5.3.1 Air Dispersion and Emission Modeling

The models that simulate the transport and dispersion of air contaminants from the point of release to potential receptors use known data on the characteristics of a contaminant release and the atmospheric conditions as input to calculate air concentrations and deposition values at almost any location specified by the user. Dispersion models can be used when monitoring is impractical or infeasible. Models also can be used to supplement air monitoring programs by filling in data gaps or interpreting monitoring results, or to assist in designing an air monitoring program. Dispersion modeling is an important tool for determining potential exposure by the air pathway.

Although dispersion modeling is a valuable tool for an air assessment, the permit writer should recognize the considerable limitations that exist when evaluating a modeling analysis. The accuracy of the models is limited by the ability of the model algorithms to depict atmospheric transport and dispersion of contaminants and by the accuracy and validity of the input data. For example, most refined models require the input of representative meteorological data from a single measuring station. In reality, a release will encounter highly variable meteorological conditions that change constantly as the release moves downwind. EPA's *Guideline on Air Quality Models - Revised* (EPA 2001) describes two types of uncertainty related to modeling. Inherent uncertainty involves deviations in concentrations that occur even if all data used for the model are accurate. Reducible uncertainty is associated with the model and the uncertain input values that will affect the results. While it is important to represent actual conditions accurately by selecting the right model and using accurate and representative data, it should be recognized that the results of all modeling are subject to uncertainty. Nevertheless, models generally are considered reasonably reliable in estimating the magnitude of highest concentrations that result from a release, although the estimate will not be necessarily time- and space-specific (EPA 2001). When applied properly, air dispersion models typically are accurate to ± 10 to 40 percent and can be used to develop a best estimate of concentrations of air pollutants (EPA 2001).

In general, a modeling analysis should follow closely the EPA modeling guidelines presented in *Guideline On Air Quality Models*, as well as information presented in user's guides and EPA risk assessment documents (e.g., *Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities*). Permit writers should refer to these documents when evaluating an approach to modeling. The permit applicant should identify clearly and justify any deviations in the application from the guidelines. Other helpful resources that aid in reviewing a modeling approach include:

- EPA. 1994. Air/Superfund National Technical Guidance Study Series. *Volume V - Procedures For Air Dispersion Modeling At Superfund Sites.* Office of Air Quality Planning and Standards. Research Triangle Park, North Carolina. February.

- EPA. 1994.

  (EPA530-R-94-021). Office of Solid Waste and Emergency Response. April.

- EPA. *Suggestions for Auditing Assessment Air Modeling Studies following the 1998 U.S. Office of Solid Waste Human Health and Ecological Risk Protocols.* U.S. EPA Region 6 Center for Combustion Science and Engineering.

The following sections discuss criteria for the selection of the model, the data that are required for a modeling analysis, and evaluation of the results of modeling. These sections describe for the permit writer how to evaluate a modeling analysis and provide information about recommended air dispersion models. Each section addresses the requirements for both screening air modeling analyses and refined air modeling analyses.

Emission Modeling

Emission modeling is a method that uses known information and assumptions about an emission source to predict the emission rate of a given contaminant. The information and assumptions used in emission modeling are incorporated into emission factors or emission equations that then are used to calculate emissions. Often, the factors and equations are based on monitoring and modeling results from several similar sources. Emission modeling should not be confused with dispersion modeling. Unlike dispersion modeling, which estimates concentrations and deposition rates of contaminants, emission modeling (or emission factors and equations) estimates the rate of release of contaminants from a source, in units of mass per time. Emission factors and equations have been developed for a wide variety of emission sources and a wide variety of release conditions. Most emission factors and equations include a built-in bias toward conservativism, so that estimated emission rates will represent the worst-case scenario. The permit writer should verify that any emission factors or emission equations used by an applicant are credible and result in conservative estimates.

Under certain circumstances, emission modeling may be used instead of emission monitoring to estimate emission rates from Subpart X units. When well-developed emission factors or equations are available for the specific type of unit and wastes, those factors may be used to estimate emissions from a unit. Use of emission modeling may be necessary when monitoring would be difficult or impossible. The most comprehensive collection of emission factors and equations is found in EPA's *AP-42 Compilation of Air Pollutant Emission Factors* (EPA 1995c). Existing "BangBox" data for OB/OD operations as presented in *Emission Factors for the Disposal of Energetic Materials by Open Burning and Open Detonation (OB/OD)* are generally acceptable for use in estimating emissions, as long as the composition of material being burned or detonated at the unit is the same as the composition of material for which the BangBox data were collected.

