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Technical Guidance Document for Air Quality Modeling

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Environmental Quality Sector	*Corporate Management Representative	Secretary General
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1.0 Introduction

This document provides general guidance on conducting an air quality modeling study. This document discusses types of models and their appropriate uses, the approach to a study, general data requirements, and methods of comparing modeling results to ambient air quality standards.

Details for each study need to be determined in consultation with the competent authority. The competent authority should also be kept apprised of progress being made, difficulties that may require assistance of the authority, and results at predetermined milestones. For example, a screening model may show the furthest distance from a source where an impact may be expected. Prior to commencing the next stage of the modeling study, the results from the screening model can be used in consultation with the competent authority to determine the size and placement of the modeling domain for a more refined model. Such consultations are expected to increase efficiency of the overall modeling study and its review procedures.

This document includes information on some specific models that are used internationally. Note that some modeling systems are open source and available at no cost from government agencies, some modeling systems are proprietary and require a purchase payment and possibly annual fees, and some modeling systems provide a user interface that executes the open source models but for a purchase cost. The modeler is cautioned to choose and implement peer-reviewed models that are state-of-the-science, widely used, and appropriate for the specific air quality modeling study.

1.1 Purpose of Modeling

The purpose for conducting an air quality modeling study is to estimate the effect on ambient air quality of a change in one or more sources that emit a pollutant of concern. Examples of reasons to conduct a study include constructing a building, widening a road, adding a new industrial facility or a new process at an existing facility, changing traffic flow to alter congestion, increasing population, and climate change.

The results of a modeling study provide information to decision makers relating to the need for dust suppression at a construction site or pollution control equipment for a new industrial process. For example, if modeling shows that the new construction may cause exceedances of an air quality standard, then an offset may be required such that new controls must be added to an existing process in order to reduce its emissions to the point where the new process can operate within applicable standards.

A modeling study needs to be designed and executed to answer relevant questions. Appropriate models and related tools must be used with high quality data (e.g., meet quality standards for data collection and processing and are appropriate for their use in the study). The entire process must be documented including all assumptions and estimates that are made. In addition to interim reports that may be required by the competent authority, the study must produce and present a final report to the competent authority. The structure of the final report will be determined by the competent authority but is expected to present results clearly with adequate interpretation and to include discussion of uncertainties in the results.

1.2 Phases of a Modeling Study

A modeling study moves through phases as it progresses from start to finish. Some of these phases must be repeated and refined based upon results obtained in a later phase, new data sources identified, or the recognized need for a different type of model. A modeling study may include the following phases:

- Scoping Phase
- Screening Model Phase
- Refined Model Phase
- Presentation of Results
- Final Report

1.2.1 Scoping Phase

The first phase identifies the issues involved and the level of detail required for an air quality modeling study. Chemicals of concern and all sources of their emissions are identified. Rough estimates are made for their expected emissions. Note that all estimates must be conservative (i.e., provide the maximum expected value); future calculations and modeling can be used to refine these estimates.

Initial information on the sources, site, and surrounding area are obtained. Sources need to be classified by phase of the project (e.g., demolition of existing buildings, preparation or grading of a construction site, construction, planned operations). The information includes current ambient concentrations from monitoring data and nearby sources of the same pollutants, relevant air quality standards, general information on terrain features, and locations of receptors of concern. Note that receptors may include both humans and ecosystems in the area of potential impact of the sources.

All gathered data, including calculations of emissions and assumptions, need to be shared with the competent authority. Some refinements may be required. If the pollutants are not on the list of toxic compounds, if their emissions are expected to be small (i.e., less than a de minimus threshold), and if no receptors of concern are located close to the sources, then modeling may not be required. Otherwise, the next step is to implement a screening model. However, if the preliminary data indicate a clear need for a detailed modeling study then the screening model phase may be omitted.

1.2.2 Screening Model Phase

A screening model, as discussed in section 2.2.1, is a simplified model designed to provide conservative estimates of downwind concentrations from an emissions source. Very little data are required on the source itself and the local meteorology. The model may estimate the location of the maximum downwind concentration or the maximum concentration at specified distances downwind.

Screening models are typically simple Gaussian plume models that use constant wind in one direction and estimate concentration along the plume's centerline. The centerline concentration is guaranteed to be conservative for a specified emission rate because winds do not blow in one constant direction. This true variation in wind direction means that concentrations are lower at locations at any distance orthogonal to the centerline than they are at the centerline.

The screening model needs to be applied to each pollutant and source. Some pollutants may be screened out from further, refined modeling by showing that their downwind concentrations will be below any level of concern. If some of the emission sources emit only those pollutants that are screened out, then those sources may be eliminated from additional, refined modeling. However, any source that emits one or more pollutants that require refined modeling must be included in that refined modeling.

Results from this phase can also be used to define the boundaries of the modeling domain for later phases of the study. The screening results show the maximum downwind concentration at any distance from the sources. The concentrations for each pollutant can be examined and compared with background concentrations (see section 4.1) and ambient air quality standards to determine the maximum distance of interest for each pollutant. The maximum of all of the maximum distances is then the starting point for defining the modeling domain for the refined modeling phase. This modeling domain may be expanded if required due to the location of receptors of interest (see section 1.3.4).

1.2.3 Refined Model Phase

This phase consists of several activities, some of which may be performed simultaneously. Activities include identifying the model to be used, determining the data that are needed by that model, gathering the data and preparing inputs to the model, executing the model, and analyzing results.

Start with identifying the pollutants of concern. These are all of the pollutants that are emitted from the sources other than those that have been eliminated via de minimus emissions in the scoping phase or by showing concentrations below levels of concern in the screening model phase.

Next, identify all sources that emit each pollutant of concern. Determine the type for each source. Select a refined model capable of simulating these types of sources. Gather sufficient data on each source to be able to calculate its emissions and model their fate and transport with the selected refined model (see sections 2.2.2, 2.2.4, and 2.2.5). If the model does not sum the concentrations from each source at each receptor, then you will need a post-processing tool to perform this task.

Work with the competent authority to identify large, nearby sources of the same pollutants. Gather all data required to model them as well.

Identify and gather other data required by the selected model. These include terrain features and possibly a digital elevation model (DEM) of the modeling domain, meteorology data for one or more surface and upper air stations, land use and land cover data, and ambient concentrations. Calculate relevant background concentrations for each pollutant of concern (see section 4.1). Define your receptor grid and any additional receptors of concern (see section 1.3.4).

Prepare all data and input files required by the selected model. Many models include one or more preprocessors to help get the data into the correct format. If you do not have experience with operating the selected model on your modeling computer, be certain that you execute any test data or scenarios included with the model; examine results for agreement with published values to show that the model is correctly installed and operating as expected.

Execute the model, which may actually be a series of computer programs. Carefully examine any message or log files produced by the programs. Fix problems found until you perform an execution without any errors and you can explain all warnings as not affecting results.

Then, carefully examine and analyze model output. This step may involve using mapping or charting software, a spreadsheet package, or post-processing tools to extract results from output files and present model predictions in a useful format. This step may identify problems with input data (e.g., missing values, data in wrong units, misplaced sources or receptors), in which case you may need to correct problems, execute the model with the updated input data, and analyze the new output. Use a versioning system to track versions of input data and match your input data with your output results.

1.2.4 Presentation of Results

Prepare your results for presentation to the competent authority. This presentation should include (1) the summary of findings from your scoping and screening phases including chemicals and sources that were screened out from further study, (2) the modeling domain and receptor locations, (3) all sources and their characteristics, (4) chemicals being modeled and relevant air quality standards, (5) overview of models that were used and justification of their selection, (6) summary of quality assurance steps during the modeling process, and (7) results produced by the models.

Results should be presented as both tables and graphics, including isopleths charts and maps of concentration showing receptors of concern. Each pollutant must be presented separately. If both deposition and concentration are of concern, then they need to be presented separately. Results may need to be presented separately for each major emission source of each chemical; this is expected to be a requirement if the total concentration (i.e., modeled concentration plus background concentration) exceeds or is close to any applicable air quality standard. If neighboring sources are included for some chemicals, then modeling results must be presented for the proposed sources, the sum of proposed and neighboring sources, and totals that include background concentrations.

If any predicted total concentration is close to or exceeding any applicable ambient air quality standard, then the competent authority may require additional modeling. Work may need to be done to reduce uncertainty in the modeling results, for example by gathering additional site-specific data. Or control strategies may need to be tested to determine if control procedures, control equipment, or process changes may be required.

1.2.5 Final Report

When all modeling has been performed to the satisfaction of the competent authority, the final report needs to be produced. This report documents the entire modeling process, including sources of data and processing steps, assumptions and estimates, problems found and how they were addressed with quality assurance procedures, and results of the study. The report should contain sufficient detail to enable the study to be replicated in the future.

1.3 Types of Data Required

Many types of data are required for an air quality modeling study. General classes of data are included here. Specific data elements are determined by the types of emission sources and models selected for the study.

1.3.1 Emissions

Air quality models typically do not calculate emissions for sources. Instead, the modeler must calculate the emissions prior to executing the air quality model and then provide those emissions in an input file. The modeler may use a source model, a spreadsheet, or some other method to calculate emissions from a source. The calculated emissions must meet the air quality model's requirements for format, time period and frequency, flux or mass, chemical species, and units of measure. Some models allow time-varying emissions and others require only one, constant value.

Note that some models compute dispersion for only one pollutant at a time, while others can handle multiple pollutants simultaneously. If the pollutants are chemically active in the atmosphere and you have a model that simulates the chemical processes, then you may need to specify the emissions in terms of chemical mechanism species instead of explicit chemicals.

Emissions of primary particles (i.e., particles that are not formed by secondary processes after they are emitted) require additional data. The unit of measure is mass per volume – typically $\mu g/m^3$. Emissions may need to be specified for preset size ranges or the modeler may be able to enter the number of size bins with the cutoff point in aerodynamic diameter and emission rate for each bin.

Document how the emissions are calculated. Include equations if the calculations are not performed using a standard model. Other important information to provide to the competent authority includes the phase of the project in which the emissions will occur (e.g., demolition, construction, or operation), operating schedule, and whether the emissions are calculated using permitted limits or expected actual emissions.

