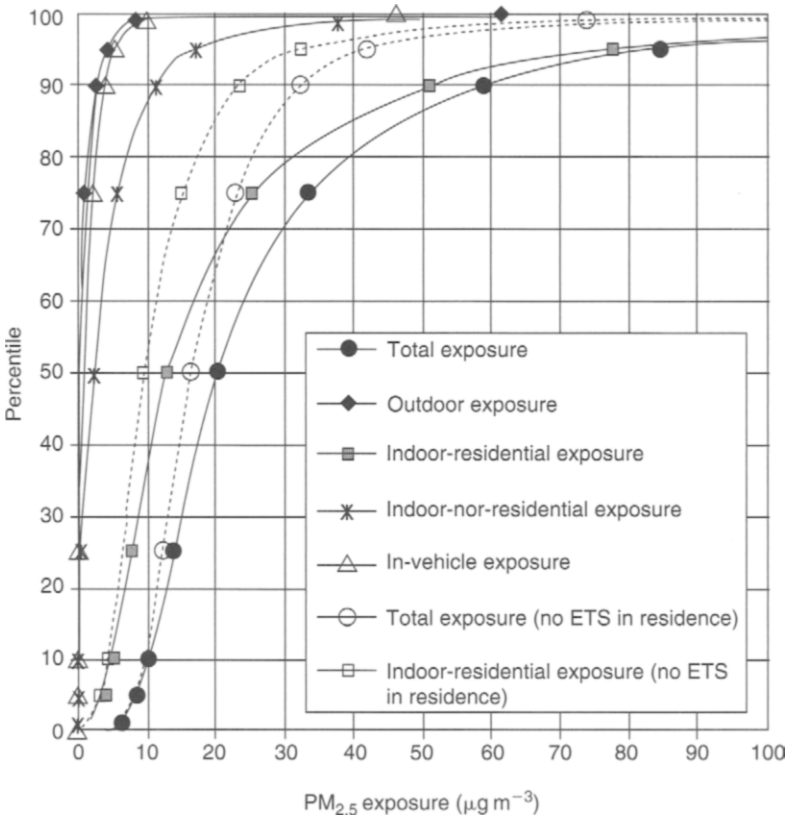

Fig. 22.15. Cumulative frequency distributions of daily total and microenvironmental $PM_{2.5}$ exposures ($\mu g\, m^{-3}$) for the simulated population of Philadelphia (solid lines). Distributions of total and indoor residential $PM_{2.5}$ exposures for the population without environmental tobacco smoke (ETS) exposure in the residence (dashed lines) are also shown. *Source*: Burke, J. M., Zufall, M. J., and Ozkaynak, A. H., *A Population Exposure Model for Particulate Matter: Case Study Results for* $PM_{2.5}$ in Philadelphia, PA: http://www.epa.gov/heasd/pm/pdf/exposure-model-for-pm.pdf; accessed on February 23, 2007.

[11] Burke, J. M., Zufall, M. J., and Ozkaynak, A. H., A Population Exposure Model for Particulate Matter: Case Study Results for $PM_{2.5}$ in Philadelphia, PA: http://www.epa.gov/heasd/pm/pdf/exposure-model-for-pm.pdf; accessed on February 23, 2007.

I. Modeling Air Toxics

The Clean Air Act Amendments of 1990 (CAAA90) included a specific health outcome provision related to toxic air pollutants. The law included 190 substances that need to be addressed because they have been known or suspected to cause cancer or other serious health effects, such as reproductive effects or birth defects, or to cause adverse environmental effects. The 1990 amendments established a range of air toxics requirements for EPA to implement that generally fall into four categories:

1. Establishing emission standards based on existing pollution control technologies, called Maximum Achievable Control Technology (MACT), for an estimated 84 000 major stationary sources within 158 industries.
2. Examining the remaining health risk (called the "residual risk") from these sources 8 years after implementing each MACT standard and, if warranted, issuing additional standards to protect public health or the environment.
3. Regulating air toxics emissions from small stationary sources, such as dry cleaners.
4. Evaluating the need for and feasibility of regulation of air toxics emissions from mobile sources, such as cars, and regulating these sources based on this evaluation.

The amendments also required the EPA to periodically assess the costs and benefits of the entire CAA. This called for an assessment of the Act's costs and benefits prior to 1990 along with projections of future economic impacts resulting from the amendments (see the earlier discussion in this Chapter regarding the regulatory impact analysis as it pertains to PM).