Another type of emission modeling technique is the mass balance technique. Mass balance is a screening technique that uses the mass of material entering a system with the mass of material leaving the system. The difference between those two known parameters is assumed to be the air emissions. This technique is applicable only to emission sources for which the mass of material both entering and leaving the system is known. A permit applicant may measure those values so that the mass balance technique can be applied.

Selection of the Dispersion Model

Selection of the proper dispersion model for analyzing the release of a contaminant to the atmosphere is crucial to the success of the modeling analysis. Dispersion models are developed for specific types of sources, atmospheric conditions, terrain, locations of receptors, and chemical and physical processes involved. Only models that are capable of assessing conditions against site-specific criteria should be used in a modeling analysis.

Dispersion models are developed for either screening or refined analyses. Screening models are easier to use and require less site-specific data than those for refined analysis. Refined models require more data, but produce more realistic results. Table 5.2 presents preferred screening dispersion models for Subpart X units and outlines each model's capabilities and features. Also provided below are summary discussions of each preferred screening model. It should be noted that Table 5.2 is not intended to be an exhaustive list of appropriate screening models for Subpart X permitting, but provides the most commonly used and most accepted screening models that may be applied to a Subpart X unit. Because of their versatility and ease of use, the SCREEN3 and TSCREEN models are the most commonly used screening models. However, the models can simulate releases only from a single source; therefore, another screening model or a refined model must be used to model sites at which there are more than one source. The CTSCREEN model is especially useful in cases in which complex terrain and multiple point sources are present.

Table 5.3 lists preferred refined dispersion models for Subpart X permitting and outlines each model's capabilities and features. Also provided below are summary discussions of each preferred refined model. As is true of the list of screening models, the list of refined models in Table 5.3 is not intended to be an exhaustive compilation of appropriate refined models for Subpart X permitting.

It should be noted that a dispersion model has been developed at the U. S. Army Dugway Proving Grounds to specifically address release and dispersion characteristics from OB/OD sources. The model is a gaussian puff model, and is called the Open Burn and Open Detonation Model (OBODM). EPA Region 4 recommends the use of the OBODM model for open burn and detonation

TABLE 5.2
PREFERRED SCREENING AIR DISPERSION MODELS AND THEIR USES

MODEL CHARACTERISTIC	SCREEN3[1]	TSCREEN[2]	CTSCREEN[3]
Source Types	Point, Area, Volume, Flare	Numerous	Point
Terrain Types	Simple, Complex	Simple, Complex	Complex
Release Mode	Continuous	Continuous, Instantaneous	Continuous
Averaging Time	1 Hour	15 Minutes to Annual	1 Hour to Annual
Land Use	Rural or Urban	Rural or Urban	Rural or Urban
Contaminant Type	Gas or Particulate	Gas, Particulate	Gas or Particulate
Applicable Range	≤ 100 km	≤ 100 km	≤ 50 km
Generic or Real Meteorological Data?	Generic	Generic	Generic
Model Chemical Reactions?	No	No	No
Model Building Wake Effects?	Yes	Yes	No
Dry Deposition Calculations?	No	No	No
Wet Deposition Calculations?	No	No	No
Model Negatively Buoyant Gases?	No	Yes	No
Single or Multiple Sources per Simulation?	Single	Single	Multiple

1 SCREEN3 dispersion model for a single source.
2 TSCREEN screening model for a single source.
3 CTSCREEN model for complex terrain.

units. For this reason, OBODM is included in this document as a preferred dispersion model for Subpart X Permitting.

SCREEN3

The SCREEN3 model is a Gaussian, steady-state dispersion model used for making simple screening evaluations for neutrally buoyant, continuous emissions from a single source. The model uses built-in worst-case meteorological conditions to predict concentrations from either point, area, volume, or flare sources. The SCREEN3 model can simulate dispersion from only one source at a time. The model is capable of simulating dispersion of gases or particulates in simple or complex terrain. Only one-hour averaging periods are calculated, so if different averaging periods are desired, generic adjustment factors must be used. (Note that reference doses and other health criteria do not require exposures of less than 1 year.) SCREEN3 is recommended for simple screening evaluations of a single, continuously emitting source.