1.3.2 Source Location

The location must be known for each source and receptor. Depending upon the needs of the selected model, the location of the property boundary and of large buildings in the vicinity of any source may be needed.

The locations should be shown on a map that includes spatial coordinates. Elevations for topography may be shown on the same map or on another map as needed for clarity. The locations then must be translated into the form required by the selected model. Examples of coordinate systems are shown below.

- Model's coordinate system – The largest (or only) source is the origin and each other physical entity is specified as distance and direction from that point.
- Geographic coordinates – Some models use latitude and longitude with decimal degrees as the unit of measure. Note that some models use negative values of longitude for the Western hemisphere.
- Projected coordinates – Some models use one map projection for a simulation, where the projection is specified in terms of a projection family and associated parameter values, a datum, a spheroid definition for the Earth, and a point of origin. All locations are then specified as distances from the origin in the x- and y-directions where the unit of measure is typically meters.
- Grid coordinates – Some models view all or a portion of the Earth as a set of grids composed of uniform, square grid cells. These models typically use a projection but then have an origin for a grid. Locations are then specified as (x,y) pairs of (grid cell column number, grid cell row number) where the origin of the grid is its lower left corner.

If locations are specified using something other than geographic coordinates, then each location should be listed using both geographic coordinates and the coordinate system used in the simulation (e.g., provide latitude and longitude as well as direction and distance if polar coordinates are used). Also, a reference map needs to be created showing how the coordinates used in the simulation align with geographic coordinates. Both sets of coordinates and the reference map need to be included in the reports submitted to the competent authority.

1.3.3 Modeling Domain

Air quality models require data on the region, which is the entire modeling domain. The modeling domain encompasses all of the sources and receptors. The size of the modeling domain depends upon the types of sources, mass of emissions, type of pollutants being emitted (i.e., toxics may need to be modeled for longer distances due to concern of effects at lower concentrations), and the models being used in the modeling study.

Carefully examine your selected air quality models and their preprocessors to determine both the required data elements and their formats. For example, relatively simple models may need to know only if the modeling domain is urban or rural, and possibly if it is flat or complex terrain. In this context, “complex” means that some point in the modeling domain is at a higher altitude than the tallest emissions source, which is usually a stack for a point source. More complex models require more detailed information on the modeling domain, including a digital elevation model (DEM), land cover, land use, and borders of large bodies of water.

Some of the regional data inform placement of receptors. If your emission sources are in a coastal area, you may not want to place receptors uniformly in all directions because you may need to analyze concentrations further inland than off-shore. A map of schools and hospitals, for example, can help you place discrete receptors throughout the modeling domain to capture impacts to sensitive subpopulations.

1.3.4 Receptors

A receptor is a specific location in the modeling domain where the model needs to provide results (i.e., concentration, deposition). Depending upon the purpose of the modeling study, some or all of the following types of receptors may be appropriate.

- General receptors – These are receptors that are placed regularly throughout the modeling domain. The distance between receptors should allow graphics or mapping software to characterize gradients of concentration or deposition. Receptors are typically spaced closer together near to the sources and further apart at longer distances. They may be specified using polar coordinates or a Cartesian grid.
- Fenceline receptors – If the modeling study needs to determine the highest concentration outside a boundary or fenceline, then place receptors at equal distances along that boundary.
- Sensitive receptors – A discrete receptor should be placed at each location with a known sensitive receptor (e.g., building air intakes, school, playground, hospital, and sensitive ecosystem).
- On-site receptors – Depending upon the purpose of the study, you may not want to report modeling results for receptors located within a boundary or fenceline; do not calculate results within that boundary or fenceline, or remove those locations and results from the analysis in a post-processing step. Note that the results should not be set to zero because that would be incorrect and would probably cause problems with your graphics or mapping software. If you cannot remove those locations and values from your results, then change the values to equal the value at the nearest fenceline receptor.

The identity and location of each receptor need to be included in the project documentation for the competent authority. Provide a reason if any receptors are removed or their results changed in a post-processing step.

1.3.5 Meteorology

Some simple screening models use preset stability classes and wind speeds to obtain the maximum concentration overall and the maximum concentration at specific distances downwind from an emissions source. Refined models, however, use at least wind speed and direction for dispersion calculations. Many models use numerous parameters from two sources of meteorology data – surface station and upper air station.

These data need to represent the spatial and climatological (temporal) aspects of the site and have the ability to characterize the transport and dispersion conditions in the modeling domain. The representativeness of the data is dependent on: (1) the proximity of the meteorological monitoring site to the modeling domain, (2) the complexity of the terrain, (3) the exposure of the meteorological monitoring site, and (4) the time period during which the data were collected. Representativeness should be

viewed in terms of the appropriateness of the data for constructing realistic boundary layer profiles and three-dimensional meteorological fields.

Where surface characteristics vary significantly over the modeling domain, the emphasis in assessing representativeness should be given to adequate characterization of transport and dispersion between the emission sources and the locations where maximum concentrations are anticipated to occur. Surface characteristics in the vicinity of the surface station should be similar to those that generally describe the modeling domain. Also, surface characteristics input to any meteorological model or preprocessor associated with the air quality model should be based on the topographic conditions in the vicinity of the surface station.

If site-specific data are available then they should be examined carefully for use in the modeling study. Spatial or geographical representativeness is best achieved by collection of the data in close proximity to the site of the emissions sources. However, collection of meteorological data on a source's property does not of itself guarantee adequate representativeness.

Only instrumentation appropriate for air quality modeling should be used; that is, the instrument specifications must include appropriate sensitivity and threshold levels. All equipment must have been sited such that the data collected are free from inappropriate local or microscale influences. Quality assurance procedures must have been followed to make certain that the instrumentation was in good working order and only high quality data are used in the study. Site-specific data should be reduced to hourly averages except turbulence data that are used to determine the Pasquill-Gifford stability class, which requires 15-minute averaging time.

The period of data should be adequate to ensure that worst-case meteorological conditions are adequately represented in the model results. If possible, all meteorological conditions for the modeling domain should be adequately represented in the data set. If the current air quality modeling study is for an emissions source that was previously modeled, and if that source's emission limitations were based on a specific year of meteorological data, then that year should be added to any longer period being used for the current study.

1.3.6 Ambient Air Monitoring Data

Ambient measurements of concentrations for specific pollutants have a variety of uses depending upon the type of modeling study. Although this discussion focuses on concentration measurements, deposition (wet or dry) measurements can be used in a similar manner.

- **Attainment** – Monitoring data reveal whether or not a location is in attainment for the relevant ambient air quality standard. If a location is not in attainment and that location will be impacted by emissions of that pollutant for a new source, then you immediately know that there are problems to address.
- **Background concentration** – Most air quality models calculate concentrations for the sources included in a simulation. Ambient concentrations, however, must be compared with ambient standards and not just the concentrations due to the sources included in a simulation. Therefore, the background concentration must be determined from one or more appropriately sited ambient monitors for the relevant pollutants.
- **Trend analysis** – Monitoring data reveal how ambient concentrations of the monitored pollutant are changing over time. If the monitored trend of concentration of a pollutant for a new source is increasing, then you may need to use a concentration higher than the current ambient concentration for the background value.
- **Chemistry** – A few models perform simplified chemistry when certain pollutants are being modeled. These may require the ambient concentration of one or more additional pollutants that participate in the chemical mechanism.
- **Source apportionment** – Speciated monitoring data are required for source apportionment calculations. These are typically performed using either speciated hydrocarbons or speciated particulate matter ($PM_{2.5}$ or PM_{10}).
- **Model validation** – Ambient monitoring data are used when validating performance of an air quality model. Model validation techniques are beyond the scope of this document.

2.0 Types of Air Quality Models

Air quality models can be classified by mathematical formulation or by objective. One formulation can meet more than one objective, just as one objective can be addressed with more than one formulation. This section discusses mathematical formulations and modeling objectives. Specific models are discussed later in section 5.0.

2.1 Mathematical Formulations

Each mathematical formulation has inherent assumptions, advantages, limitations, and requirements for its implementation. This section presents information to help you select the formulation most appropriate to the requirements of your modeling study.

2.1.1 Empirical or Statistical

An empirical model is an application of mathematics to a series of related data values for the purpose of establishing a relationship among dependent and independent variables. Various types of relationships (e.g., linear, exponential, logarithmic) can be tested to fit the data set. Statistics are applied to determine the values of parameters required for the specific formulation, as well as to estimate how well the resulting equation fits the data (i.e., goodness-of-fit).

Empirical models should be used with caution. They may be considered valid only within the range of the data from which they were derived. That is, interpolation between data values is acceptable, but extrapolation to a set of conditions outside the range of data may yield invalid results. One example is when an equation predicting concentration of a neutrally-buoyant chemical at a location downwind from a source is derived from a set of measurement data from a field study. The equation may provide the best fit of the equation to the data, which were measured in an unstable atmosphere (e.g., hot afternoon with bright sun) in an open, flat field with a particular range of wind speeds. The equation may be used to predict concentration of a similar chemical released in a similar location under similar physical circumstances. However, the equation would not be expected to give reasonable results in mountainous terrain, in the winter, at night, in a coastal region, or for a chemical that is not neutrally-buoyant (e.g., gas with density greater than air).

Also, empirical models are based on mathematics instead of physical science. That is, the relationships developed within the data set may not have connections to principles of physics, chemistry, biology, or other physical sciences. These types of models, therefore, cannot be used to draw conclusions of how processes work in the underlying physical system.

2.1.2 Gaussian

Gaussian models have the assumption of normality inherent in their formulation. For example, the distribution of wind direction is described as a Gaussian (standard normal) distribution described by a mean direction and a standard deviation from the mean direction. Additional assumptions include (1) the standard deviation of concentration in the along wind direction is 0 (no diffusion in the direction of plume travel), (2) the wind speed is constant, (3) the standard deviation of concentration within the plume in the crosswind direction is equal to the standard deviation in wind direction at the distance downwind from the source, (4) the standard deviation of concentration in the vertical direction is determined by atmospheric stability and distance downwind from the source, and (5) the duration of constant release is equal to or greater than the travel time from the source to the location of interest.