Air toxics originate from a variety of sources (see Fig. 22.16). Of the numerous compounds that are classified as air toxics, however, about 60% are represented by just five pollutant classes (see Table 22.5). The EPA has completed MACT standards for major stationary sources. The EPA establishes the federal standard, but the state and local air pollution control agencies generally implement the EPA's emission standards. These agencies can choose to impose more stringent requirements than the federal standards, and some state and local agencies have developed innovative air toxics programs that go beyond the federal program, which is enabling them to address air toxics that would be insufficiently covered by EPA's standards.

The CAA residual risk program (i.e. the risk remaining after technology-based standards have been in place), must try to determine whether the most highly exposed individuals face excess cancer risk of more than 1 in 1 million (risk = 1×10^{-6}). In cases where estimated risks exceed this threshold, the EPA must develop a new residual risk standard to provide an ample margin of safety for those potentially affected individuals. In fact, the EPA generally uses a lifetime cancer risk of 1 in 10 000 (risk = 1×10^{-4}) as the upper boundary of acceptability. The ample margin of safety decision must

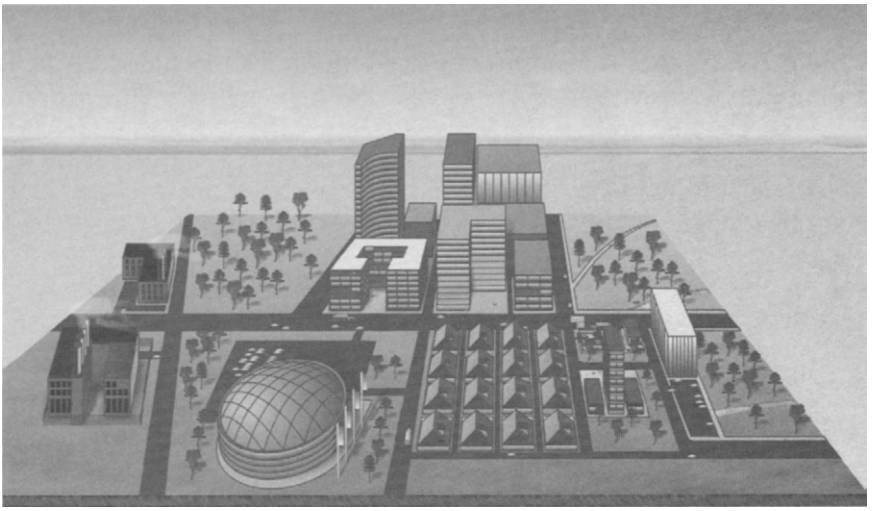

Fig. 22.16. Common sources of air toxics emissions. *Source*: US Government Accountability Office, *Clean Air Act: EPA Should Improve the Management of Its Air Toxics Program.* Report No. GAO-06-669, June 2006.

also consider costs, technological feasibility, uncertainties, and other relevant factors. In this feasibility step, EPA must also assess whether to adopt more stringent standards to prevent adverse effects to wildlife, aquatic life, or natural resources considering cost, energy, and other pertinent details.

EPA is not expected to complete the residual risk reviews until the year 2012, rather than by the 2008 date given in the amendment. These reviews are intended to provide information on any potential adverse health effects that may warrant further regulation. According to the US Government Accountability Office (GAO)[12]:

> EPA does not have reliable data on the degree to which its programs have reduced risks. Furthermore, the data that are available suggest that the agency still has substantial opportunities to control emissions from mobile and small stationary sources.
>
> EPA faces significant challenges in implementing the air toxics program, many of which stem from its relatively low priority within the agency. Importantly, the agency lacks a comprehensive strategy for managing its implementation of the remaining air toxics requirements. Senior EPA officials said that the program's agenda is largely set by external stakeholders who file litigation when the agency misses deadlines. For example, EPA currently faces a court order to issue emissions standards for small stationary sources. Previous reports by GAO identified inadequate funding for the air toxics program as a challenge, and key stakeholders—including senior EPA officials, environmental advocates, and state and local agency officials—said resource constraints continue to pose a major challenge. The percentage of funding for the air toxics program relative to all clean air programs ranged from 18% to 19% between 2000

[12] US Government Accountability Office, *Clean Air Act: EPA Should Improve the Management of Its Air Toxics Program.* Report No. GAO-06-669, June 2006.