SCREEN3 is available on EPA's Support Center for Regulatory Air Models (SCRAM) bulletin board, which is part of the OAQPS Technology Transfer Network:

Telephone Number: (919) 541-5742
Baud Rate: 200, 9600, or 14.4K baud
Line Settings: 8 data bits, no parity, 1 stop bit
Terminal Emulation: VT100 or ANSI
Internet TTN site: http://ttnwww.rtpnc.epa.gov
SCRAM site: http://134.67.104.12/html/scram/scram.htm

TSCREEN

TSCREEN is a screening modeling system for toxic releases that consists of four different dispersion models: 1) SCREEN3 for neutrally buoyant, continuous releases; 2) PUFF for neutrally buoyant, non-continuous releases; 3) RVD for dense gas jet releases; and 4) the Britter-McQuaid Model for continuous or puff dense gas area sources. When executing TSCREEN, the user enters parameters for the source and receptors, and the appropriate model is selected within the modeling program. TSCREEN uses generic, worst-case meteorological data to calculate downwind concentrations. The modeling system is versatile in its ability to simulate dispersion from many different types of toxic emission sources. As in the case of SCREEN3, only one source can be entered in the model per simulation. TSCREEN is recommended for screening evaluations of single sources of toxic air contaminants. TSCREEN is available on EPA's SCRAM bulletin board. See the SCREEN3 summary for details on access to SCRAM.

CTSCREEN

CTSCREEN is the screening mode of the CTDMPLUS model for calculating downwind concentrations from point sources in complex terrain. CTSCREEN and CTDMPLUS are identical, except that CTSCREEN uses generic, worst-case meteorological data rather than the extensive site-specific meteorological data used in CTDMPLUS. CTSCREEN can be used in a screening analysis for point sources when complex terrain affects dispersion of contaminants. See the individual listing below for information about CTDMPLUS. CTSCREEN is available on EPA's SCRAM bulletin board.

ISC3

The Industrial Source Complex 3 (ISC3) model is a Gaussian plume model that can predict short- or long-term concentrations of pollutants from continuous emissions of point, area, and volume sources. The model can simulate the downwash effects of buildings on point sources, can simulate multiple sources per run, and is appropriate for use to a distance of 50 kilometers. The model recently has been modified to include dry and wet deposition, an algorithm for complex terrain, and an improved algorithm for modeling area sources.

ISC3 is preferred for most refined modeling applications when there are continuous emissions of neutrally buoyant, nonreactive pollutants. The ISC3 model is not the best model in cases in which a release of a pollutant is instantaneous or intermittent or those in which the pollutant is significantly heavier than air. ISC3 treats chemical reactions only by simulating exponential decay of a pollutant. If complex chemical reactions of a pollutant in the atmosphere are important, a different model may be more appropriate.

ISC3 requires entry of detailed data on the source and receptors and preprocessed hourly meteorological data. Depending on the features used, additional data are required, such as information about building dimensions and particle size. Because ISC3 requires entry of complex data to use various model features, analyses should be performed by an experienced modeler. The ISC3 model is available on the SCRAM bulletin board.

RAM

The RAM model (Gaussian-plume multiple source air quality algorithm) is a steady-state Gaussian plume model capable of predicting concentrations of contaminants from point or area sources. The model assumes level terrain and can assess concentrations for short-term averaging periods (from one hour to one day). RAM can estimate concentrations in rural or urban areas, but is recommended specifically for use in urban areas. Although use of the RAM model is acceptable, within those limiting conditions, the ISC3 model generally is preferred because of its updated features and algorithms. RAM is available from the National Technical Information Service (NTIS).

CTDMPLUS

CTDMPLUS is a refined point source Gaussian air quality model for use in all stability conditions for complex terrain applications. The model requires entry of considerable surface and upper air meteorological data, and uses extensive data on terrain to define the shapes of individual hills. The model associates each receptor with a particular hill. CTDMPLUS is recommended specifically for continuous, elevated point sources near terrain that is higher than the top of the source's stack. CTDMPLUS is available on EPA's SCRAM bulletin board.

