

Chapter 9 Assessing Air Quality: Modeling

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9.1 Introduction

Models have been used for decades to approximate physical systems and make estimates about the nature of the system under study. The types of models most frequently used in air toxics exposure assessments are mathematically-based models, which attempt to approximate all of the important physical and chemical processes affecting contaminant fate and transport within the environment. The physical and chemical processes are described as a set of mathematical expressions which characterize the behavior of contaminants released into the environment.

One specific type of model, called an **air quality model**, is used by EPA to understand the impact of pollution on air quality for a variety of purposes. For example, under the Clean Air Act (CAA), EPA uses air quality models to facilitate the regulatory permitting of industrial facilities, demonstrate the adequacy of emission limits, and project conditions into future years. For several of the criteria pollutants, regulatory requirements call for the application of air quality models to evaluate future year conditions as part of State Implementation Plans to achieve and maintain the National Ambient Air Quality Standards (NAAQS). Model simulations are also used to assist in the selection of monitoring locations.

Air quality models, when combined with emissions inventory and meteorological data, can be used as part of risk assessments that may lead to the development and implementation of regulations or voluntary reduction measures. For example, under National Air Toxics Assessments (NATA), EPA has conducted a national-scale assessment using air quality models for some 33 priority air toxics (see Chapter 2) to identify broad national air toxics issues and to help focus efforts. This Chapter provides an overview of air quality modeling used in air toxics risk assessments.

9.2 Air Quality Modeling

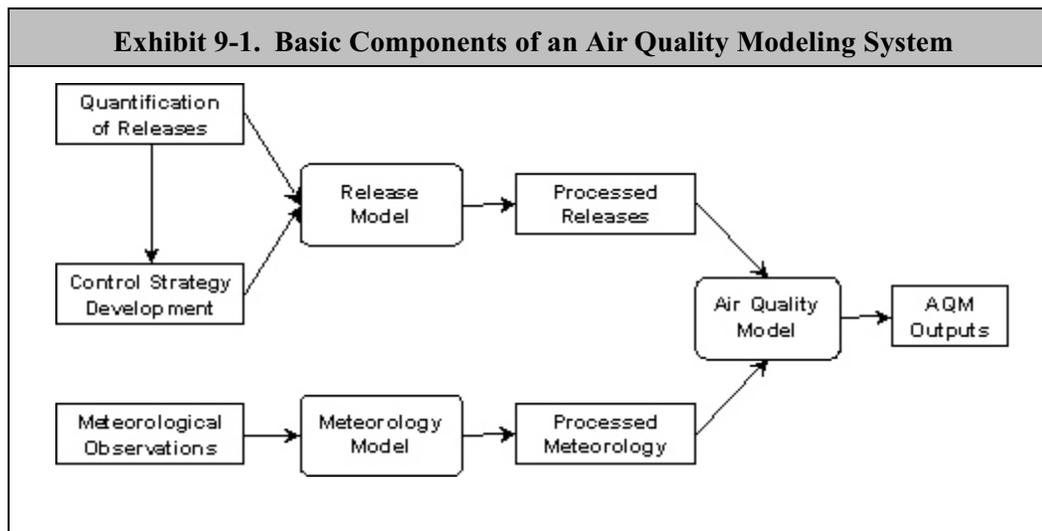
A variety of methods, data, and tools used for modeling the fate and transport of air toxics released to the environment have been developed; for a summary of methods, the reader can refer to Chapter 3 and other parts of EPA's *Residual Risk Report to Congress*.⁽¹⁾ While the Report to Congress is oriented toward assessment of residual (i.e., post-Maximum Achievable Control Technology [MACT]) risks from facilities regulated by the Clean Air Act, it also provides a good, general overview of general modeling procedures for air toxics assessments at the local scale. Another key reference for air quality models is the EPA's Support Center for Regulatory Air Models (SCRAM) website (<http://www.epa.gov/ttn/scram/>).⁽²⁾

9.2.1 The Overall Structure of an Air Quality Model

Air quality models provide estimates of ambient air concentrations and/or deposition rates for one or more chemicals emitted from one or more sources. All air quality modeling systems are comprised of three major components (see Exhibit 9-1) which, when combined, provide a picture of predicted fate and transport of air toxics once released into the environment:

- An emissions (release) model (Chapter 7 discusses developing the emissions inventory);
- A meteorology model (Chapter 8 discusses atmospheric phenomena and physical properties that affect the fate and transport of air toxics after release); and

- An air quality model that predicts the movements of chemicals through the atmosphere along with any physical and chemical changes that may occur (e.g., chemical reactions that degrade the pollutant).



Specifically, the emissions and meteorology data are fed into the model (or the various components of the model) which are then run through various algorithms that simulate the physical and chemical processes in the atmosphere to provide estimated concentrations of chemicals (e.g., for inhalation exposure assessment, the exposure concentration at the point of exposure). Depending upon the specific model application being used, the release and meteorological data may simply be input to a single air quality model that includes both release and meteorological modules or the release and meteorological modules may be separated initially to “pre-process” the data and subsequently combined for the remaining calculations.

Air quality models provide estimates of ambient air concentrations at specific points distant from the source(s) being modeled. These are either predetermined within the model or selected by the analyst. In the simplest models (e.g., SCREEN3), the points are laid out along a vector (straight line) from the source. Many other models use a grid system to calculate ambient concentrations at specific exposure points at specified “nodes”(see Exhibit 9-2). The model does not always automatically provide an estimate of concentration at every desired location, and extrapolation to desired locations is often required. A discussion of where and how to choose exposure points is provided in Chapter 11.