TABLE 22.5

The Five Most Commonly Emitted Air Toxics, 2002

Pollutant	Percentage of total air toxics emissions	Primary sources of emissions	Health effects
Toluene	18	Mobile sources	Impairment of the nervous system with symptoms including tiredness, dizziness, sleepiness, confusion, weakness, memory loss, nausea, loss of appetite, and hearing and color vision loss; kidney problems; unconsciousness; and death.
Xylenes	13	Mobile sources, asphalt paving	Irritation of the skin, eyes, nose, and throat; headaches, dizziness, memory loss, and changes in sense of balance; lung problems; stomach discomfort; possible effects on the liver and kidneys; unconsciousness; and death.
Hydrochloric acid	12	Coal-fired utility and industrial boilers	Eye, nose, and respiratory tract irritation; corrosion of the skin, eyes, mucous membranes, esophagus, and stomach; severe burns; ulceration; scarring; inflammation of the stomach lining; chronic bronchitis; and inflammation of the skin.
Benzene	9	Mobile sources, open burning, pesticide application	Drowsiness, dizziness, vomiting, irritation of the stomach, sleepiness, convulsions, rapid heart rate, headaches, tremors, confusion, unconsciousness, anemia, excessive bleeding, weakened immune system, increased incidence of cancer (leukemia), and death.
Formaldehyde	7	Mobile sources, open burning	Irritation of the eyes, nose, throat, and skin; severe pain; vomiting; coma; limited evidence of cancer; and death.

US Environmental Protection Agency and Agency for Toxic Substances and Disease Registry

and 2003 and declined to 15% in 2004 and 12% in 2005. EPA has not estimated the level of resources necessary to comply with the remaining requirements of the 1990 amendments, according to a senior program official. We believe that such estimates would help inform congressional oversight and appropriations decisions. Senior EPA officials and other stakeholders also cited a lack of information on the benefits of regulating air toxics as a major challenge, which, in turn, reinforces the program's relative priority because the agency cannot demonstrate its effectiveness. The stakeholders identified a number of other challenges, but perceptions varied by stakeholder group. For example, EPA and industry stakeholders rated the large number of statutory requirements as a challenge, while environmental stakeholders rated a lack of reliable data on air toxics sources and their emissions as a challenge.

The EPA is required to conduct a National Air Toxics Assessment (NATA) as a part of the national air toxics program, which

- expands air toxics monitoring;
- develops emission inventories;
- conducts national and local-scale air quality analyses;
- characterizes risks associated with air toxics exposures;
- conducts research on health and environmental effects and exposures to both ambient and indoor sources;
- conducts exposure modeling.

This helps EPA set program priorities, characterize risks, and track progress toward meeting goals, especially providing trends in air quality as the United States transitions from technology-based standards to a greater number of risk-based standards (see Fig. 22.17).

As part of the NATA program, EPA conducted a national screening-level assessment using 1996 emissions inventory data to characterize air toxics risks nationwide. This helped to characterize the potential health risks associated with inhalation exposures to 33 air toxics and diesel PM. These 34 air toxics were identified as priority pollutants in EPA's Integrated Urban Air Toxics Strategy.[13]

The Assessment System for Population Exposure Nationwide (ASPEN) is the model used to estimate toxic air pollutant concentrations. It is based on

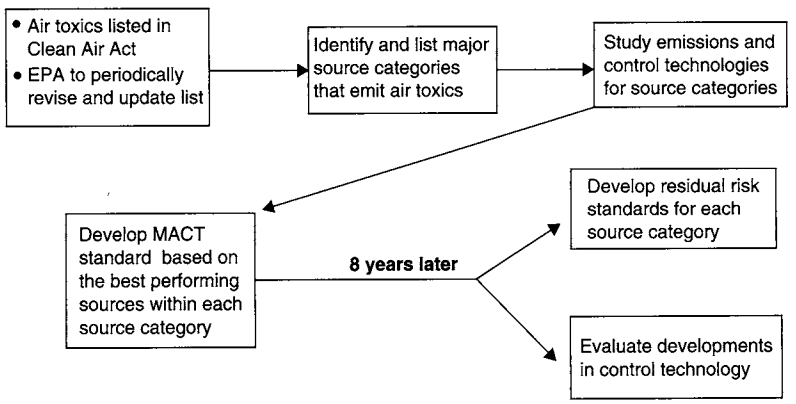

Fig. 22.17. Overview of the regulatory process for major stationary sources of air toxics, including MACT standards and 8-year technology and residual risk reviews. *Source*: US Government Accountability Office, *Clean Air Act: EPA Should Improve the Management of Its Air Toxics Program*. Report No. GAO-06-669, June 2006.