INPUFF

INPUFF is a Gaussian integrated puff model for evaluating downwind concentrations or deposition fluxes from continuous or noncontinuous sources. INPUFF is capable of modeling multiple sources at as many as 100 receptors and for as many as 144 meteorological periods. Moving or stationary sources may be simulated with puffs that disperse over a gridded wind field. The puffs from a source are released in a series of user-specified time steps. INPUFF usually is applied to noncontinuous sources and is the most common model for use for OB/OD operations. INPUFF is a suitable model for OB/OD releases under most circumstances, but it does have significant limitations including: use of dispersion parameters for long-term releases, rather than short-term releases; use of plume rise equations for continuous sources; and unrealistic simulation of atmospheric turbulence. Unfortunately, there are few alternative models available to address OB/OD releases. The limitations of INPUFF should be recognized when evaluating a modeling plan that uses the model.

INPUFF can be used for OB/OD releases but it was not developed to model OB/OD type processes. The limitations of INPUFF should be recognized when evaluating a modeling plan.

When INPUFF is used to model OB/OD operations, source parameters should be input into the model to best fit the actual release characteristics of the source. Because INPUFF is not able to specifically address OB/OD type releases, the input parameters must be modified to fit the input requirements of another source type, and still exhibit the release and dispersion characteristics of the OB/OD operation.

Open burn operations are usually characterized as point sources so that buoyancy plume rise can be taken into account. When running the model for open burn sources, the buoyancy-induced dispersion option should be selected. Input values will vary depending on the type of material being burned, and the location and construction of the burn pan. As a guide, the checklist gives typical open burn values of 3700 °K for exit temperature and 0.1 to 10 meters per second for exit velocity. An open burn operation may be considered a continuous release if the burn lasts for a long time (1 hour or longer), but will usually be considered a short-term release.

Open detonation sources should be characterized as a volume source with initial lateral and vertical dimensions equivalent to the expected maximum extent of the blast cloud. There are several methods for identifying the extent of the cloud. Stoner and Kirkpatrick (1995c) suggest one method for determining the cloud size by first calculating the initial source volume using the POLU model, which estimates total detonation gases and initial temperature. These results are entered into INPUFF as a ground-level source with plume rise. As part of this method, the cloud is limited to a maximum height using estimates made from high-explosive algorithms developed by the Defense Nuclear Agency. Other methods for determining the cloud extent may also be used. In general, any method used to determine the cloud dimensions should be well documented and justifiable.

When an OB/OD source is located in complex terrain, a model such as CALPUFF should be used to properly address the terrain issues. However, for screening analyses, INPUFF may be used if conservative assumptions are incorporated into the analysis to account for the complex terrain. One example of this is to assume that the cloud height is ground level and all the receptors are at ground level. INPUFF is available from NTIS.

CALPUFF

The CALPUFF model is a complex modeling system that can estimate concentrations of pollutants from non-steady-state emission sources. This model can simulate the effects of meteorological conditions that vary according to time and space, chemical transformation, and physical removal. CALPUFF is also capable of simulating building downwash and transport over complex terrain and over water, or coastal transport. It can be used for point, area, volume, or line sources. The CALPUFF modeling system has several modules, each intended for performing a separate operation. One recently added module treats buoyant rise and dispersion from area sources. This module may be useful for modeling OB/OD sources. Because CALPUFF is a complicated modeling system, and because EPA has not fully recommended its use, review of a CALPUFF analysis by experts is recommended. CALPUFF is available on EPA's SCRAM bulletin board.

OBODM

The Open Burn/Open Detonation Dispersion Model (OBODM) is intended for use in evaluating the potential air quality impacts of the open air burning and detonation (OB/OD) of obsolete munitions and solid propellants. OBODM uses cloud/plume rise, dispersion, and deposition algorithms taken from existing models for instantaneous and quasi-continuous sources to predict the downwind transport and dispersion of pollutants released from OB/OD operations. The model can be used to calculate gravitational deposition for emissions from multiple OB/OD sources for either a single event of up to a year of sequential hourly source and meteorological inputs. The program is designed for use on IBM-compatible PCs using the MS-DOS (Version 2.1 of higher) operating system with keyboard and optional mouse-control. It will also run under most WINDOWS environments.

OBODM is available on EPA's SCRAM Bulletin Board http://www.epa.gov/scram001

DEGADIS

The Dense Gas Dispersion Model (DEGADIS) uses mass and momentum balances and laboratory and field scale data to simulate the release and transport of pollutants (EPA 1995). It is used for negatively or neutrally buoyant releases of toxic, nonreactive gases or aerosols. It is applicable for ground-level, low-momentum area releases; or upwardly directed stack releases. The release may be instantaneous, continuous, or of finite duration, or may vary over time. The model simulates only one set of meteorological conditions, so the modeled time frame should not exceed one to two hours. Another limitation affecting the model is that dispersion is assumed to take place over flat, unobstructed terrain. DEGADIS is not equipped to address terrain that is complex or that has extensive surface roughness.