Gaussian models may be expanded in several ways. The surface of the Earth can be a perfect reflector such that any mass from the plume that touches the surface is reflected back up into the plume. Similarly, an elevated inversion layer in the atmosphere can be a perfect reflector. Some models allow a low level inversion layer below the release height of the pollutant to be a perfect reflector, trapping the plume above the ground. When the low level inversion layer breaks down after sunrise, then the plume is allowed to mix down to ground level in a process known as fumigation.

Also, Gaussian models are not limited to the plume paradigm. Some models have the source emit a series of puffs. Each puff has Gaussian characteristics as it disperses and travels downwind, but now all puffs are forced to travel in the same direction. This allows the model to use varying wind speed and direction within a Gaussian construct. In this type of model, the concentration at a specific point cannot be directly calculated as in the plume model. Instead, the concentration at that point

must be calculated for each puff impacting that point at the specified time; these concentrations are then summed to obtain the total predicted concentration.

Note that Gaussian models do not allow the mass within the plume to interact with the mass through which the plume (or puff) is traveling. Therefore, the only chemistry supported by a Gaussian model is first-order transformation.

It is possible, however, to compute deposition within a Gaussian model. If the model is designed to provide conservative estimates of concentration, then the deposited mass is not removed from the plume. In this type of construct the deposition and concentration may be calculated independently (i.e., in separate model executions).

Steady-state Gaussian plume models should not be applied at distances greater than can be accommodated by the steady-state assumptions inherent in such models. This limitation is generally considered to be 50 km. Long-range transport models should be used beyond this distance if a refined model is needed.

2.1.3 Lagrangian

Lagrangian models do not utilize the steady-state assumption. Instead, they are built on probability distributions for wind speed and direction. Therefore, they can support constant, time-varying, and intermittent emission sources. Lagrangian models require more computational resources (i.e., computer memory, CPU speed, and disk storage) than Gaussian models.

Two paradigms of Lagrangian models are particle and puff. In a particle model each particle is separately emitted from the emission source and separately moved throughout the modeling domain based on the probability of wind speed and direction. Each emitted particle may represent the same amount of mass when it is emitted, so more particles are emitted for higher emission rates and fewer particles for smaller emission rates. Deposition can be accommodated by changing the mass represented by a specific particle.

In a puff model each puff is emitted from the source with an initial length, width, and height and containing a specified number of particles, each of which represents the same amount of mass when it is emitted. The particles within the puff are separately moved based on the probability of wind speed and direction, but retain their identity within the same puff. Therefore, the puff changes shape as it moves throughout the modeling domain. A puff may be split into multiple puffs due to impaction with terrain features or buildings. Puffs that occupy the same space may be joined into one puff. Deposition can be accommodated by removing particles from puffs that impact the ground.

Lagrangian models also support four-dimensional wind fields, where the wind speed and direction vary throughout the horizontal extent and vertical layers of the modeling domain and over time. The modeling domain is divided into grid cells for the purpose of meteorology. As individual particles travel through the modeling domain they are moved either by the vector of the grid in which they are located or by an interpolated vector calculated from the adjacent grid cells.

Neither the particle nor the puff paradigm allows the emissions being transported to truly interact with the ambient atmosphere. Therefore, Lagrangian models do not support full atmospheric chemistry.

Long-range transport models (e.g., models for distances beyond approximately 50 km) are typically built using Lagrangian principles. Example applications include illustrating the movement of power plant plumes through mountain ranges and valleys and showing the movement of plumes from volcanic eruptions.

2.1.4 Eulerian

Eulerian models are typically used for urban-to-global scale air quality modeling studies and employ five-dimensional data sets. The modeling domain is divided into three-dimensional grid cells, each of which is homogeneous (e.g., a well-mixed reactor). Pollutants are advected between grid cells in the x- and y- directions (horizontal) and the z-direction (vertical), which are the first three dimensions. The fourth dimension is time and the fifth dimension is chemical species.

All relevant chemical species are included in the model in the form of a chemical mechanism. Therefore, Eulerian models are well-suited for full atmospheric chemistry. Some species are handled explicitly in the chemical mechanism, but most species are simulated using species unique to the chemical mechanism. For example, formaldehyde may be modeled explicitly, but higher

aldehydes may be lumped together into one model species. Similarly, methane and ethane may be modeled explicitly, but higher alkanes may be divided into pseudospecies in the chemical mechanism, where each mechanism species represents a functional part of the alkane. Eulerian air quality models typically allow the modeler to select which chemical mechanism to use for the specific study among several mechanisms supported by the model.

Output time steps are typically one hour, although the computational time steps within the model are based upon the requirements of the simulation and may be as small as a few seconds. For example, if the first layer of the atmosphere is very small due to concerns about effects of processes very close to the ground, such as winds moving in a different direction along mountain slopes, then the time step for the advective solver is smaller to support numerical stability in the solution. Similarly, if some chemical species have very fast reaction rates then the time step for the chemical solver is smaller.

Within each grid cell, at each time step fresh emissions are added to the cell, mass is deposited to the ground due to wet deposition (if it is precipitating at that location and time) and dry deposition, the mix of chemicals are reacting, and mass is horizontally and vertically advected. The cell-based approach causes a few difficulties. First, because the mass emitted to a cell is immediately well-mixed throughout the cell, effects of large emissions at a point are muted in the chemistry. Also, emissions may be moved to other grid cells very quickly even if their emission point was at the opposite end of the cell. Considerable research has been devoted to methods of reducing numerical diffusion caused by three-dimensional vectors moving mass between block-shaped cells.

These effects can be reduced by using small grid cells, but at high computational cost. Reducing the length of a side of the grid cell by a factor of 4 results in increasing computation time by a factor of 16 (4^2). Also, the vertical dimension may need to be reduced, further increasing the computation time. Constructs such as nested grids allow the modeler to put more computational effort into subregions of concern without increasing the cost throughout the modeling domain.

The time required to execute the model is, therefore, related to the size of the grid cells, number of grid cells, number of chemical species, and relative reaction times, as well as the requirements of other processes. The modeler, therefore, must balance the need for spatial resolution and explicit treatment of chemicals against computational costs as measured in computing time and data storage needs. Eulerian models are typically executed in high performance computing environments that employ multi-processor computers (parallel-processors) and possibly vector or shared memory capabilities.

Eulerian models also require a vast amount of data, which spawns the need for numerous related models and pre- and post-processors. Eulerian models are, however, customarily used to investigate air quality issues related to tropospheric ozone, $PM_{2.5}$ formation, secondary organic aerosols, and visibility.

2.1.5 Hybrid

A hybrid approach combines two or more of the other mathematical types of models. Two examples are the Lagrangian-Gaussian and the plume-in-grid approaches. In both examples the reason for combining approaches is to reduce overall computing cost while attaining improved results over using just one approach.

The Lagrangian-Gaussian hybrid starts as a Lagrangian model. This gives a more detailed solution close to the source than a steady-state Gaussian plume model. However, the computational cost increases with the number of particles that need to be tracked throughout the modeling domain. Therefore, when the particles are very old and far from the source, they are tested to determine if they can be approximated by a Gaussian distribution. If so, then a Gaussian construct is substituted and the number of particles being tracked is reduced.

The plume-in-grid approach addresses the problem of immediate dilution from a point emission source to the well-mixed grid cell. This approach has been used primarily for large power plant plumes from coal-fired electric generating units (EGUs). The EGU plume is very rich in NO_x, which has a large effect on atmospheric chemistry. Reducing the size of all grid cells in the modeling domain is too expensive. The plume-in-grid superimposes a plume model onto the Eulerian model. A reactive plume is emitted from the large point source and is simulated as a series of layers. The outermost layer can entrain ambient air, where the NO_x reacts with the other chemical species. As the plume advects, reacts, and disperses it grows in size. When the width of the plume approximates the size of the grid cells through which it is traversing, the plume effectively ceases to exist and its mass is added to the appropriate grid cells.

2.2 Objectives of Models

Many models have been built to meet specific modeling objectives. Therefore, it is important to select a model that meets the requirements of a specific air quality modeling study. This section discusses the types of models that are used most frequently. Examples of models that meet each of these objectives are also presented.

2.2.1 Screening

A screening model needs to quickly and easily estimate maximum downwind concentrations from an emissions source of nonreactive pollutants. The model must require less data than a more refined model. The results must be conservative; that is, the model must estimate higher concentrations than those estimated by a more refined model. Therefore, a screening model is typically a steady-state Gaussian plume model.

If the scoping phase of an air quality modeling study does not show a clear need for a refined model, then use a screening model to try to screen pollutants out from additional modeling. That is, if a screening model's maximum downwind concentration for one pollutant and for all emissions sources of that pollutant when added to the background concentration is substantially less than the ambient air quality standard, then refined modeling should not be required for that pollutant.

A screening model should be executed using a source's design capacity (i.e., 100% load), a higher load if the source may be able to operate at greater than design capacity, 75% load, and 50% load, and a range of operating conditions. The goal is to determine a set of conditions that cause the highest downwind concentration. If the pollutant is not screened out from further modeling, then the set of conditions that is determined to cause the highest concentration using the screening model must be used in addition to the design capacity in subsequent refined modeling.

Examples of screening models are:

- SCREEN3 – see section 5.1 for more details. This model is available from the U.S. EPA (www.epa.gov/scram001/dispersion_screening.htm#screen3).
- AERSCREEN – new screening model under development. When promulgated this model will be available from the U.S. EPA (www.epa.gov/scram001/dispersion_screening.htm#aerscreen).

2.2.2 Local Scale Modeling

Local scale modeling is usually performed for new or expanding industrial sources, large industrial facilities, large construction projects, and major road construction projects. This type of modeling is more refined than screening models.

Local scale models are customarily built using Gaussian principles. Supported types of sources include elevated point (e.g., stack, flare), area, volume, and line. If the model does not directly support a line source, it is simulated as a series of adjacent area sources (e.g., road).

Local scale models typically include effects of buildings close to sources on elevated plumes (i.e., building downwash). When modeling the effects of a building on concentration, determine the projected length, width, and height of the building for each wind direction. Either the user's guide or the technical reference manual for the model should provide details on these calculations for the specific model.

Local scale models should also calculate effective plume height, which changes during the simulation based on the difference between ambient temperature and the exit temperature from the stack. The temperature difference causes buoyant plume rise. Exit velocity causes plume rise due to momentum or stack tip downwash due to low exit velocity in high wind conditions.