Air Toxics Modeling Issues

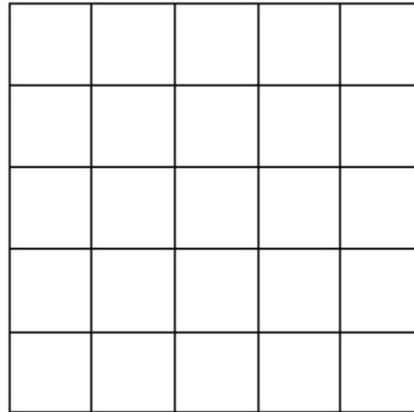
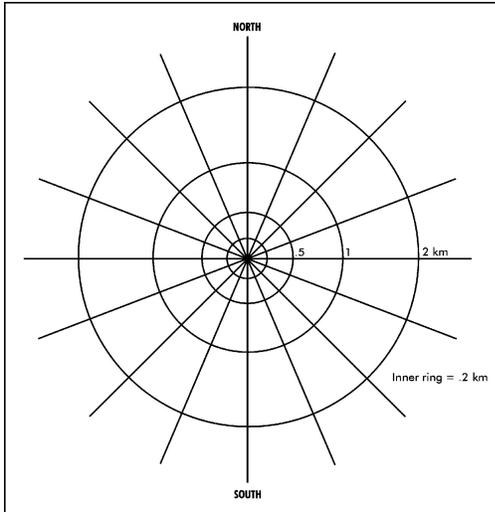
A recent study identified several issues that affect uncertainties associated with air toxics modeling, including:

- Uncertainties associated with emissions;
- Meteorological conditions that are difficult to simulate (e.g., calm conditions, complex terrain, land/sea breezes, precipitation events);
- Spatial coverage, temporal resolution, and detection limits in monitoring data;
- Chemical transformations in the atmosphere;
- Removal via dry and wet deposition;
- Indoor sources; and
- Population activity patterns.

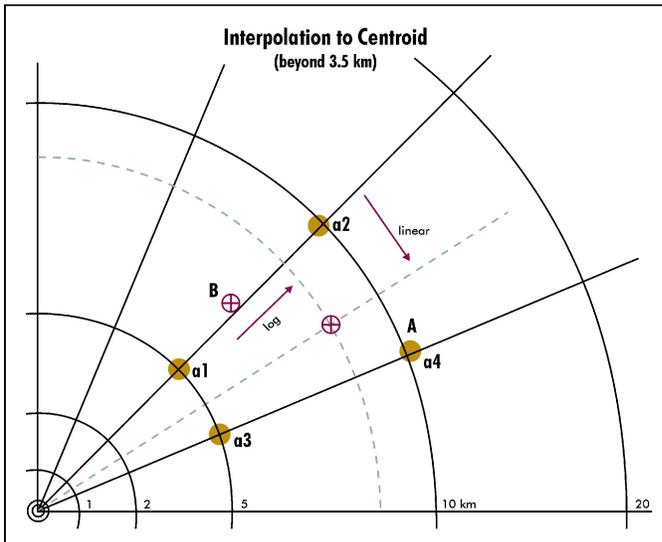
The study recommended a combination of modeling and monitoring for air toxics exposure assessments. For further information, see:

Coordinating Research Council and U.S. Department of Energy. 2002. *Critical Review of Air Toxics Modeling*, August 2002. CRC Project Number A-42-1, available at: <http://www.crao.com>.

Exhibit 9-2. Model Grids and Interpolation



Many air quality models calculate ambient concentrations at specific exposure points at specified “nodes” using either a polar coordinate grid system (i.e., the intersections of a series of concentric circles and radial lines [above, left]) or on a standard Cartesian coordinate system (above, right). (Note that the nodes, in both of these types of grids, are simply the points where two lines intersect.) The locations of these nodes often do not fall precisely on the locations of interest for a given risk assessment.

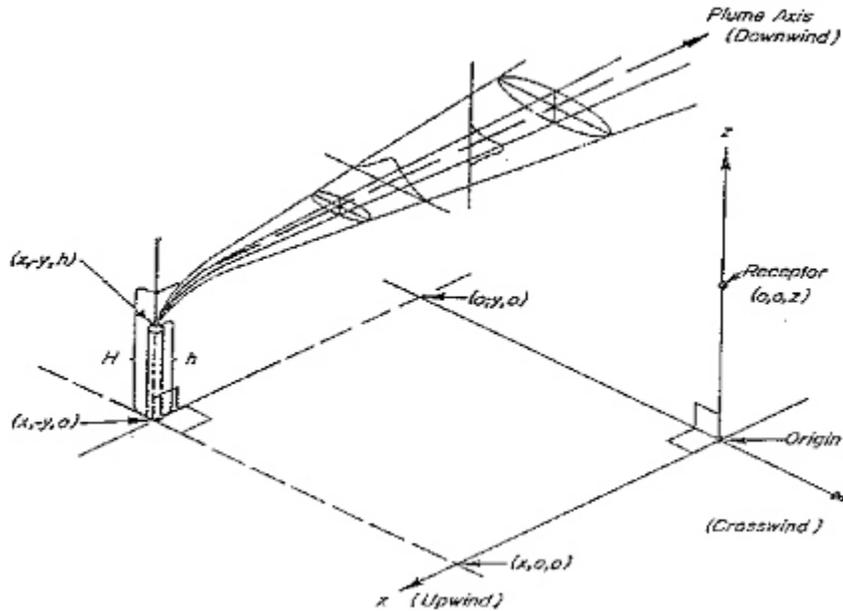


In cases where the nodes and locations of interest do not align, a process of interpolation is used to estimate the ambient air concentration at the location. For polar grids, a two-step interpolation is used, starting with the modeled concentrations at the nearest locations (e.g., a1, a2, a3, and a4 in the graph to the left). The first interpolation is in the radial direction (i.e., along the two adjacent radial lines [a1,a2] and [a3, a4] in the graph). The concentration is estimated at the intersection of each radial line with the concentric circle that intersects the receptor location (at the same radial distance from the source as the internal point). This interpolation is performed under the assumption that the

logarithm of the concentration decreases in proportion to the increase in the logarithm of the distance from the source (i.e., a log-log interpolation). The second interpolation is in the azimuthal direction (i.e., along the concentric circle that intersects the internal point). This interpolation is performed under the assumption that the change in concentration is proportional to the distance around the circle between the two radial lines (i.e., linear interpolation).