[13] A list of the 34 selected toxics can be found at: http://www.epa.gov/ttn/atw/nata/34poll.html.

the EPA's ISCLT, which simulates the behavior of the pollutants once they are emitted into the atmosphere. ASPEN uses estimates of toxic air pollutant emissions and meteorological data from National Weather Service stations to estimate air toxics concentrations nationwide.

ASPEN incorporates a number of critical pollutant concentration variables, including

- rate of release;
- location of release;
- the height from which the pollutants are released;
- wind speeds and directions from the meteorological stations nearest to the release;
- breakdown of the pollutants in the atmosphere after being released (i.e. reactive decay);
- settling of pollutants out of the atmosphere (i.e. deposition);
- transformation of one pollutant into another (i.e. secondary formation).

The model estimates toxic air pollutant concentrations for every census tract in contiguous United States, Puerto Rico, and the Virgin Islands. Census tracts are land areas defined by the US Bureau of the Census and typically contain about 4000 residents each. These census tracts are usually smaller than 2 square miles in size in cities, but much larger in rural areas.

NATA is intended to identify ambient concentrations of air toxics attributable to anthropogenic (human-generated) emissions, within 50 km of each source. However, for many pollutants, ambient concentrations have "background" components attributable to long-range transport, resuspension of previous emissions, and non-anthropogenic sources. To estimate ambient concentrations of air toxics accurately, these background concentrations must be addressed. In the 1996 assessment, with exception of diesel PM, background concentrations were based on measured values of 13 pollutants. The background concentrations used in the 1996 NATA are provided in Table 22.6.

The modeled estimates for most of the pollutants are generally lower than the measured ambient annual average concentrations when evaluated at the monitors. However, when the maximum modeled estimate for distances up to 10–20 km from the monitoring location are compared to the measured concentrations, the modeled estimates approach the monitored concentrations. This may be the result of spatial uncertainty of the underlying data (emissions and meteorological), as well as the tendency of existing air toxics monitoring networks to characterize the higher (if not maximum) air pollution impact areas in the ambient air. Also, the model estimates are more uncertain at the census tract scale, but are more reliable at more extensive geographic scales, such as a county or state. Further, ASPEN and underlying data are used to estimate exposures and risks (see Fig. 22.18).

TABLE 22.6

Background Concentration Estimates Used in the National-Scale Air Toxics Assessment

Pollutant	Background concentration ($\mu g\, m^{-3}$)
Benzene	0.48
Carbon tetrachloride	0.88
Chloroform	0.083
Ethylene dibromide	0.0077
Ethylene dichloride	0.061
Formaldehyde	0.25
Hexachlorobenzene	0.000093
Mercury compounds	0.0015
Methylene chloride	0.15
Polychlorinated biphenyls	0.00038
Perchloroethylene (tetrachloroethylene)	0.14
Trichloroethylene	0.081

Source: US Environmental Protection Agency.