Some local scale models simulate elevated area sources, elevated volume sources, or buoyant area sources. More specialized sources, such as horizontal jets, evaporative pools, and dense gas, are seldom supported by local scale models. Specialized models are required for these sources.

The local scale models output concentrations and/or deposition at receptor locations specified by the user. The model may allow the user to specify a grid of receptors (e.g., Cartesian grid, polar grid) or discrete receptor locations. A receptor that is placed above ground level is called a flagpole receptor. For further information on placing receptors, see section 1.3.4.

Reporting options include listing the top N values for each receptor (e.g., top 10 values), the maximum values for multiple time periods (e.g., hour, 3-hr average), and values for all receptors and all hours. Note that if the maximum values are output for all receptors, the time period associated with the maximum value will not be the same for all receptors due to hourly changes in wind speed and direction.

The modeler usually needs to extract the required values from the output for further analysis and reporting to the competent authority. Transfer tables of values to an appropriate graphics package that can show isopleths. The preferred output is isopleths of maximum concentrations for each pollutant on a diagram of the entire modeling domain to show maximum extent of impact. Also, provide a more detailed diagram showing isopleths close to the facility. Two versions of these diagrams should be created – with and without background values. If deposition is of concern, then also include diagrams of deposition for each pollutant of concern. If a method of emissions control may be considered for any source, then also include diagrams showing isopleths for just that source, as well as diagrams for all sources with and without background values.

All diagrams and tables of values are to be included in reports to the competent authority.

Examples of industrial source/facility models are:

- **AERMOD** – see section 5.2 for more details. This model is available from the U.S. EPA (www.epa.gov/ttn/scram/dispersion_prefrec.htm#aermod).
- **Industrial Source Complex (ISC)** – This model changed from a preferred model to an alternative model when AERMOD was promulgated, but is still available from the U.S. EPA (www.epa.gov/scram001/dispersion_alt.htm#isc3).
- **AUSPLUME** – This model from the Environmental Protection Authority of Victoria in Australia is derived from the original ISC model (1979). AUSPLUME is available from the Australia EPA Victoria (www.epa.vic.gov.au/air/epa/ausplume-pub391.asp). This model supports stack, area, and volume sources in flat terrain with simple winds (i.e., one wind direction in the entire modeling domain each hour).
- **AUSPUFF** – This non-steady-state Gaussian puff model is by Australia's Commonwealth Scientific and Industrial Research Organisation (CSIRO). AUSPUFF uses a three-dimensional meteorology data set.
- **Atmospheric Dispersion Modelling System (ADMS 4)** – This model from Cambridge Environmental Research Consultants (CERC) supports point, area, volume, line, and jet sources. For further information see www.cerc.co.uk/software/adms4.htm.
- **AirWare** – This is a large modeling system from Environmental Software and Services of Austria (www.ess.co.at/AIRWARE/product.html). Note that this modeling system runs the AERMOD model (above).

2.2.3 Source-Apportionment

The purpose of a source-apportionment model is to estimate the relative impact of specific types of sources at a designated location (i.e., a receptor). Also known as receptor models, chemical and physical characteristics of gases and particles that are measured at the source and receptor are used both to identify the presence of and to quantify source contributions to receptor concentrations. Because this type of model is typically based on linear algebra principles, this is a good example of a statistical model.

The primary assumption of source-apportionment models is that each type of source is associated with a unique combination of pollutants that are measured in the ambient air. This unique combination forms a fingerprint for that source type. Examples include gasoline evaporation, diesel truck exhaust, tanker engine exhaust, and painting. Therefore, the fingerprints that are used need to accurately represent their respective source types. If they don't (e.g., diesel fuel has a different sulfur content in the area where the model is applied), then the results of the model will be incorrect.

In addition to the source fingerprints, monitoring results are used for one ambient monitoring location. Note that the same pollutants that are used in characterizing the sources must be measured in the ambient air. For example, if five hydrocarbons and seven metals are required to distinguish several sources from each other, then the ambient measurements must include at least those same five hydrocarbons and seven metals.

Two cautions apply to source-apportionment models. First, speciated data are required for source-apportionment modeling; measurements of total mass for particles or total hydrocarbons are insufficient. Second, the species used in characterizing the

sources either should not participate in atmospheric chemistry or should have very long lifetimes in the atmosphere. That is, this method does not work well when the source characteristics vary with time in the atmosphere, which is equivalent to changing over distance, or when the pollutants involved react with other pollutants in the atmosphere.

A variety of source-apportionment models are available with differing data requirements. Some utilize a time series of ambient speciated data from one monitoring site. Others may include additional types of data, such as wind speed or wind direction. Also, some models are built using standardized libraries of statistical and computational functions, allowing those models to be free or very low cost. Other models are built using functions from or as add-on components to proprietary software packages, requiring additional expense and possibly training on the associated software. All of these factors should be considered when selecting a model for a study.

Examples of source-apportionment models are:

- **Chemical Mass Balance model (CMB)** – see section 5.3 for further information. This model is available free of charge from the U.S. EPA.
- **Unmix** – This model is another receptor model from the U.S. EPA and is available free of charge from www.epa.gov/heasd/products/unmix/unmix.htm. Its approach to source-apportionment is different from that in CMB.
- **Positive Matrix Factorization (PMF)** – This model has also been released from the U.S. EPA and is available free of charge from www.epa.gov/heasd/products/pmf/pmf.htm. This model is currently being enhanced to allow factors such as wind speed, wind direction, and weekday/weekend indicators.

2.2.4 Long-range Transport

Long-range transport models are used when receptors are over 50 km from the source or when the plume of a large facility travels through mountains and valleys. Gaussian-type models are not appropriate for these conditions. Lagrangian or Eulerian models may be suitable for these distances.

Examples of long-range transport models are:

- **CALPUFF** – see section 5.4 for further information. This model is available free of charge.
- **Lagrangian Atmospheric Dispersion Model (LADM)** – This is a Lagrangian particle model that uses synoptic scale meteorology to perform near-source and regional calculations in complex terrain. This model is considered too computer-intensive to simulate more than a few days. For further information see www.dar.sciro.au/ladm/index.html.

2.2.5 Regional Photochemical

If large amounts of pollutants that participate in atmospheric chemistry are to be emitted, then the potential effect on regional air quality should be examined using a photochemical model. Relevant pollutants of concern include tropospheric ozone and particulate matter, which includes PM_{10} and $PM_{2.5}$. Results of this modeling study can be directly compared to the appropriate ambient air quality standards because all relevant sources of pollution in the modeling domain are included in this type of model.

Applicable chemicals include volatile organic compounds (VOCs) (e.g., short-chain hydrocarbons, monocyclic aromatic compounds), chemicals containing either reduced or oxidized forms of nitrogen, and any other chemicals included in the model's chemical mechanism.

Due to the amount of data and modeling effort involved in implementing a regional photochemical model, one industrial facility is not expected to initiate this effort. However, if data and relevant model simulations are available for the region of concern, then a source emitting large quantities of relevant pollutants may be required to use these existing data with new information on the source to perform special simulations. If this is required, the competent authority will provide additional guidance.

Examples of regional photochemical models are:

- **Community Multiscale Air Quality Model (CMAQ)** – see section 5.5 for more information. This is an open source model being maintained under the auspices of the U.S. EPA. It is a community model in that members of the modeling community make enhancements to the model and provide those enhancements to the rest of the modeling community in a prescribed manner. This model has undergone extensive peer review and is considered to be state-of-the-science.

- **Comprehensive Air Quality Model with extensions (CAMx)** – This is an open source modeling system for the integrated assessment of gaseous and particulate air pollutants. For further information see www.camx.com/.
- **MUSE** – This is a multilayer dispersion model for reactive species in the local-to-regional scale from Aristotle University of Thessaloniki. MUSE requires the MEMO meteorological model. For further information see www.ess.co.at/ISIREMM/a53.html.
- **The Air Pollution Model (TAPM)** – This model is an Eulerian/Lagrangian model that takes its meteorology input from the Bureau of Meteorology Limited Area Prediction System. TAPM requires the Chemical Transport Module (CTM) for more complete chemical mechanism. For further information see www.cmar.csiro.au/research/tapm/index.html.

3.0 Types of Sources

Air quality models typically support one or more general types of sources. The user is responsible for calculating the emissions and describing the source. The air quality model then simulates the transport, transformation, and fate of those emissions.

Note that these same names for types of sources mean something different in the context of regional models vs. other types of air quality models. This section does not address terminology associated with regional models.

3.1 Point

A point source is a single emission source at a known location. Industrial stacks and flares are two examples of a point source. Each source usually emits multiple pollutants. The emission rate is specified in units of mass/unit time.

Characteristics of the source include its diameter (i.e., inside diameter from which the exiting emissions emerge) and the physical height above ground where the emissions exit to the atmosphere. Characteristics of the emissions are the pollutants and rate of emissions, exit temperature from the source, and exit velocity from the source. Point sources are assumed to have emissions exit in the “up” direction; if the emissions exit in a different direction then the source is considered to be a jet, not a point source.

The height to be modeled may be different from the height of the stack. Taller stacks disperse pollutants faster than shorter stacks. This means that the concentrations close to the stack are lower for taller stacks, but the mass and rate of pollutant being emitted are the same. For this reason, some older facilities built taller stacks than necessary, treating the additional height like a control device. Because the emissions were not reduced, some modeling studies must use the appropriate height (i.e., Good Engineering Practice [GEP] stack height) instead of the physical height of the stack.

The air quality model should use these data to calculate the effective stack height, which varies with temperature. The effective stack height may be higher or lower than the height of the stack. The effective stack height is increased from plume momentum, which is caused by a high exit velocity, and plume buoyancy, which is caused by an exit temperature greater than the ambient temperature at the height of the stack. The effective stack height may be decreased by stack-tip downwash, which is caused by the exit velocity being much less than the wind speed at the height of the stack.

If you have one or more sources that are elevated, have a substantial exit velocity, and are emitted at a temperature other than ambient, then select a model that appropriately calculates effective stack height.