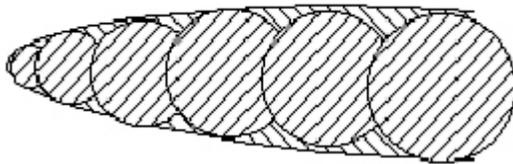
Illustrations of Three Common Types of Air Quality Models

Gaussian Plume Models: Model a continuous release downwind from a source

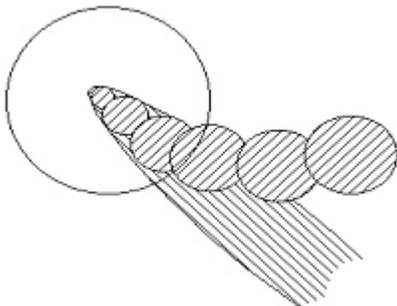


Gaussian plume models estimate the transport and mixing of pollutants in the dispersing plume as it moves downwind from the source. They assume that dispersion in the vertical and lateral dimensions will take the form of a normal Gaussian curve, with the maximum concentration at the center of the plume.^(a)

Gaussian Puff Models: Model either Steady-state or Non-steady state releases



Steady-State Approach: Plume = Puff



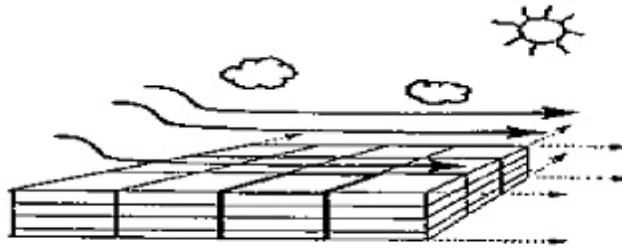
Non Steady-State Approach: Puffs follow Air

Puff models use a series of overlapping puffs to represent emissions. As shown by the illustration of the non-steady state approach, changes in wind direction over time and through space bring about changes in the plume's shape.^(b)

Illustrations of Three Common Types of Air Quality Models (continued)

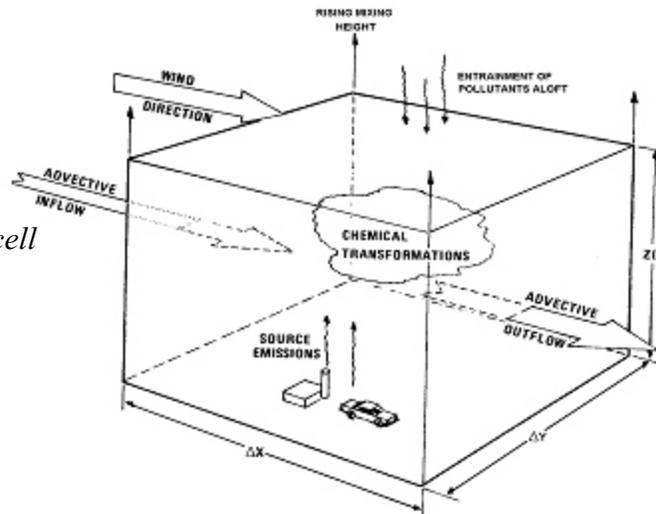
Numerical Grid Models: Model reactive pollutants in complex topography

Modeling Domain



Numerical grid models assume that emissions from area and line sources are mixed throughout the volume of each surface cell within the modeling domain. Emitted species react with each other and the incoming solar radiation with resulting chemical reactions taking place. Point source emissions, typically emitted from elevated stacks, are emitted into upper layers of the modeling domain based on a plume rise calculation. The point source emissions are then mixed throughout the volume of the elevated layer. Some models may modify this widespread dispersal by including a plume in grid module which acts to minimize the instantaneous mixing across the grid cell volume. These reactions are simulated to generate volume-average concentrations as a function of time within each cell.^(c) The cells of the grid, representing discrete portions of the atmosphere, are superimposed on the modeling domain.^(d)

Individual surface cell



^a U.S. Environmental Protection Agency. 1970. Office of Air Programs, prepared by Turner, D.B. *Workbook of atmospheric dispersion estimates*. Publication AP-26. NTIS PB 191 482.

^b National Oceanic and Atmospheric Administration. 2003. Prepared by Irwin, J.S. *Modeling Air Quality Pollutant Impacts*. Research Triangle Park, NC, 15 Oct. 2003. Available at: <http://www.meteo.bg/EURASAP/40/paper1.html>.

^c U.S. Environmental Protection Agency. 1984. Office of Research and Development, prepared by Schere, K.L. and Demerjian, K.L. *User's guide for the photochemical box model (PBM)*. Research Triangle Park. EPA-600/8-84-022a

^d Systems Applications International. 1991-1993. Urban Airshed Modeling National Training Workshops.

Results from air toxic modeling are highly dependent upon the quality of data used as input to the models. The degree to which a user has reliable information on releases, meteorology, and setting will determine the accuracy of the modeled concentrations. Because model inputs are only estimates, even the most sophisticated models will have inherent uncertainties and will have the potential to underestimate or overestimate actual concentrations. (Monitoring data can assist in this regard as a way of evaluating the modeled results and to look for important gaps in the emissions inventory – see Chapter 10).

The uncertainty associated with the meteorology data includes measurement of key variables of wind speed/direction and atmospheric stability, and to a lesser extent, temperature and precipitation. Uncertainty is also associated with the terrain specification. Use of a model designed for flat terrain will likely provide inaccurate estimates of concentrations if the terrain is actually more complex (e.g., a facility located in a river valley modeled as being located on flat terrain).

In addition to the model inputs, uncertainties also arise from the model formulation used to describe the physical and chemical processes that take place in the atmosphere. In general, models are most accurate in simulating long-term averages of ambient concentrations and deposition rates in settings with simple topography.

9.2.2 Types of Models: Scientific Principles

In general, air quality models can be categorized as one of two types: **steady-state** and **non-steady state** models. The movement of mass away from the source (i.e., **advection**) and **turbulent diffusion** (e.g., dispersion) are modeled in both types of models. The steady-state model assumes that no variations occur over a certain time period (typically, one-hour); the non steady-state allows time-varying changes, but this capability imposes the need for additional model inputs, increased computation resources, and increased model formulation complexities. For additional information on air dispersion modeling, refer to NOAA's Real-time Environmental Applications and Display sYstem (READY) website.⁽³⁾

- **Steady-state models** are models which assume no time-varying processes occur over the period of interest. Hence, material released travels infinitely in only one direction over the time period (e.g., one hour). Often, these models assume that the material is distributed normally (also termed a “Gaussian distribution”) and are thus called “Gaussian plume” models (see illustration above). The steady-state model typically uses meteorological information obtained near the source and assumes it holds true throughout the modeling region (e.g., a 50 kilometer radius). Wind direction, wind speed, and atmospheric stability are used to predict concentrations. This type of model is most widely used for stationary sources and for non-reactive pollutants (although models can take into account deposition and simple linear decay). The models are least applicable in areas with rapid time-varying conditions, over spatially varying terrain and land use, over large spatial scales (> 50 km), and where complex atmospheric chemistry takes place.
- **Non-steady state models** are models which can simulate the effects of time- and space-varying meteorological conditions on pollutant transport, transformation, and removal. The modeling region is typically divided into grid cells, and the model simulates movement of pollutants between cells by taking into account advection, degradation, and other physical

and chemical processes. These models are often used for chemically reactive pollutants or where there is complex topography or meteorology (e.g., complex sea breeze circulation). They require complex wind flow characterization and other detailed meteorological information for dispersion. For chemical transformation, they require information on the important chemical compounds as well as chemical kinetics to properly characterize the transformation and removal of air toxics. These models often take the form of grid models with the calculation of the physical and chemical processes taking place at each grid location. Other model types include “puff models” (illustrated above), which use a series of overlapping puffs to represent emissions. The calculations of the physical and chemical processes are made for each “puff.”