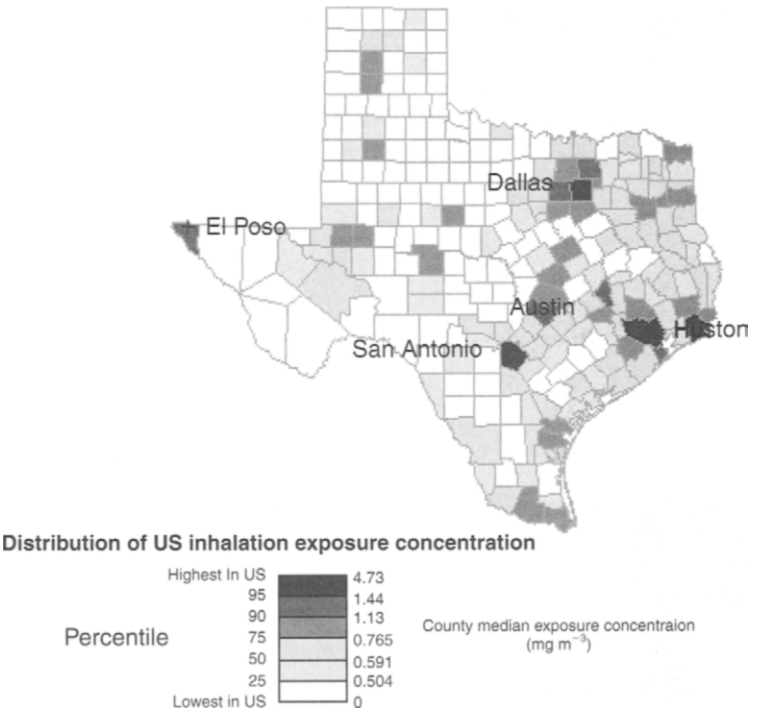

Fig. 22.18. Estimated county median exposure benzene concentrations in Texas in 1996. A county's shading indicates its exposure concentration compared with all other counties in the nation. The exposure concentration value displayed is the county median in micrograms of benzene per cubic meter of air ($\mu g\, m^{-3}$). Similar maps can be generated for other states and various air toxics at the US Environmental Protection Agency's National Air Toxics Assessment website: http://www.epa.gov/ttn/atw/nata/mapexpo.html.

VI. MODEL PERFORMANCE, ACCURACY, AND UTILIZATION

A. Methodology of Assessing Model Performance

A number of statistics have been suggested [39, 40] as measures of model performance. Different types of models and the use of models for different purposes may require different statistics to measure performance.

In time series of measurements of air quality and estimates of atmospheric concentration made by a model, residuals d can be computed for each location. The residual d is the difference between values paired timewise:

$$d = M - E \tag{22.27}$$

where M is the measured value and E is the value estimated by the model.

A measure of bias $\bar{d}$ is the first moment of the distribution of these differences, or the average difference:

$$\bar{d} = \frac{1}{N}\sum d \tag{22.28}$$

A measure of the variability of the differences is the variance S^2, which is the second moment of the distribution of these differences:

$$S^2 = \sum(d - \bar{d})^2/N = \frac{\sum d^2}{N} - \left(\frac{\sum d}{N}\right)^2 \tag{22.29}$$

The square root of the variance is the standard deviation.

The mean absolute error (MAE) is

$$\text{MAE} = \Sigma\,|d|\,/\text{N} \tag{22.30}$$

The mean square error (MSE) is

$$\text{MSE} = \Sigma d^2/N \tag{22.31}$$

The root-mean-square error is the square root of theMSE. Note that since the root-mean-square error involves the square of the differences, outliers have more influence on this statistic than on the MAE.

The fractional error (FE) [41] is

$$\text{FE} = (M - E)/0.5(M + E) \tag{22.32}$$

The mean fractional error (MFE) is

$$\text{MFE} = \Sigma\,\text{FE}/\text{N} \tag{22.33}$$

The FE is logarithmically unbiased; that is, an M which is k times E produces the same magnitude FE (but of opposite sign) as an M which is $1/k$ times E.

In addition to analyzing the residuals, it may be desirable to determine the degree of agreement between sets of paired measurements and estimates. The linear correlation coefficient r_{EM} is

$$r_{EM} = \frac{N\Sigma E \cdot M - \Sigma E \Sigma M}{\{[N\Sigma E^2 - (\Sigma E)^2][N\Sigma M^2 - (\Sigma M)^2]\}^{0.5}} \tag{22.34}$$

The slope b and intercept a of the least-squares line of best fit of the relation $M = a + bE$ are

$$\text{Intercept:} \quad a = \frac{\Sigma E^2 \Sigma M - \Sigma E \Sigma E \cdot M}{N\Sigma E^2 - (\Sigma E)^2} \tag{22.35}$$

$$\text{Slope:} \quad b = \frac{N\Sigma E \cdot M - \Sigma E \Sigma M}{N\Sigma E^2 - (\Sigma E)^2} \tag{22.36}$$

The temporal correlation coefficient at each monitoring location can be calculated by analysis of the paired values over a time period of record. The spatial correlation coefficient at a given time can be calculated by analysis of the paired values from each station. For the spatial correlation coefficient to have much significance, there should be 20 or more monitoring locations.

Techniques to use for evaluations have been discussed by Cox and Tikvart [42], Hanna [43], and Weil *et al.* [44]. Hanna [45] shows how resampling of evaluation data will allow use of the bootstrap and jackknife techniques so that error bounds can be placed about estimates.