3.2 Area

An area source is typically at ground level; many models do not simulate an elevated area source. Pollutants are emitted uniformly across the surface of the source. If one part of a source has a different emission rate, specified as mass/unit area/unit time, than another part then the source must be divided into multiple, uniform sources. Examples of area sources are landfills, parking lots, land being graded for construction, and treatment ponds or impoundments.

The source should be drawn on a map of the modeling domain, showing the actual boundaries of the source. Some models consider an area source to be a circle of the same surface area as that specified by the user with center point at the centroid of the area source. If there are receptors close to the area source, however, the concentration or deposition from a circular source

is not the same as that from a rectangular source of the same area; the wind traversing a rectangle has a different length of travel than that traversing a circle.

If the source is oddly shaped (i.e., cannot be sufficiently described as a rectangle at an orientation from North), then break it up into a series of adjacent rectangles. Note the shape requirements of your model; it may have a maximum length-to-width ratio.

Your air quality model may allow you to group these sources into one source for reporting purposes. If not, you need to sum their estimated concentrations at each receptor location as a post-processing step.

3.3 Volume

A volume source is similar to an area source, but with a nonzero thickness (i.e., minimum height and maximum height above ground level). Pollutants are emitted uniformly from the volume of the source. If one part of a source has a different emission rate, specified as mass/unit volume/unit time, than another part, then the source must be divided into multiple, uniform sources. Examples of volume sources are parking garages with open sides and a bank of exhaust fans from an industrial building.

3.4 Line

A line source is a source that has a uniform emission rate, specified as mass/unit length. Roads are the most common types of line sources. Some specialized models are available for traffic-induced air pollutant concentrations close to roads.

Very few air dispersion models explicitly simulate a line source. Instead, a line source is represented as a series of adjacent area sources. Refer to the documentation for your model to determine how you should handle road attributes such as multiple lanes, median, and shoulders. You may need to represent a bend in the road as appropriately-sized and oriented rectangles.

Air quality models rarely simulate roads on a grade (i.e., not flat), overpasses, or underpasses. If your modeling project has these needs, then you need to find a specialty model in consultation with the competent authority.

3.5 Mobile

Mobile sources are sources that move while emitting pollutants. Examples of mobile sources are automobiles, trucks, railroad locomotives, aircraft and ground support equipment, and ships. Emissions for one vehicle are specified in units of mass/unit distance traveled.

Air quality models do not attempt to simulate a moving source. Instead, the emissions from the moving source are allocated to the underlying fixed surface, such as the road on which the automobiles and trucks are moving; the road is then considered to be the source in the air quality model (see sections 3.2 and 3.4).

3.6 Biogenic

Biogenic sources are natural sources, including volcanoes and lightning. Barren land is commonly considered an area source that emits particulates as wind blows over it.

Vegetation is the most common type of biogenic source in air quality modeling. Although the presence and type of vegetation affects air movement on a local scale, it is seldom considered an emissions source on that scale. Emissions from vegetation are very important in regional air quality modeling studies because those chemicals are highly reactive in the atmosphere.

3.7 Chemically Reactive

If the pollutants emitted by a facility are chemically reactive in the atmosphere, then two types of modeling may be required. First, the emissions should be modeled using the same type of model as would be required if nonreactive chemicals were being emitted from that source. The results of this modeling reveal the expected area of impact and provide an estimate of the extent of the impact if the chemicals were nonreactive.

The results of this phase of the modeling study need to discuss the potential effects due to reactivity. These effects include formation and destruction of other chemicals already in the atmosphere at the area of impact, expected change in concentration of those chemicals, comparison of the changed concentration with applicable air quality standards, and atmospheric lifetime of the chemicals formed. If the atmospheric lifetime of the chemicals formed is greater than the distance that they are expected to travel within the expected area of impact, then any additional modeling would need to appropriately enlarge the modeling domain.

Depending upon the results of this nonreactive modeling phase, an additional phase may be required. This requires applying a regional photochemical model to a regional modeling domain. A pair of simulations needs to be performed. The first simulation must use all emissions in the modeling domain for all emission sources except the new emissions for the sources being studied. The second simulation uses all of the same inputs (e.g., emissions, meteorology, initial conditions, and boundary conditions) as the first, plus the new emissions. These two simulations are required because all of the pollutants in the atmosphere must be allowed to interact in the model; using just the new emissions would not produce appropriate results. The results of the two simulations are then compared (e.g., subtract concentrations throughout the modeling domain for the first simulation from those for the second simulation for each chemical species) to determine the effect of the new emissions on air quality.

The results of this modeling study need to include maps and discussions of the potential effect of the new emissions at time periods of interest. Location and values of the maximum change in concentration need to be shown, as well as comparisons of the change in concentration at the locations of high concentrations before adding the new emissions. The time periods of interest include hourly maximum and may also include annual, seasonal, or other periods depending upon the pollutants of concern.

3.8 Special Types

Some types of sources require specialized model formulations. These types are typically part of accident release scenarios, which are emissions of short duration. Examples include jet (e.g., failure of a valve on a high-pressure pipe), tank rupture, denser than air gas, buoyant (i.e., emitted gas is lighter than air and rises to an altitude of neutral buoyancy) and evaporative (i.e., spill of volatile liquid, where emission rate changes as the liquid evaporates over time).

Specialized models should be selected in consultation with the competent authority.

4.0 Special Considerations

Many factors are considered when designing an air quality modeling study. In addition to the types of sources, pollutants, and regional characteristics to be modeled, you need to decide whether or not certain other factors are important. For example, one emission source may have large buildings nearby, so when that source is included in a study the model needs to estimate effects of those buildings on downwind concentrations. Similarly, if a pollutant of concern has an ambient air quality standard, then you need to determine the ambient air concentration of that pollutant when the proposed sources are not operating.

4.1 Background Concentration

Background concentrations are an essential part of the total air quality concentration to be considered in determining source impacts. Background air quality includes pollutant concentrations due to natural sources, nearby sources other than the one currently being modeled, and unidentified sources. Simply stated, for a local air quality modeling study the background concentration of a pollutant is the ambient concentration of that pollutant when the source being modeled is not operating and all other sources are operating. Therefore, the background concentration may be added to the modeled concentration at each receptor location to determine the expected total concentration of that pollutant at that location. This total concentration may then be compared to the applicable air quality standard to determine if the locations of the receptors may be expected to be within air quality guidelines when the source being modeled is emitting the pollutant.

If there are other sources of the same pollutants that are not operating for the time period when the background measurements were made, then those sources must also be modeled. This discussion is applicable for other sources under construction. If sources that are operating are undergoing expansion that will affect the ambient concentration of the same pollutants, then the additional emissions due to the expansion must also be modeled. Also, if other sources were operating at reduced capacity or

on a reduced schedule, then the additional emissions that were not being emitted must be calculated and modeled. All of these sources and their parameters should be identified and modeled in consultation with the competent authority.

For a regional modeling study the background concentration is the ambient concentration measured upwind of each lateral boundary of the modeling domain. For example, when the wind is blowing from the North the ambient concentration just to the North of the northern boundary of the modeling domain is the background concentration for that boundary. These background concentrations are then treated as the boundary conditions for the regional model. Alternatively, and especially for pollutants treated as lumped species in a chemical mechanism in the regional air quality model, the boundary conditions can be extracted from a model with similar capabilities that has been previously executed for a larger modeling domain but the same time period, meteorology, and emissions. In this case the boundary conditions can be set for each time period of the model (usually hourly).

Note that “clean conditions” have lower values than a background concentration. Clean conditions may be determined in an area not impacted by any obvious sources (e.g., away from any city or industrial activity).

4.2 Stack Parameters

The stack height and inside diameter, gas exit temperature, and volume flow rate or exit gas velocity need to be determined for operation at 100, 75, and 50 percent load for each stack. Some models require additional data including the elevation at the base of the stack.

Note that the physical height of the stack may not be the stack height required by the model or for the modeling study. Most models calculate the effective stack height using exit velocity for plume rise due to momentum, the difference between stack exit temperature and ambient temperature for buoyant plume rise, and the ratio of exit velocity to wind speed for stack tip downwash. Some models, however, require the modeler to calculate the final height of the plume centerline and, possibly, the distance downwind from the stack to final plume height. These calculations must be shared with the competent authority and included in the project’s report.

4.3 Buildings

A building that is close to a point source’s stack may affect the dispersion of the emissions from that stack. This effect, which is known as building downwash or building-induced dispersion, alters the concentration and deposition values downwind of the affected stack. Note that a building that is either upwind or downwind of a stack may cause these effects.

Refined models should include building effects in their dispersion calculations. To prepare the data required by the model, start with a map showing all point sources and buildings close to them. Obtain the dimensions of each building. Check the model’s documentation to determine which buildings need to be included and how to provide the relevant data on each building. For example, you may need to designate all buildings affecting each source, the building’s dimensions (length, width, and height), and the distance from the stack to the building. A model may require you to enter the building dimensions for each of a set of predefined wind directions, in which case the length is the length of the building in the alongwind direction and the width is the width of the building in the crosswind direction. The model may also specify the point on the building to which you need to specify the distance from the stack and how to specify the distance (e.g., distance in North-South and in East-West directions to the nearest corner of the building).

4.4 Averaging Times

The averaging times used in a modeling study need to match those of relevant air quality standards. In general, air quality models provide output on an hourly basis. Some also provide maximum hourly for a year, top N values (e.g., top 10 hourly averages) for a year, or annual hourly average. If the model that you are using does not provide results for the specific time period that you need, then you can transfer the hourly results to a spreadsheet for post-processing. Provide documentation of these calculations with the documentation of your modeling study.

Air quality models generally do not provide output for time periods less than one hour. For acute exposure averaging time (e.g., 3-minute average concentration) you need to convert from the 1-hour average values to the required time period. Provide documentation of these calculations with the documentation of your modeling study.

4.5 Terrain

Air quality models generally consider three general classifications of terrain.

- **Flat** – No elevations are considered. This is equivalent to having the entire modeling domain located at the elevation of mean sea level. The terrain does not affect the concentration or deposition associated with the plume.
- **Simple** – No elevation in the modeling domain is above the height of the shortest stack. The terrain may have a limited effect on the plume's behavior.
- **Complex** – At least one location in the modeling domain has an elevation higher than at least one stack. The plume is expected to impact the terrain (i.e., plume impaction) and may have the highest ground-level concentration at that location. The plume may split into two or more smaller plumes as it meanders through the terrain.