Another type of non-steady state model, the atmospheric trajectory model, uses meteorological data and mathematical equations to simulate transport in the atmosphere. The position of a parcel of air with time are calculated based on externally provided meteorological data such as wind speed and direction, temperature, humidity, and pressure. Model results depend on the spatial and temporal resolution of the meteorological data used, and also on the complexity of the model itself. Simpler models may deal with only two-dimensional transport by winds assuming the material emitted into the parcel stays at the same level, while more complex models may include 3-dimensional chemical and thermodynamic processes such as aerosol formation, convection, and turbulent diffusion.

9.2.3 Modeling Deposition

Deposition is the transfer of chemicals from the plume to the earth’s surface (i.e., to soil, water bodies, or living organisms such as plant surfaces). Although the primary route of exposure for many air toxics is inhalation of ambient concentrations, deposition rates can be important for the multimedia fate and transport assessments required for persistent bioaccumulative hazardous air pollutant (PB-HAP) substances (see Chapter 18). Air quality models all simulate ambient air concentrations, and many also simulate deposition. Based on the simulated ambient air concentration at a location, the **deposition flux** (i.e., mass of pollutant deposited per unit area) can be simulated based on a number of assumptions (see Chapter 8 for a discussion of mechanisms of deposition). Two types of deposition are usually modeled:

- **Dry deposition** is determined from the ambient air concentration and the deposition velocity. Particle-phase air toxics are the principal pollutants removed through dry deposition by particle settling. In addition, semi-volatile toxics (air toxics that exist both in the gas and particle phases) can also be removed through dry deposition. Dry deposition of some vapor-phase air toxics is also possible for some chemicals (e.g., divalent mercury).
- **Wet deposition** is determined from a combination of the ambient concentration and a **scavenging ratio**. The scavenging ratio accounts for the propensity of the modeled chemical to partition into precipitation in the atmosphere, based on physical and chemical characteristics of the pollutant, the nature of the precipitation (liquid or frozen), and the precipitation rate. The term “scavenger” is a general term that can apply to anything chemical or physical that removes a pollutant from the atmosphere. In this example, rain is a scavenger because it is removing (by dissolution) an air toxic from the atmosphere and transferring it to a surface.

9.2.4 Screening vs. Refined Models

The overall accuracy and precision of results determined by a model is generally proportional to the complexity of the model, which in turn affects input data requirements and overall resources.

- **Screening-level models** are designed to provide conservative (i.e., high) estimates, and are useful for applications such as identifying facilities and/or air toxics that appear likely to contribute the greatest risk among a group of sources and chemicals released. Data requirements are generally low (e.g., emission rates, some stack parameters), and running the models is generally easy and requires few resources.
- **Refined models** take into account more complex chemical behavior and a greater degree of site-specific information, generally producing more accurate results. Data requirements are higher (e.g., site-specific meteorology, terrain, chemistry data), and application of more refined models may require expert judgment in developing model inputs and setting model options. Some models can be used both as a screening model and refined model if additional site-specific information is used in the application.

The selection of a model for a specific application depends on a number of factors, including:

- The nature of the pollutant (e.g., gaseous, particulate, reactive, inert);
- The meteorological and topographic complexities of the area of concern;
- The complexity of the distribution of sources;

Exposure Concentrations: Units are Important

Air toxics exposure concentrations (ECs) should in general be reported as $\mu\text{g}/\text{m}^3$. Dose-response values often are reported as parts per million (ppm), parts per billion (ppb), or mg/m^3 . In the risk characterization step, ECs are compared to dose-response values, and therefore the units for the EC must match the units for the dose-response values.

The conversion from mg/m^3 to ppm can be expressed as:

$$\text{Concentration [ppm]} = \text{Concentration [mg/m}^3] \times 24.45 \text{ [L/mole]} / \text{MW}$$

and the conversion from ppm to mg/m^3 is:

$$\text{Concentration [mg/m}^3] = \text{Concentration [ppm]} \times \text{MW} / 24.45 \text{ [L/mole]}$$

where MW is the molecular weight of the air toxic in g/mole and 24.45 is the volume in liters of one mole of an ideal gas at 1 atmosphere and 25 degrees Celsius.

Note also that $\text{ppb} = 1,000 \times \text{ppm}$ and that here, ppm is volume-based. Also, $\mu\text{g}/\text{m}^3 = 1,000 \times \text{mg}/\text{m}^3$.

Tip: In the development of the analysis plan, stipulate that all laboratory and modeling results be reported in $\mu\text{g}/\text{m}^3$. This will save time (and reduce computational errors) in the remaining phases of the risk assessment.

- The spatial scale and temporal resolution required for the analysis;
- The level of detail and accuracy desired for the study and the amount of uncertainty that the analyst/risk manager is willing to accept; and
- The technical expertise of user.

For example, steady-state models are not considered appropriate for downwind distances beyond a 50 km range, primarily because the steady-state wind speed and direction over that distance become unrealistic over the typical one-hour simulation period. This is especially true where complex terrain or meteorology is present.

Because screening models are applied with fewer resources and data to provide conservative estimates of concentrations, screening models are often applied prior to any refined modeling in order to narrow the set of sources or air toxics to be modeled. Such an iterative approach is generally recommended by EPA, where screening results are used to generate a subset of potentially higher-risk sources or chemicals for more refined assessment. General guidance on screening-level modeling has been published by EPA.⁽⁴⁾ Additional guidance on air modeling is incorporated into EPA's Guideline on Air Quality Models.⁽²⁾

Risk assessors generally work out the development of a modeling protocol to be used in the assessment during the planning/scoping and problem formulation phase of the assessment. Providing this protocol will help establish the modeling approach for not only review and comment by interested parties up front, but will help to establish technical credibility and provide for consensus building among all interested parties.