The use of various statistical techniques has been discussed [46] for two situations. For standard air quality networks with an extensive period of record, analysis of residuals, visual inspection of scatter diagrams, and comparison of cumulative frequency distributions are quite useful techniques for assessing model performance. For tracer studies the spatial coverage is better, so that identification of maximum measured concentrations during each test is more feasible. However, temporal coverage is more limited with a specific number of tests not continuous in time.

The evaluations cited in the following sections are examples of the use of various measures of performance.

B. Performance of Single-Source Models

Since wind direction changes with height above ground and plume rise will cause the height of the plume to vary in time, it is difficult to model accurately plume transport direction. Because of this transport wind

direction error, analyses of residuals and correlations are not frequently utilized for assessment of single-source model performance. Instead, cumulative frequency distributions of estimated and measured concentrations for specific averaging times at each location are examined, as well as comparison of the highest concentrations such as the five highest for each averaging time of interest, e.g., 3 and 24 h.

The performance of one specific model, CRSTER [47], for the second-highest once-a-year 24-h concentrations, is summarized in Fig. 22.19 in terms of ratios of estimates to measurements. Overestimates by more than a factor of 2 occur for all receptors whose elevations are near or exceed stack top. The value ΔE is the elevation of the receptor minus the elevation of the stack base; h is the physical stack height. Over seven sites, having stacks varying from 81 to 335 m, for receptors having elevations above the stack base less than 0.7 of the stack height, the second-highest, once-a-year 24-h estimates were within a factor of 2 of the measurements for 25 of 35 monitoring stations.

Comparisons [49] of measured concentrations of SF_6 tracer released from a 36-m stack, and those estimated by the PTMPT model for 133 data pairs over Pasquill stabilities varying from B through F, had a linear correlation coefficient of 0.81. Here 89% of the estimated values were within a factor of 3 of the measured concentrations. The calculations were most sensitive to the selection of stability class. Changing the stability classification by 1 varies the concentration by a factor of 2–4.

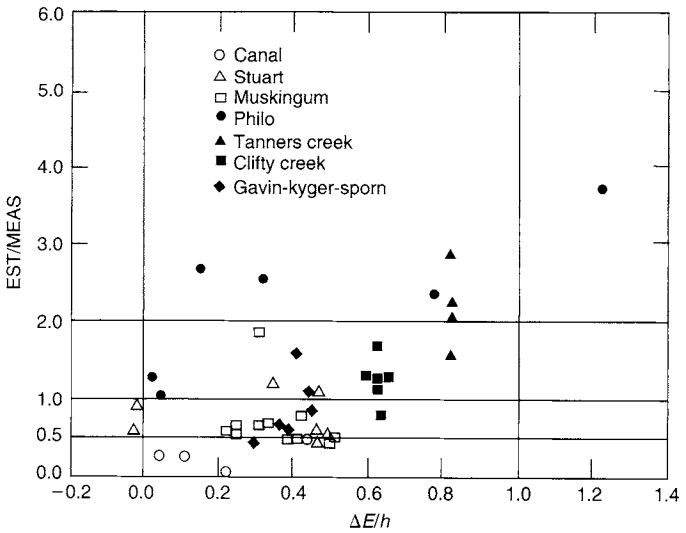

Fig. 22.19. Ratio of second-highest 24 h estimated concentrations from the CRSTER model [47] to measured concentrations as a function of the excess of receptor elevation over stack base evaluation ΔE relative to the stack height h. Names with each symbol are power plants. *Source*: From Turner and Irwin [48].

C. Performance of Urban Models for Nonreactive Pollutants

Because there are multiple sources of most pollutants in urban areas, and because the meteorology of urban areas is modified so that the extremes of stability are avoided, concentrations tend to vary much less in urban than in rural areas.

For sources having a large component of emissions from low-level sources, the simple Gifford–Hanna model given previously as Eq. (22.19), $\chi = Cq_a/u$, works well, especially for long-term concentrations, such as annual ones. Using the derived coefficients of 225 for PM and 50 for SO_2, an analysis of residuals (measured minus estimated) of the dependent data sets (those used to determine the values of the coefficient C) of 29 cities for PM and 20 cities for SO_2 and an independent data set of 15 cities for PM is summarized in Table 22.7. For the dependent data sets, overestimates result. The standard deviations of the residuals and the MAE are about equal for particulates and sulfur dioxide. For the independent data set the mean residual shows only slight overestimation, and the standard deviation of residuals and MAE are considerably smaller.