The type of terrain both at the source and throughout the modeling domain must be considered when selecting a model. For example, a model that is designed for flat terrain is not able to appropriately simulate movement of pollutants in the atmosphere above complex terrain. On the other hand, a model that is designed for complex terrain may be used for flat terrain.

4.6 Receptors

Receptors must be placed appropriately to answer the questions posed by the modeling study. A screening model may not use receptors per se; it provides a distance from the source to a maximum concentration downwind along the plume centerline, or a maximum concentration at specific distances downwind along the plume centerline. A regional model may provide concentrations within each grid cell in the modeling domain, so the value at a receptor is either the value for the grid cell that contains the receptor or is interpolated from the values at the centroids of the containing and adjacent grid cells.

When modeling an industrial source or a facility, a regular grid of receptors is superimposed on the modeling domain. The receptors may be specified as either a Cartesian grid or a polar grid. Because concentrations of a pollutant being dispersed generally are higher at smaller distances from the source, more receptors are typically placed closer to the source and fewer are placed further away. This placement helps to show the relative concentration gradients throughout the modeling domain. Define a polar grid by placing its origin at the centroid of the largest emission source. Specify 36 directions (i.e., at 10-degree increments) and radii at increasing distance from the origin (e.g., at 50-m increments to 500-m, then at 100-m increments, etc. until at 1-km increments far from the source).

Additional, discrete receptors need to be placed at points of concern. For example, placement of receptors along the facility's property line (i.e., fenceline receptors) will identify the highest concentration leaving the facility's property. Other receptors may be placed at potentially sensitive receptors, such as schools, hospitals, nursing homes, and large apartment complexes. An elevated receptor (i.e., flagpole receptor) may be placed at the location and altitude of air intakes to buildings close to the source.

Note that using regular grids may put receptors at inappropriate locations. Therefore, placement of the receptors should be viewed on a map of the modeling domain at an appropriate scale to see their placement with respect to major buildings or bodies of water. It may not be reasonable to report concentrations at a location appearing to be within or adjacent to a large building (e.g., hotel complex); unless the model adequately simulates concentrations within the wakes and eddies formed by a building, such concentrations would be misleading and erroneous. Similarly, receptors located within the fenceline of the facility may be inappropriate for the study. Values computed at these types of locations may need to be removed prior to performing the final analysis, but their original placement and reason for removal need to be included in the project's documentation.

4.7 Meteorology Data

The list of required parameters is determined by the models in the modeling study.

For local-scale models, site-specific meteorology data are preferred. Large industrial facilities frequently have on-site surface meteorology stations that automatically measure and record wind speed and direction, temperature, humidity, and other data. Before these data may be used for a modeling study, they must have passed rigorous quality assurance procedures and routine equipment inspection equivalent to requirements imposed by the appropriate certifying authority. The data need to be on at least an hourly basis and for a period of at least one year.

If such site-specific meteorology data are not available, then data from the closest certified surface station that is representative of the conditions at the site should be used. A station is representative of the site if similar conditions exist at both locations (e.g., land use, land cover, topography, coastal or inland). Sometimes the most representative station is not the one closest to the site. Five years of data are preferred. In addition to surface data, upper air data for the same time period as the surface data may be required by the model.

When a large region is being modeled, identify all sources of appropriately quality-assured meteorological data that are available and applicable. Large modeling domains typically require more than one surface station to adequately characterize the wind field, but the data from all stations must be for the same time period. Also, the selected air quality model must be capable of utilizing data from more than one station; this capability requires either a compatible meteorology model or a preprocessor for the air quality model.

4.8 Large, Adjacent Sources

If the study utilizes an industrial source/facility model and if there is one or more large sources of the same pollutants of concern located nearby such that their modeling domains overlap yours, then those nearby sources should be included in the modeling study. This poses challenges that need to be addressed: obtaining the required data for the other sources, and calculating appropriate background concentrations.

To successfully model the other sources you need the same data for them as for your own. These include information required to calculate emissions, characteristics of each emissions source, location and dimensions of each large building close to any source, and detailed topography. If the competent authority has a copy of the modeling work performed for those sources for the same pollutants as you are modeling, then you may be able to get access to those data. However, emissions included in their modeling study may not be the same as what they currently emit. Also, if the modeling results for your facility indicate that your emissions plus background are close to one or more air quality standards, then you may need to model the maximum permitted emissions instead of reported or previously modeled emissions.

Obtaining appropriate background concentrations is also more difficult if those sources operate during the time period covered by the ambient monitoring data. The background concentration needs to include all sources except those of your modeling study (see section 4.1). If you are modeling emissions that will occur in the future, then they are not in the ambient measurements that represent background concentrations. But, if the other sources have been operating, then you need to make certain that the ambient measurements you use are all upwind of those sources or were made when those sources were shut down.

Also, the report of this study needs to document all calculations and assumptions related to these sources. All modeling results need to clearly indicate effects of emissions from your sources, effects of emissions from these other sources, and background concentrations.

5.0 Specific Models

This section provides some more detailed information on specific models that are used in regulatory applications in the U.S. and other countries. All of these models are available free of charge over the Internet.

5.1 SCREEN3

SCREEN3, which is available from www.epa.gov/scram001/dispersion_screening.htm#screen3, is the screening model for the Industrial Source Complex Model version 3 (ISC3), which has been replaced by the AERMOD modeling system. AERSCREEN, which is a new screening model for AERMOD, is currently in development. Its release will be announced at www.epa.gov/scram001/dispersion_screening.htm#aerscreen.

5.1.1 Purpose, Strength, and Weaknesses

SCREEN3 is a basic, Gaussian screening model. It is an MS-DOS application. On a computer running Microsoft Windows, SCREEN3 can be started either from a command window or by double-clicking on the SCREEN3.EXE program in a file browser.

SCREEN3 handles one source at a time. It uses a built-in set of meteorological conditions to determine the maximum concentration at downwind locations. For each distance it calculates the concentration and provides the atmospheric stability class, wind speed at 10 m above stack base, wind speed at stack height, mixing height, plume height, and dispersion parameters σ_y and σ_z. It also calculates the downwind distance for the maximum concentration and provides the atmospheric stability class, etc. for those conditions.

Concentrations are calculated for one-hour averaging time only. This model does not calculate wet or dry deposition.

5.1.2 Types of Sources

Point, Flare, Area, and Volume sources are supported.

5.1.3 Special Considerations

Some support is included for complex or simple terrain and for building downwash calculations.

5.1.4 Output

When you exit the program, it automatically saves its output to the file SCREEN.OUT in the program's directory. If you want to keep this output, you need to rename the file so it is not overwritten the next time the program is executed. It also saves a file SCREEN.DAT that contains your inputs. Although this file is in text format and can be read by any text editor, such as Notepad, the format of the information is cryptic.

If you want to make a slight modification to your inputs and run the model again, you can edit the SCREEN.DAT file. To execute SCREEN3 using the edited file for input, you need to open a command window, navigate to the directory containing SCREEN3.EXE and your input data file, and follow the instructions in the SCREEN3 Model User's Guide.

5.2 AERMOD

The AERMOD modeling system is the refined industrial source/facility model preferred by the U.S. EPA and available free of charge from www.epa.gov/ttn/scram/dispersion_prefrec.htm#aermod. The model includes the AERMET meteorology preprocessor, AERMAP terrain preprocessor for terrain that is not flat, AERSURFACE preprocessor for surface characteristics, and the AERMOD air dispersion model. The modeling system is distributed for a PC running Microsoft Windows, but the source code is available and has been successfully recompiled and executed under the Red Hat Linux operating system.

5.2.1 Purpose, Strength, and Weaknesses

The American Meteorological Society/Environmental Protection Agency Regulatory Model Improvement Committee (AERMIC) was formed to introduce state-of-the-art modeling concepts into air quality models from the U.S. EPA. Through AERMIC, the AERMOD modeling system was introduced that incorporated air dispersion based on planetary boundary layer (PBL) turbulence structure and scaling concepts, including treatment of both surface and elevated sources and both simple and complex terrain.

AERSURFACE is a tool that processes land cover data to determine the surface characteristics for use in AERMET.

AERMET ingests surface meteorological data, upper air soundings, and site-specific meteorological data. It then performs quality assurance tests on the data and reports problems found. The output file contains the hourly meteorology-related data for input to AERMOD.

AERMAP processes Digital Elevation Model (DEM) data and creates a file for use by AERMOD. This file contains elevation and hill height scaling factors for each receptor specified for the air quality modeling study.

AERMOD includes the Plume Rise Model Enhancements (PRIME) model for calculating the effects of near and far wakes of buildings close to a point source. This model also supports variable emission rates, multi-year operation, and short-term events. Specific hourly emissions may be provided for some or all sources in a simulation.

Multiple receptor grids, including both Cartesian and polar, may be specified for a single simulation. Discrete receptors, including flagpole receptors, may also be specified.

5.2.2 Types of Sources

Point, Area, and Volume sources are supported. Line sources may be simulated as either a series of adjacent volume sources or as elongated area sources.

Sources may also be grouped together in a single run. AERMOD then produces results for each group.

5.2.3 Special Considerations

This modeling system was extensively tested and underwent rigorous peer review prior to its promulgation by the U.S. EPA for regulatory work. The model itself and supporting documents are expected to continue to evolve to accommodate the best available science.

5.2.4 Output

AERMOD provides the standard types of output values expected for this type of model (e.g., high values by receptor, maximum N values, hourly values) for each receptor, averaging period, individual source, and source group as specified by the user. Results are available for concentration and deposition (wet and dry). These files are text files, which can be transferred to the user's preferred graphics software for creating isopleths.

Other output options are available for specific needs. One example is a file of all occurrences when a value equals or exceeds a user-specified threshold for averaging period and source group as specified by the user.

5.3 CMB8.2

The Chemical Mass Balance version 8.2 model is available free of charge from the US EPA (www.epa.gov/scram001/receptor_cmb.htm). CMB8.2 is provided as a 32-bit Microsoft Windows application.