9.2.5 Specific Data Required for Modeling

As described above, meteorology, terrain, and emissions data are processed and used as primary input data for air quality models. Depending on the level of refinement of the model, the required input data for an air quality model will include (but not necessarily be limited to) the following parameters:

- **Emission rate.** In general, the rate at which emissions are released into the atmosphere are specified as a rate of release for each chemical in units of mass per unit time.
- **Physical/chemical characteristics of emissions.** These data are closely related to emission rates (i.e., from measurements and/or emission factors; see Chapter 7). For some models, the phase of emission must be specified (e.g., gas, particulate, or semi-volatile). For chemicals present as particulate matter or as semi-volatile substances, particle size distribution and fraction of particle phase as a function of temperature, for each chemical, may be necessary inputs. In some cases, information may only be available on the basis of total volatile organic compounds or total particulates. This information may be speciated based on the emissions source type through the use of sources such as EPA's SPECIATE database. (The most recent version of SPECIATE, Version 3.2, was last updated with new profiles in October 1999.)⁽⁵⁾
- **Type of release point.** The required input data, modeling approach, and model selected for assessment can depend on the type of release being modeled. Chapter 4 discussed types of sources from a regulatory perspective (e.g., stationary, mobile). The following discussion is focused on types of sources from a modeling perspective.

- **Point sources** (modeling sense) are releases from stacks and isolated vents, and typically have plume rise associated with the release due to the buoyancy or momentum of the effluent.
 - **Area sources** (modeling sense) are sources which are usually low level or ground level releases with no plume rise (e.g., fugitive emissions from the summary of equipment leaks across a facility; uncontrolled emissions that escape from the windows along a building wall; releases of dust from a road or work site; slag dumps; storage ponds). Depending on the type of area source, the modeler may opt to evaluate it as emissions occurring from a two-dimensional surface (i.e., an area source in the modeling sense) or as a three-dimensional volume source (see below). If a large number of sources are to be modeled, a common approach is to spread these sources uniformly across the modeling domain if no appropriate spatial surrogate is available. Alternatively, these sources may be allocated based on spatial surrogates. Typical examples include census tract population and commercial, residential and industrial land-uses.
 - **Volume sources** are releases that are modeled as emanating from a 3-dimensional volume (such as a box) . Examples include releases from conveyor belts or the collective releases from the gas pumps at service stations. Volume sources differ from area sources in that they have a vertical dimension to their release. Like area sources, they do not have plume rise.
 - **Line sources** are releases that are modeled as emanating from a two-dimensional area. Examples include rail lines and roadway segments. Line sources differ from area sources in that they have aspect ratios (length to width) much higher than 10:1. Like area sources, they do not have plume rise.
 - **Specialized release types** include multiple parallel release lines that result in increased buoyant dispersion (e.g., coke ovens, aluminum smelters); dense gas release; and exothermic gas release, jet-plume release and horizontal venting that may be defined and modeled using special techniques or models depending on the characteristics of the emission source.
- **Release point parameters.** Depending on the type of source being modeled, the user may need to specify the physical characteristics of the release point. Key parameters may include the following:
 - Release height above ground level (e.g., stack height, average height of fugitive emissions).
 - Area of the release point (for point sources, stack diameter; for area sources, length and width of the area across which releases occur).
 - Other stack parameters of the release stream for point sources that can alter the effective release height, which include temperature, stack orientation, the presence of obstructions to flow (i.e., rain caps), and exit velocity or flow rate. Flow rate is expressed in terms of the total volume of material released per unit of time. In general, most of the flow rate is made up of nontoxic exhaust gases, with a small fraction being composed of chemical contaminant.
 - Facility building dimensions, if building downwash (i.e., the effects on plume dynamics due to structures located near the source) is modeled.
 - **Location of special receptors.** The location of known sensitive receptors (e.g., a school or day-care center) may be a critical input when determining where to model ambient concentrations. If these special receptor locations are not identified, the model will only

provide concentration estimates at the nodes of the modeling grid that is initially laid out around the source.

- **Information on the surrounding land-use and terrain heights.** For dispersion models, classification of the surrounding area as urban or rural is usually required (this classification can affect the rate of dispersion). In addition, more refined modeling that takes into account complex terrain (e.g., ground surfaces higher than release height elevation) will require terrain elevation data.
- **Chemical-specific data.** If transformation/removal is being modeled, rates of transformation or removal for the chemicals being modeled are required (transformation processes are discussed in Chapter 8).
- **Boundary or background concentrations.** Ideally, emissions from modeled source(s) are responsible for the modeled concentrations. However, background concentrations, or boundary conditions in the case of grid models, may be important contributors to the total concentrations. This is particularly relevant where modeled concentrations are compared to observed concentrations. There are three basic approaches to estimating background concentrations:
 - Default values based on supporting documentation from the literature (this is the simplest approach);
 - Data collected from monitoring stations within the study area; and
 - Estimates made from larger regional scale models that cover the study area.

For grid type models, users should be aware that with a smaller modeling domain, there is more potential for the boundary concentrations to play a more important role in determining the total concentration.

In general, air quality modeling results will be most sensitive to the emission rate when studying a single or few release points. However, when studying multiple release locations over a broad area, source location becomes the most important parameter. For a Gaussian-type dispersion model (e.g., ISC3, AERMOD; see Section 9.2.7 below), the ambient concentration will be directly proportional to the emission rate (enabling the use of unit emission rates). Other inputs, especially stack height and distance to fence line, can also affect the results because these parameters can have a direct impact on the location of higher ambient chemical concentrations and potential off-site receptors. In general, however, the sensitivity of air modeling results to specific input parameters can vary widely according to site-specific and chemical-specific factors. Site-specific analyses are generally required to derive accurate sensitivity results for a specific air modeling application. Additional discussion on sensitivity analysis can be found at the EPA Region 6 Air Modeling for Combustion Risk Assessments website.⁽⁶⁾

9.2.6 Sources of Air Quality Models and Information

Numerous models (both screening and refined) have been developed by EPA, other government agencies, and private sources. EPA models in particular undergo extensive evaluation and statistical measures of performance. Some private industry models are also available to the user at little or no charge. (If a public domain model is not available and a private model must be

used, the user should request information about the theoretical basis for the model and the result of any peer review.) Important sources of information include EPA's *Guideline on Air Quality Models*⁽²⁾ and *Dispersion Modeling of Toxic Pollutants in Urban Areas: Guidance, Methodology and Applications*.⁽⁷⁾ Both are available at EPA's SCRAM website (<http://www.epa.gov/ttn/scram/>), EPA's primary resource for Agency air modeling information.⁽²⁾ At the SCRAM site, EPA maintains an up-to-date collection of the executable files, source codes, and user guidance for EPA air quality models. The EPA Office of Air Quality Planning and Standards maintains an on-line Air Pollution Training Institute (APTI) that is managed by the Education and Outreach Group (EOG) and offers additional information and training opportunities for air quality modelers.⁽⁸⁾

9.2.7 Examples of Air Quality Models

A variety of models are available for air toxics risk assessments, with some models having been designed for specific air toxics application. The SCRAM website provides detailed information regarding individual models, including software/code for each model, user's manuals, and other support documentation.