A version of the Gifford–Hanna model was evaluated [50] using 1969 data for 113 monitoring stations for PM and 75 stations for SO_2 in the New York metropolitan area. This version differed from Eq. (22.19) in considering major point source contributions and the stack height of emission release. This model produced results (Table 22.8) comparable to those of the much more complicated Climatological Dispersion Model (CDM) [51].

The urban RAM model was evaluated [52] using 1976 sulfur dioxide data from 13 monitoring locations in St. Louis on the basis of their second-highest once-a-year concentrations. The ratio of estimated to measured 3-h average concentrations was from 0.28 to 2.07, with a median of 0.74. Half of the values were between 0.61 and 1.11. For the 24-h average concentrations the rations ranged from 0.18 to 2.31, with a median of 0.70. Half of the values were between 0.66 and 1.21. Thus, the urban RAM model generally underestimates concentrations by about 25%.

TABLE 22.7

Residual Analysis for the Gifford–Hanna Model (Eq. (22.19))

Pollutant	N	$\bar{M}$	S_M	$\bar{E}$	S_E	$\bar{d}$	S_d	$\lvert\bar{d}\rvert$
Particulate	29	110.7	27.8	171.9	111.5	−61.2	103.7	81.3
SO_2	20	89.8	83.1	116.25	72.0	−26.5	101.2	82.5
Independent data set particulate	15	91.6	38.7	93.2	51.7	−1.6	24.9	21.3

Note: N is the number of cities, M is measured, E is estimated from the model, d is residual (measured − estimated) and S values are standard deviations.
Source: Data are from Gifford and Hanna [23].

TABLE 22.8

Residual Analysis Using 1969 New York Data[a]

Model	Pollutant	N	$\bar{M}$	S_M	$\bar{E}$	S_d	$\lvert\bar{d}\rvert$
CDM	Particulate	113	82	23	74	22	16
6B	Particulate	113	82	23	67	25	19
CDM	SO_2	75	135	72	138	52	37
6B	SO_2	75	135	72	127	56	38

[a] Adapted from Turner *et al.* [50].
Note: N is the number of monitoring stations, M is measured, E is estimated from the model, d is residual (measured − estimated), and S values are standard deviations.

TABLE 22.9

Residual Analyses of Three Photochemical Models

	Ozone (ppm)			
Model	N	$\bar{d}$	S_d	$\lvert\bar{d}\rvert$
Photochemical box model	10	−0.033	0.041	0.039
Lagrangian photochemical model	10	−0.004	0.110	0.080
Urban airshed model	10	0.074	0.033	0.074

Note: N is the number of days, d is residual (measured – estimated), and S is the standard deviation.
Source: Adapted from Shreffler and Schere [53].

D. Performance of Photochemical Models

The performance of photochemical models is evaluated by their ability to estimate the magnitude, time, and location of occurrence of the secondary pollutant oxidant (ozone). Several photochemical models were evaluated using 10 days' data from St. Louis (Table 22.9). Among those evaluated were the PBM [6], which features a single variable-volume reacting cell. This model is most appropriate for use with light winds, so that most of the emissions will remain in the cell and react, rather than being rapidly transported through the downwind side of the cell. The maximum measured concentrations for the 10 days ranged from 0.08 to 0.18 ppm; the maximum model estimates ranged from 0.07 to 0.22 ppm.

The second model evaluated was the Lagrangian Photochemical Model (LPM) [54], a trajectory model. Backward trajectories were first determined so that starting positions could be used which would allow trajectories to reach station locations at the times of measurement. Measured concentrations ranged from 0.20 to 0.26 ppm and estimated concentrations from 0.05 to 0.53 ppm.

The third model evaluated was the Urban Airshed Model (UAM) [55], a three-dimensional grid-type model. The area modeled was 60 by 80 km, consisting of cells 4 km on a side. There are four layers of cells in the vertical, the bottom simulating the mixing layer. The model provides both spatially and temporally resolved estimates. Hour-averaged estimates of each pollutant species at each monitoring site within the model domain are given. Measured concentrations ranged from 0.17 to 0.24 ppm and estimated concentrations ranged from 0.10 to 0.17 ppm. The model underestimates the concentration at the point of the observed maximum each day.

Seinfeld [33] indicates that photochemical models estimating peak ozone concentrations in urban areas are generally within 30% of measured peaks.