The CMB receptor model consists of a solution to linear equations that express each receptor chemical concentration as a linear sum of products of source contributions and source profile abundances (i.e., the mass fraction of a chemical or other property in the emissions from each source type). The source profile abundances and the receptor concentrations, with appropriate uncertainty estimates, serve as input data to CMB. In order to distinguish among source type contributions, the measured chemical and physical characteristics must be such that they are present in different proportions in different source emissions and changes in these proportions between source and receptor are negligible or can be approximated. The CMB model calculates values for the contributions from each source and the uncertainties of those values.

5.3.1 Purpose, Strength, and Weaknesses

The CMB model is applicable to multi-species data sets, the most common of which are chemically characterized particulate matter (PM) and volatile organic compounds (VOC). CMB model results are used to determine to what extent different sources contribute to ambient concentrations. This information can be used with insights gained from dispersion models to justify emissions reduction strategies.

One or more ambient sampling locations may be used in a single analysis, although one location is typically the focus of this type of study. The user selects pollutant species, ambient monitoring data sets (i.e., one data set is one set of speciated data for one location, date, and time period), and source profiles.

Note that the source profiles must accurately represent the sources in the vicinity of the monitoring site. That is, a profile of evaporated gasoline from southern California in the U.S. probably does not accurate represent the local profile of evaporated gasoline. Therefore, a country- or region-specific profile may be needed for some source categories.

5.3.2 Types of Sources

This model does not simulate source emissions directly. However, any relevant category of source may be used for which a local emission point has relevant chemical species that may impact the monitoring site being studied.

5.3.3 Special Considerations

There are three important considerations when using this model. First, the profile of any source that is used in the modeling study must accurately represent the local profile of that type of source. Second, the person defining the simulation needs to have knowledge of the types of sources that probably impact the monitoring site. Third, the simulation must use at least as many species as source profiles.

Some of the calculations for best fit are performed iteratively with user input. The underlying mathematics performs best fit calculations using the data that are supplied. This best fit may produce inappropriate results, such as negative values associated with one or more source profiles. The user then must remove the source profile associated with the most negative results and execute another simulation until all calculated weights are positive. The user must also watch for collinearity among source profiles, which indicates that certain profiles are too similar for the model to distinguish between them within the monitoring data. The user is then responsible for selecting the source profiles to eliminate from the simulation.

5.3.4 Output

Because CMB is a statistical model, its results are statistics. The impact of each source profile on the ambient values, the percentage of mass explained by the results, and various measures of goodness-of-fit and uncertainty are provided.

5.4 CALPUFF

The CALPUFF modeling system may be downloaded free of charge from the US EPA from www.epa.gov/scram001/dispersion_prefrec.htm#calpuff, which provides a link to www.src.com/calpuff/calpuff1.htm to obtain the models themselves. The CALPUFF components are provided as executables and sample input files for the Microsoft Windows operating system. The models are also provided in source code format with versions for HP UNIX and Sun UNIX. PC-based GUIs for the major components are not available for the UNIX versions. All versions may be executed from text-based control files.

The CALPUFF Modeling System includes three main components: CALMET, CALPUFF, and CALPOST. Additional preprocessing programs interface the model to standard meteorological and geophysical datasets. CALMET is a meteorological model that develops hourly wind and temperature fields on a three-dimensional, gridded modeling domain. Associated two-dimensional fields (e.g., mixing height, surface characteristics) are included in the CALMET output. CALMET is capable of ingesting fields produced from the MM5 mesoscale meteorological model.

CALPUFF is a non-steady-state Lagrangian Gaussian puff model that advects puffs of material emitted from sources, simulating dispersion and some transformation processes. Modules are included for complex terrain, overwater transport, coastal effects, building downwash, and wet and dry removal from the plume. CALMET provides the meteorological fields. Temporal and spatial variations in the meteorological fields are explicitly incorporated in the resulting distribution of puffs throughout a simulation period. CALPUFF outputs either hourly concentrations or hourly deposition fluxes at selected receptor locations.

5.4.1 Purpose, Strength, and Weaknesses

CALPUFF is most appropriate for long-range transport (i.e., 50 to several hundred kilometers from source to receptors) of emissions from point, volume, area, and line sources. CALPUFF handles spatiotemporal variations of wind fields produced by CALMET, including stagnation, wind reversals, coastal effects, and vertical wind sheer effects. Specialized terrain modules handle terrain impingement, steep-walled terrain influences on lateral plume growth, and divided streamline, in which the flow is divided into a lift component that travels over the obstacle and a wrap component that is deflected around the obstacle. It also supports vertical wind shear via puff splitting.

CALPUFF does not include a photochemistry mechanism, but is appropriate for both gaseous and particulate pollutants that are inert or undergo quasi-linear chemical reactions (e.g., SO_2 and $SO_4^{=}$). This model includes special sulfate and nitrate particulate components and liquid water content variables (i.e., cloud water/ice and precipitation water/ice) to support regional haze analyses.

One weakness is in how the user configures the model. If a study requires a larger modeling domain or needs to increase the maximum value of some other parameters, then the program must be recompiled with these new settings using a supported publisher and version of a FORTRAN compiler. Also, some of the input and output files are formatted for access by a FORTRAN program and are not user-readable or editable.

The run-time for the model is influenced by the number of puffs in the simulation. The user specifies the number of sources and receptors for the simulation. The technical options and mean wind speed, which are factors determining the residence time of each puff within the modeling domain, plus the terrain and wind shear, which can cause puffs to be split into multiple independent puffs, can affect run-time by one or two orders of magnitude.

5.4.2 Types of Sources

CALPUFF supports point, area, volume, and line sources. Emission rates can vary over time. Also, CALPUFF supports buoyant area sources; their location, size, shape, and other characteristics are allowed to change over time.

5.4.3 Special Considerations

The CALPUFF modeling system includes specialized pre- and post-processors to help transfer data between its components and other software. The output files are not text files; they are designed to be read by a program written in FORTRAN. Therefore, these files should be accessed with the CALPOST post-processor.

5.4.4 Output

CALPOST processes the CALPUFF output files and produces summary tables, calculated values, lists of top N values at each receptor, and output files for input to certain graphics packages. Extinction coefficients and related measures of visibility can also be calculated for selected averaging times and locations. POSTUTIL allows the re-partitioning of nitric acid and nitrate to account for the effects of ammonia limitation on aerosols for visibility.

5.5 CMAQ

The Community Multiscale Air Quality Model (CMAQ) is the Eulerian model preferred by the U.S. EPA for urban-to-continental scale air quality studies that consider photochemistry. CMAQ itself includes numerous components and preprocessors and requires specific software libraries. It is designed for use by modelers who are experienced in compiling FORTRAN libraries and source code, editing shell scripts, and using a wide range of computing tools in a Linux or UNIX operating environment on a multiprocessor computer.

Access the following Web sites for the model itself, its documentation, and links to other libraries that you may need to download and compile on your computer system. Note that this software requires the PGI Workstation compilers from Portland Group (www.pgroup.com); an appropriate license for these compilers must be purchased for your development computer.

- www.epa.gov/asmdnerl/CMAQ/CMAQscienceDoc.html

- www.epa.gov/asmdnerl/CMAQ/cmaq_model.html
- www.cmaq-model.org/
- plus links to other sites for additional components

5.5.1 Purpose, Strength, and Weaknesses

CMAQ is a one-atmosphere model, which means that its chemical mechanism simulates the chemistry and physical interactions of gases and particles with the environment through which they move. The model simultaneously handles cycles and interactions of tropospheric ozone, oxidized and reduced forms of nitrogen and sulfur, secondary organic aerosols, sea salt, particulate matter, and toxic compounds.

The model can be executed with nested modeling domains such that a global or hemispheric model provides boundary conditions for the coarsest grid and results of each grid provides boundary conditions for the next, finer nested grid. The model currently does not support two-way nesting, which is a construct wherein the results of the finer grid also affect the computations of the next coarser grid.

The Advanced Plume Treatment (APT) is an available plume-in-grid option. If there are large, elevated NOx sources impacting the region of greatest focus in the modeling study, then APT can be applied to those sources.

5.5.2 Types of Sources

Point, Area, On-road Mobile, Nonroad Mobile, and Biogenic sources are supported. Note that Point and Area sources have a different definition in the context of regional Eulerian models than for the Gaussian and Lagrangian models discussed earlier in this document.

5.5.3 Special Considerations

CMAQ supports many science options and chemical mechanisms. The modeler must select the desired options and configure the model in shell scripts before compiling it. These selections should be made by an experienced modeler familiar with the region of interest because some science options perform better than others for certain types of regions. Also, the model and all of its preprocessors must be compiled using the same options for them to work together.

When compiling the model, libraries, and preprocessors, note that some cannot be executed as multiprocessor applications. This means that some libraries need to be compiled into both single-processor and multiprocessor versions. Each executable program must link against the appropriate version of the libraries.

Gathering and processing the emissions data is a complex effort. Also, a mesoscale meteorology model, such as MM5, must be executed prior to CMAQ. When simulating a specific episode of poor air quality, an expert in MM5 (available from www.mmm.ucar.edu/mm5/) is required to work with that model until its results adequately simulate meteorological observations throughout the modeling domain. If the MM5 predictions of wind direction, timing of frontal boundaries, temperature, humidity, or mixing heights are incorrect, then the air quality predictions calculated by CMAQ will have lower accuracy.

5.5.4 Output

CMAQ outputs results as five-dimensional matrices in NetCDF-formatted files (see www.unidata.ucar.edu/software/netcdf). The five dimensions are grid cell number in x-direction, grid cell number in y-direction, layer, hour of the simulation, and chemical species. The associated value is concentration. Wet deposition and dry deposition are output in four-dimensional matrices because there is only one layer associated with deposition.

The Visualization Environment for Rich Data Interpretation (VERDI), which is the latest graphics tool for analyzing CMAQ output, is available free of charge from www.verdi-tool.org. Note that this package has replaced the older PAVE software that has been in use world-wide for analyzing, documenting, and publishing results of regional Eulerian modeling studies. Other utilities are available to extract data from NetCDF to other formats so it can be used with other graphics software if desired.

6.0 Atmospheric Dispersion Modelling in Europe

6.1 Summary of the 2008 air quality directive

The "Directive 2008/50/EC of the European Parliament and of the Council on ambient air quality and cleaner air for Europe" was officially adopted by the European Parliament on the 21 May 2008. In addition, reference is also made to the directive on heavy metals, as this is still valid. In this guidance document we refer to these collectively as the 'air quality directive' or simply 'Directive'. When necessary specific distinction between the two will be made.