The extent to which a specific air dispersion model is suitable for the evaluation of air toxic source impacts depends upon several factors, such as the nature of the pollutant (e.g., gaseous, particulate, reactive, inert), the meteorological and topographic complexities of the area, the complexity of the source distribution, the spatial scale and resolution required for the analysis, and the level of detail and accuracy required for the analysis. For example, steady-state Gaussian plume models are not considered appropriate for downwind distances outside of the 0.1 km to 50 km range. Because of the assumption in Gaussian models of a steady wind speed and direction over the entire modeling domain for each hour, a > 50 km distance may be inappropriately long in many areas, especially where complex terrain or meteorology is present. In such cases, a non-steady state model would be more appropriate.

Exhibit 9-3 provides an overview of the key physical processes simulated in the most widely used air quality models oriented toward assessment of risks from facilities. Exhibit 9-4 shows the spatial and temporal scales over which these air quality models are typically applied. Exhibit 9-5 identifies some common applications for these air quality models.

Finer scale models, such as CAL3QHC and CALINE4, are most typically applied to exposure studies from mobile sources.

The UAM-TOX and CMAQ models are examples of models which can simulate photochemically active air toxic species, including secondary formation of pollutants like formaldehyde. Because the complex secondary formation processes are nonlinear and can occur at locations distant from the emission source, these models are designed to be applied to an exhaustive set of sources over a large region, rather than to individual facilities or small groups of facilities. The models more typically applied to single or

The Draft Guidance on the Development, Evaluation, and Application of Regulatory Environmental Models recommends best practices to help determine when a model, despite its uncertainties, can be appropriately used to inform a decision. The Knowledge Base (KBase) is a web-accessible database of information on some of EPA's most frequently used models. The draft guidance recommends what information about models to document, while the Knowledge Base is the repository where this information is documented. Both products are available at the CREM internet site at <http://www.epa.gov/crem>.

multiple facilities include SCREEN3, ISCST3, ISCLT3, AERMOD, ASPEN, CALPUFF, and UAM-TOX. Brief descriptions of these models are provided below. Some modeling studies have combined the application of a regional model with a neighborhood-scale model in order to address secondary and background concentration contributions, while capturing finer spatial resolution for primary pollutant predictions.

Community Multi-scale Air Quality (CMAQ) Modeling System

The CMAQ modeling system has been designed to approach air quality as a whole by including state-of-the-science capabilities for modeling multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation. In this way, the development of CMAQ involves the scientific expertise from each of these areas and combines the capabilities to enable a community modeling practice. CMAQ was also designed to have multi-scale capabilities so that separate models were not needed for urban and regional scale air quality modeling.

The target grid resolutions and domain sizes for CMAQ range spatially and temporally over several orders of magnitude. With the temporal flexibility of the model, simulations can be performed to evaluate longer term pollutant climatologies as well as short term transport from localized sources. With the model's ability to handle a large range of spatial scales, CMAQ can be used for urban and regional scale model simulations. By making CMAQ a modeling system that addresses multiple pollutants and different spatial scales, CMAQ has a "one atmosphere" perspective that combines the efforts of the scientific community. Improvements will be made to the CMAQ modeling system as the scientific community further develops the state-of-the-science. Additional information about CMAQ can be found at: <http://www.epa.gov/asmdnerl/models3/cmaq.html>.

SCREEN3

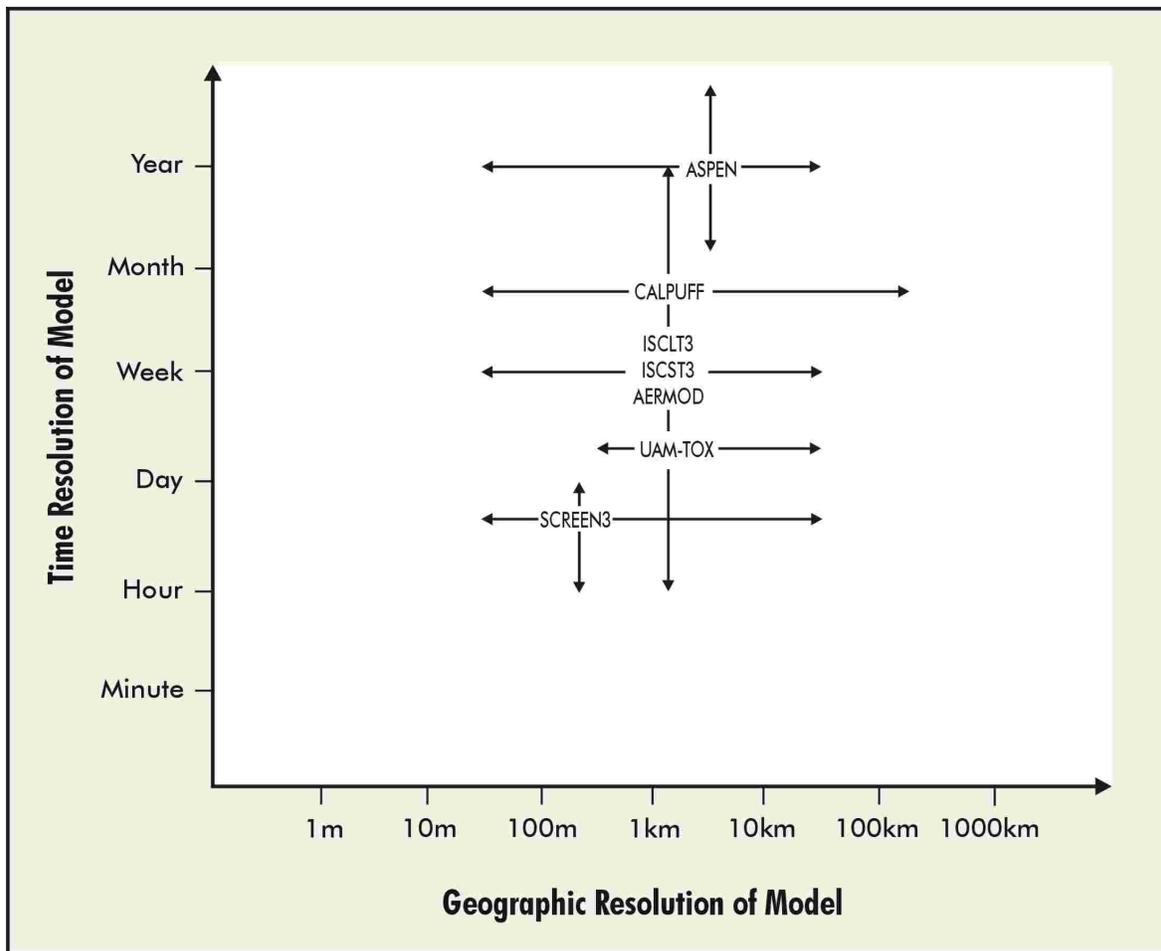
- Screening-level Gaussian dispersion model that estimates an hourly maximum ambient concentration based on an average, constant emission rate (concentration results can be scaled up to annual average using simple conversion factors as specified in EPA guidance;⁽⁴⁾ results are not direction-specific (i.e., wind direction is not taken into account).
- Data requirements are relatively low; uses site-specific facility data (e.g., stack height, diameter, flow rate, downwash); does not use site-specific meteorology data.
- Data processing requirements are low; easy to use for quick assessment of a single facility.
- Model does not estimate deposition rates.