E. Utilization of Models

For the air quality manager to place model estimates in the proper perspective to aid in making decisions, it is becoming increasingly important to place error bounds about model estimates. In order to do this effectively, a history of model performance under circumstances similar to those of common model use must be established for the various models. It is anticipated that performance standards will eventually be set for models.

F. Modeling to Meet Regulatory Requirements

In the United States if the anticipated air pollution impact is sufficiently large, modeling has been a requirement for new sources in order to obtain a permit to construct. The modeling is conducted following guidance issued by the US EPA [56, 57]. The meeting of all requirements is examined on a pollutant-by-pollutant basis. Using the assumptions of a design that will meet all emission requirements, the impact of the new source, which includes all new sources and changes to existing sources at this facility, is modeled to determine pollutant impact. This is usually done using a screening-type model such as SCREEN [58]. The impacts are compared to the modeling significance levels for this pollutant for various averaging times. These levels are generally about 1/50 of the National Air Quality Standards. If the impact is less than the significance level, the permit can usually be obtained without additional modeling. If the impact is larger than the significance level, a radius is defined which is the greatest distance to the point at which the impact falls to the significance level. Using this radius, a circle is defined which is the area of significance for this new facility. All sources (not only this facility, but all others) emitting this pollutant are modeled to compare anticipated impact with the NAAQS and with the PSD increments.

The implementation of CAAA90 requires not only permission for new sources but also permits for existing facilities. There is also a requirement for reexamination of these permits at intervals not longer than 5 years. The permit programs are set up and administered by the states under the review

and guidance of EPA. These programs include the collection of permit fees sufficient to support the program. Implementation of CAAA90 will require the application of MACT on an industry-by-industry basis as specified by EPA. Following the use of MACT, a calculation will be made of the residual risk due to the remaining pollutant emissions. This is accomplished using air quality dispersion modeling that is interpreted using risk factors derived from health information with the inclusion of appropriate safety factors.

Because of their inclusion of the effects of building downwash, the ISC2 (Industrial Source Complex) models [16], ISCST and ISCLT (short-term performing calculations by hourly periods and long-term using the joint frequencies of wind direction, wind speed, and Pasquill stability, commonly referred to as STAR data) are recommended. The ISC2 models differ only slightly from the earlier ISC models (several small errors that make little difference in the resulting calculations were corrected). The recoding of the model to result in ISC2 was requested by EPA to overcome a difficult-to-understand code that had resulted from a number of changes that had been incorporated. The ISC models will make calculations for three types of sources: point, area, and volume. There are recognized deficiencies in the area source algorithm incorporated in the ISC models.

Models are continuing to improve, but many challenges remain. Combined with better measurements and analytical procedures, the new models are crucial to air pollution control and planning decisions.

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QUESTIONS

1. Assuming that the buoyancy flux parameter F is greater than 55 in both situations, what is the proportional final plume rise for stack A compared to stack B if A has an inside diameter three times that of B?
2. How much greater is the penetration of a plume through an inversion of 1°C per 100 m than through an inversion of 3°C per 100 m? Assume that the wind speed is 3 m s^{-1}, ambient air temperature is 29 K and the stack characteristics are $T_s = 415$ K, $d = 3$ m, and $v_s = 20$ m s^{-1}.
3. What is the steady-state concentration derived from the box model for a 10 km city with average emissions of 2×10^{-5}g $m^{-2}s^{-1}$ when the mixing height is 500 m and the wind speed is 4 m s^{-1}?
4. In formulating and applying a gradient transfer model, what are two of the major difficulties?
5. What is the advantage in using trajectory models for estimating air pollutant concentrations at specific air monitoring stations?
6. What is the major difficulty in estimating the maximum short-term (hours) impact of two point sources 1 km apart?
7. Using simplified techniques for estimating the concentrations from area sources, what is the annual average PM concentration for a city with an average wind speed of 3.6 m s^{-1} and area emission rate of $8-10^{-7}$g $s^{-1}m^{-2}$?
8. What are the major limitations in modeling pollutant transformations in urban areas?
9. From the results of the application of the EURMAP model to Europe, what pollutant and mechanism seem to cause the least pollution by a nation to itself?
10. Which measure of scatter is likely to be larger, the mean absolute error or the root-mean-square error?
11. Contrast the fractional error for a measurement of 20 and an estimate of 4 to the fractional error for a measurement of 4 and an estimate of 20.