This chapter summarizes the air quality directive in regard to the thresholds, limit values, critical levels, reduction targets, target values, etc. It is not intended as a replacement for the directives and the reader should refer directly to the directive document for confirmation of the summary provided here.

6.1.1 Concepts and definitions

In this section a number of terms and concepts necessary to understand the Directive are given. Many of these are provided in the Directive already, however some terms are not defined and these are also given an interpretation here. The list given here is intended to supplement those provided in the Directive and are listed under topics. These descriptions are intended to guide the reader, for an official interpretation of all terms the reader is referred to the directive itself.

Table 1. List of the terms and their definition contained in the Directive

Concept	Meaning
Pollutant levels and values	
Limit value	A pollutant level not to be exceeded, in regard to human health, for every year.
Critical level	A pollutant level not to be exceeded, in regard to vegetation protection, for every year.
Margin of tolerance	Relates to the limit value and is given as a percentage. This provides, under specified conditions, a flexibility for compliance with the limit value.
Target value	A pollutant level that one tries to avoid. Generally applicable over longer periods, 3 – 5 years.
Alert threshold	A short term pollutant level for which immediate steps must be taken.
Information threshold	A pollutant level for which immediate information to the public must be given.
Upper assessment threshold	A pollutant level, beneath the limit value, where a combination of modelling and monitoring (and/or indicative measurements) may be used for assessment.
Lower assessment threshold	A pollutant level, beneath the upper assessment threshold, where a modelling (or objective-estimation techniques) may be used for assessment.
Long-term objective	A pollutant level to be obtained in the long term.
Exposure levels and values (related to PM2.5)	
Average exposure indicator (AEI)	This is the urban background pollutant level and has been introduced in relation to PM2.5
Exposure concentration obligation	A level applied to the AEI that should be obtained over a given (3 year) period.
National exposure reduction target	A percentage reduction in the AEI to be achieved over a given period.
Measurement types	
Fixed measurements	These are measurements with the most strict data quality objectives , which are to be used when the pollutant is above the upper assessment threshold.
Indicative measurements	These are measurements with less strict data quality objectives than normal fixed measurements. For some pollutants, e.g. particulates, this has the same data quality objective as modelling.

Concept	Meaning
Objective-estimation techniques	These are methods (not specified) with even less strict data quality objectives than the indicative measurements. The quality objectives are around 100%.
Other defined concepts	
Proportionate measures	These are not defined explicitly but can be considered to be 'all necessary measures not entailing disproportionate costs'
Contributions from natural sources	Contributions from emissions not caused directly by human activities. These are: volcanic eruptions, seismic activities, geothermal activities, wild-land fires, high wind events, sea sprays, the atmospheric re-suspension or transport of natural particles from dry regions
Undefined concepts	
Combine	The text in the directive often refers to a 'combination' of monitoring and modelling. This is not defined explicit.
Supplement	The text in the directive often refers to a 'supplementary' methods or assessment. Nowhere is this defined but it is understood to refer to all other methods than the use of fixed measurements.

6.1.2 Where does the Directive not apply?

The Directive is applied within individual zones and these zones are defined by the Member States. The air quality requirements for health apply everywhere within the zone but with the following exceptions :

a. any locations situated within areas where members of the public do not have access and there is no fixed habitation
b. on factory premises or at industrial installations to which all relevant provisions concerning health and safety at work apply
c. on the carriageway of roads and on the central reservations of roads except where there is normally pedestrian access to the central reservation.

These exceptions are a change from previous directives and indicate that the health related assessments are intended to be applied where people live, work and play. Note that these exceptions appear to exclude exposure during road transport activities. E.g. the directive does not cover the environment within a bus but will cover the ambient environment when the public steps out of the bus. It also does not seem to cover cyclists whilst on the road but does cover cyclists on bicycle paths.

In regard to the protection of vegetation and natural eco-systems the Directive is intended to cover regional background levels of pollutants within any zone in areas where eco-systems are dominant, i.e. not in urban areas. Specifics regarding this, in regard to modelling, are discussed in section 3.5 of this document.

6.2 Interpretation of the EU directives in regard to modelling

In 2008 a new European air quality directive was ratified by the European parliament . This directive replaced earlier directives with the intention of simplifying and streamlining reporting, as well as the introduction of new limit values concerning $PM_{2.5}$. Whilst previous directives had based assessment and reporting largely on measurement data, the new directive places more emphasis on the use of models to assess air quality within zones and agglomerations. Modelling is featured in the new air quality directive, referred to in the rest of this document as 'the Directive', in the following ways:

- It allows a reduction of up to 50% in the number of monitoring stations when suitable modelling is available.
- It can be used exclusively when concentrations are likely to be below the lower threshold value.
- It can be used in conjunction with monitoring when concentrations are below the upper threshold value.
- It is implicitly required if source apportionment, e.g. natural sources, is to be assessed.
- It is implicitly required if transboundary pollution is to be assessed.
- It is implicitly required if abatement measures are to be applied and assessed.
- It is implicitly required for air quality forecasting and the effective implementation of short term action plans.

Air Quality Modelling

The increased focus on modelling allows the Member States more flexibility in reporting assessments and the potential to reduce the often costly activity of air quality monitoring. Though measurements remain the cornerstone of air quality assessment the more widespread use of models opens up the potential for complete spatial and temporal coverage as well as providing tools to assess mitigation strategies that are also required under the Directive.

Modelling, like monitoring, requires expert implementation and interpretation. Models must also be verified and validated before they can be confidently used for air quality assessment or management.

6.2.1 Why use models?

Historically air quality assessment has been based on monitoring data as this has been seen to be as close as we come to the truth. Even though modelling is often seen as being more uncertain than monitoring there are three major reasons for using models for air quality assessments.

1. The spatial coverage of monitoring is extremely limited. Modelling can provide complete spatial coverage of air quality.
2. Modelling can be applied prognostically (i.e., it can be used to predict the air quality as a result of changes in emissions or meteorological conditions.
3. Modelling provides an improved understanding of the causes and links that determine air quality.

In regard to the directives there are distinct advantages in using models for reporting, e.g.

- Models can provide assessment within zones in areas where monitoring is not carried out.
- The number of monitoring sites can be reduced significantly, saving costs.
- Models can be used to develop and detail measures taken to improve air quality.

Modelling, however, does not provide all the answers and there are a number of limitations attached to them, e.g.

- Models require extensive input data, particularly emissions and meteorology, which are not always reliable or easily acquired.
- Models remain uncertain in their predictions and extensive validation is required before models can be applied and believed.
- The ability of models to represent the real world is very limited, e.g. spatial resolution and process descriptions. Models remain a representation of reality.
- Effective and quality controlled modelling requires expert users under most situations.

6.2.2 Model applications in the air quality directives

Models may be applied to a range of applications relevant to the Directive; however, modelling is only explicitly named in regard to the application of assessment. In this document we will consider the wider range of applications, which typically involve the following types of applications.

1. Assessment
   – Models can be used to supplement or even replace monitoring data under specified conditions. These conditions are related to the various categories of pollutant levels and are described below.
   – Given adequate quality and resolution a model can be used to reduce the number of measurements by up to 50% (not including ozone), unconditional on the pollutant levels.
   – Given adequate quality and resolution of the model it can be used to reduce the number of measurements of ozone by one-third.
2. Mitigation and planning
   – When recommending mitigation plans or measures, models need to be used for a thorough assessment. The use of models is not stated explicitly in the Directive for this management activity, but it is not possible to do assessment properly without the appropriate models.
3. Source apportionment

– Though not directly written into the directives, source apportionment studies will generally be required to assess the contribution from natural sources, neighbouring countries, resuspended road sand, and sea salt. Monitoring of these contributions everywhere in a zone or agglomeration would not be possible, so modelling is the most likely methodology that can be used for this application.

6.2.3 When can models be used for assessment?

The Directive defines a range of situations where models may be applied for assessment instead of, or in combination with, fixed measurements.

1. Models can always be used to supplement fixed measurement data no matter the pollutant levels. The advantage of this is that the number of monitoring stations may be reduced.
2. *Article 6 of* the Directive stipulates when, and in what way, modelling may be used for air quality assessment, not including ozone, based on the level of pollutants. These are:
   – To supplement monitoring when a zone is in exceedance of the upper assessment threshold
   – In combination with monitoring when a zone is in exceedance of the lower assessment threshold
   – To replace monitoring when a zone is below the lower assessment threshold
3. *Article 9.2 and Annex II.B* state that, when monitoring data are not available for 5 years (i.e., the period for which the threshold levels are to be assessed), then short term measurement campaigns combined with modelling may be used to determine both upper and lower exceedance thresholds.

6.2.4 Combined use of measurements and models for assessment

In *Articles 6* and *9* of the Directive the combined use of measurements and modelling is encouraged and allowed for in reporting when exceedances are below the upper assessment threshold. There are no specifics provided as to the level of combination or how the combination can be made. There is clearly a multitude of methods available for combining monitoring and modelling, ranging from advanced data assimilation methods to simple validations of models. The general concept is most likely to be that locally validated models can be used for assessment in the areas where monitoring is not available but where the characteristics of both locations are similar.

6.2.5 What types of models can be used?

The directive does not provide any recommendations for the actual models to be used. As long as the model complies with the quality objectives (*Annex I*) then it may be applied. The following general criteria should however apply:

- The model has the appropriate spatial and temporal resolution for the assessment.
- The model is well validated and documented.
- The model contains the relevant physical and chemical processes suitable for the type of application, the scale and the pollutant for which it is applied. In other words, the model is ‘fit for purpose’.

6.3 Model Documentation System

A comprehensive listing of air quality models used in Europe can be found at the EIONET Model Documentation System web site (http://air-climate.eionet.europa.eu/databases/MDS/index_html). The Model Documentation System provides guidance to any model user in the selection of the most appropriate model for an application. The number of models available at the moment is 124. Inclusion of a model in the system is by no means associated with any form of endorsement for using the particular model: it helps select the most appropriate by using the specifications submitted by the modellers.

Air Quality Modelling

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