Exhibit 9-3. Key Modeling Attributes of Some Widely Used Air Quality Models for Residual Risk Assessment

Modeling Attribute	SCREEN3	ISCST3	ISCLT3	AERMOD	ASPEN	CALPUFF	UAM-TOX
Point	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Volume	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Area	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Meteorology	Built-in worst-case meteorology	Hourly (National Weather Service) or site-specific equivalent	Frequency array of meteorology data	Hourly (National Weather Service) or site-specific equivalent	Multiple hourly observations (National Weather Service or site-specific equivalent)	Hourly user-defined 3-D fields, usually from a meteorological model with multiple meteorological stations	Hourly user-defined 3-D fields, usually from a meteorological model with multiple meteorological stations
Wet Deposition	No	Yes	No	Yes*	Yes	Yes	Yes
Dry Deposition	No	Yes	Yes	Yes*	Yes	Yes	Yes
Complex Terrain	Yes	Yes	No	Yes	No	Yes	Yes
Overwater Effects	No	No	No	No	No	Yes	No
Vertical Wind Shear	No	No	No	Yes	No	Yes	Yes
Building Downwash	Yes	Yes	Yes	Yes	Yes	Yes	No
Model Formulation and Plume Distribution	Steady-state, Gaussian	Steady-state, Gaussian	Steady-state, Gaussian sector average	Steady-state Gaussian stable & neutral conditions, bi-Gaussian in unstable conditions	Steady-state, Gaussian sector average	Non-steady-state, Gaussian puff	Non-steady-state grid model
Chemical Transformation	None	Simple decay	Simple decay	Simple decay (SO ₂)	Difference between precursor inert and precursor decay	Simple psuedo-first-order effects	Complete chemical mechanism for most gas-phase toxics
Relative Complexity	Simple	Moderate	Moderate	Moderate	Moderate	Complex	Complex

*AERMOD version 02222 is now available for review and comment on EPA's SCRAM website (<http://www.epa.gov/scram001/>). This version includes algorithms for dry and wet deposition as well as an improved downwash algorithm known as PRIME.

Exhibit 9-4. Spatial and Temporal Scales of Widely Used Air Quality Models



This figure illustrates the geographic and temporal resolution of several widely used air quality models. For example, the screening-level model SCREEN3 has a spatial resolution of 50 m to 50 km, but a temporal resolution of 1-24 hours. In contrast, ISCST3 has the same spatial resolution (50 m to 50 km), but has a temporal resolution from 1 hour to 1 year.

Industrial Source Complex - Short Term (ISCST3)

- Gaussian dispersion model (more advanced than SCREEN3); estimates average annual ambient concentration by modeling hourly emissions, and meteorology includes removal effects for wet and dry deposition flux for any locations specified by the user.
- Data requirements are higher than for SCREEN3; requires hourly, site-specific, processed meteorological data, physical characteristics of emissions, and terrain information. Model can accommodate variable emission rates.
- More expertise is required to use model (compared to SCREEN3); user should possess specific technical and computer skills.

Exhibit 9-5. Typical Applications for Common Dispersion Models						
	Averaging Period	Terrain Type	Single Source		Multiple Sources	
			Rural	Urban	Rural	Urban
Screening Models	Short Term (1-24 hour average)	Simple	SCREEN3	SCREEN3	ISCST3, AERMOD	ISCST3, AERMOD
		Complex	SCREEN3, ISCST3	SCREEN3, ISCST3	ISCST3	ISCST3
	Long Term (Monthly-Annual)	Simple	ISCLT3	ISCLT3	ISCLT3, ASPEN	ISCLT3, ASPEN
		Complex	ISCST3	ISCST3	ISCST3	ISCST3
Refined Models	Short Term (1-24 hour average)	Simple	ISCST3, AERMOD	ISCST3, AERMOD	ISCST3, AERMOD	ISCST3, AERMOD, UAM-TOX
		Complex	AERMOD, CALPUFF	AERMOD, CALPUFF	AERMOD, CALPUFF	AERMOD, UAM-TOX, CALPUFF
	Long Term (Monthly-Annual)	Simple	ISCST3, AERMOD	ISCST3, AERMOD	ISCST3, AERMOD	ISCST3, UAM-TOX, AERMOD
		Complex	CALPUFF, AERMOD	CALPUFF, AERMOD	CALPUFF, AERMOD	CALPUFF, UAM-TOX, AERMOD

Industrial Source Complex - Long Term (ISCLT3)^(a)

- Similar to ISCST3, but uses seasonal frequency distribution of meteorological inputs rather than hourly data; runs more rapidly than ISCST3, but can only produce concentrations averaged over a relatively long period of time; not considered as accurate as ISCST3.
- Unlike ISCST3, it cannot simulate wet deposition or complex terrain (terrain higher than the stack height).

^aEPA is no longer actively updating the model with improvements or additional capabilities. It still is one of EPA's preferred models and can be used in appropriate situations. For most single or limited source applications, the ISCLT3 model can be used without any overwhelming computational burden.

AMS/EPA Regulatory Model (AERMOD)

- Replacement model for ISCST3 using new or improved algorithms on the parameterization of the earth's boundary layer turbulence and state-of-the-science dispersion modeling; deposition algorithms should be available soon.
- Like ISCST3, is a Gaussian formulated model.
- Similar to ISCST3, but includes dispersion algorithm for both convective and stable boundary layers and allows plume penetration into elevated inversions.
- Incorporates new algorithms for building downwash.
- Unlike ISCST3, it simulates vertical profiles for wind, turbulence, and temperature.
- No wet or dry deposition (although planned future improvement).
- Requires surface characteristics as inputs (e.g., albedo, Bowen ratio, surface roughness), which allow user to differentiate between different types of terrain.

ASPEN

- A Gaussian dispersion model used to estimate toxic air pollutant concentrations over a large scale domain from regional to continental scale. (This is the model used for NATA risk characterization analyses.)
- Employs a dispersion algorithm similar to ISCLT3.
- However, unlike ISCLT3, it includes treatment of wet deposition for particles, and more detailed treatment of chemical transformation than ISCLT3 or ISCST3, although less detailed than UAM-Tox.
- In contrast to ISCLT3, ASPEN can utilize meteorological information from several locations, and includes a simplified treatment of secondary formation of gaseous air toxics.

CALPUFF

- A Gaussian puff model designed for long-range transport (> 50km) assessment, but may also be applied for near-source in situations with complex meteorology. As described previously, a puff represents a continuous plume as a number of discrete packets of pollutant material.
- Has all the functional capabilities of ISCST3, but also includes capabilities for including 3-dimensional wind fields, vertical wind shear, and overwater effects.
- Not as extensively evaluated and tested as ISCST3 model.
- Requires a substantially higher level of air quality modeling expertise to use the model (compared to ISCST3).

UAM -Tox (Urban Airshed Model - Toxics Version)

- A three-dimensional, grid-type model used to model pollutants in urban areas. Derived from the Urban Airshed Model (UAM), designed to calculate ozone concentrations under short-term, episodic conditions lasting three to four days resulting from emissions of oxides of nitrogen (NO_x), volatile organic compounds (VOC), and carbon monoxide (CO).
- Simulates the most photochemically active air toxics (i.e., acetaldehyde, 1,3-butadiene, and formaldehyde), as well as secondary formation of acetaldehyde and formaldehyde, tracking primary and secondary fractions separately.
- Requires a substantially higher level of air quality modeling expertise to use this model (compared to ISCST3).

9.2.8 Emissions from Soil

In addition to the air quality models described above, it is sometimes necessary to model emissions of chemicals from soil. Emissions from soil may occur as a result of the volatilization of chemicals from contaminated soil or as a result of the resuspension of study area soils. Models that predict emission rates for volatile chemicals or dust require numerous input parameters, many of which are study area-specific. For volatile chemicals, emissions models are available from several EPA sources.⁽⁹⁾ Emissions due to suspension of soils may result from wind erosion of exposed soil particles and from vehicular disturbances of the soil. To predict soil or dust emissions, a number of modeling approaches have been developed. These include EPA's fugitive dust model for a site-specific assessment.⁽¹⁰⁾ For road dust, other techniques are generally used.⁽¹¹⁾ After emissions have been estimated or measured, air dispersion models can be applied to estimate air concentrations receptor points.

In addition, chemicals in contaminated soils and groundwater may also evaporate into homes and buildings through cracks in the floor. The models used to assess these types of exposures (often called "basement models" because this type of problem can be exacerbated when a room is buried in the contaminated medium) are commonly used by hazardous waste site cleanup risk assessors to determine whether people living on or near contaminated sites are being adversely affected by chemicals evaporating into their living or working spaces. This type of analysis is less common for ambient air toxics risk assessment of the type that will generally be performed in an urban setting or in the evaluation of source impacts on nearby populations. However, this issue does come up on occasion and the topic is mentioned here for completeness.

One of the primary vapor intrusion models is the Johnson and Ettinger model (http://www.epa.gov/oerrpage/superfund/programs/risk/airmodel/johnson_ettinger.htm), and EPA has developed a users guide for evaluating vapor intrusion into buildings through the use of this model (<http://www.epa.gov/superfund/programs/risk/airmodel/guide.pdf>).

Another chemical, radon, is also an issue for homes and buildings in certain parts of the country (see Chapter 2). EPA's Indoor Environments Division (<http://www.epa.gov/iaq/>) provides a comprehensive set of informational materials on risks associated with radon and mitigation methods (see <http://www.epa.gov/iaq/radon/pubs/>).

9.3 Air Quality Modeling Examples

EPA's Air Toxics Community Assessment and Risk Reduction Projects Database has been compiled to provide a resource of planned, completed, and ongoing community-level air toxics assessments across the country. The projects included in the database provide examples of the applications of air quality modeling at real-world sites. Project descriptions and related information can be obtained from the database website at:

<http://yosemite.epa.gov/oar/CommunityAssessment.nsf/Welcome?OpenForm>.

Additional Reference Documents

Although the list of following documents are now somewhat dated in terms of computational limitations for application of the models, the documents do provide overall methodology and guidance on procedures to consider when conducting air toxic modeling:

Guidance on the Application of Refined Dispersion Models for Hazardous/Toxic Air Releases, USEPA/OAQPS, Research Triangle Park, NC, EPA-454/R-93-002, May 1993.

Air/Superfund National Technical Guidance Study Series, Volume V - Procedures for Air Dispersion Modeling at Superfund Sites, EPA/OAQPS, Research Triangle Park, NC, February, 1994.

Dispersion Modeling of Toxic Pollutants in Urban Areas, Guidance, Methodology And Example Applications, EPA/OAQPS, Research Triangle Park, NC, EPA-454/R-99-021, July 1999.

Guidelines on Air Quality Models. 40 CFR Part 51 and Part 52, Appendix W; Environmental Protection Agency, AH-FRL-5531-6.

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