DEGADIS requires entry of the characteristics of the release and its chemical and physical properties, data on receptors, and standard meteorological data. If an aerosol release is being modeled, the density of the release also must be entered into the model. Although DEGADIS is appropriate for a wide range of sources, it is particularly valuable in characterizing releases of pollutants that are very dense compared with air. An external input file or an interactive computer program can be used to run DEGADIS. DEGADIS is available on EPA's SCRAM bulletin board.

HGSYSTEM

HGSYSTEM is a computer program that incorporates several different dispersion models for various types of toxic releases. The modeling package can estimate one or more consecutive phases between a spill of a toxic substance and near-field and far-field dispersion of a pollutant. The pollutant being modeled can be a two-phase, multicompound mixture of nonreactive compounds or hydrogen fluoride. The modeling system can simulate chemical reactions only for hydrogen fluoride. HGSYSTEM assumes flat, unobstructed terrain and can be used for continuous, finite-duration, instantaneous, and time-dependent releases. HGSYSTEM can be used to determine short-term (one hour or less) concentrations of toxic releases under one set of ambient conditions. HGSYSTEM is available from the American Petroleum Institute.

SLAB

The SLAB model is used for modeling the dispersion of dense gas releases from a ground-level evaporating pool, an elevated horizontal jet, a stack or elevated vertical jet, or an instantaneous volume source. If two or more different types of releases require evaluation, they must be processed in separate model simulations. The SLAB model uses only one set of meteorological conditions, so only short-term concentrations can be calculated. The model assumes that the release consists of nonreactive dense gases or aerosols and that no deposition occurs. SLAB calculates concentrations by using numerical integration in space and time to solve the basic conservation equations. SLAB is available on EPA's SCRAM bulletin board.

Source Type Specification

In part, selection of the proper dispersion model depends on the type of emission source or sources that must be modeled. Each source must be classified as a point, area, volume, or line source. Some models allow for identification of other types of sources that are subsets of the four types listed above. An example of such a sub item is a flare, which is a type of point source. In addition, each source must be classified as a continuous, instantaneous, or intermittent source; as a vapor-phase or particulate emission source; and, when modeling gaseous contaminants, as neutrally buoyant or negatively buoyant. These determinations will affect the selection of a model.

Releases from point sources are those from stacks or vents; they exhibit well-defined exit parameters such as temperature, flow rate, and stack height. Releases from area sources are emitted at or near ground level and over a given surface area. Area source emissions are entered into a model in units of mass per time per area. Releases from volume sources are those that occur over a given area (like area sources), and also within a certain depth. Volume sources can be ground level or elevated sources. When entering data for a volume source, a model requires the initial lateral and vertical dimensions of the source. Releases from line sources are releases from roadways or other sources that emit over a long and narrow space. Some models simulate line sources with a series of volume or area sources adjacent to one another.

In general, a permit writer should evaluate the description of a source or proposed source and decide whether an applicant's representation of the source in a modeling analysis is reasonable. As can be anticipated, the choice of the type of source to be used sometimes can be left to professional judgment and based on how a source best fits into the definition of a given type of source.

Sources must also be classified as continuous, instantaneous, or intermittent. The most common dispersion models are Gaussian, steady-state models, such as ISC3. These types of models can simulate dispersion from continuous sources. For instantaneous or intermittent releases, a "puff" model may be used. This differentiation is of particular importance for OB/OD operations, from which emissions occur over a very short period during OD operations and from a few minutes to one hour during OB operations. TSCREEN incorporates a puff model into its screening system, and INPUFF and CALPUFF and OBODM are puff models that can be used for screening or refined analyses. A puff model should be used when the travel time of the plume from the source to a receptor is longer than the duration of the emissions.

If a gaseous contaminant cloud emitted by a source has a significantly higher density than air, it will be negatively buoyant and should be modeled with a dense gas model (DEGADIS, HGSYSTEM, or SLAB). When uncertain whether a vapor cloud should be modeled with a dense gas model, the vapor cloud's Richardson Number (Ri) should be calculated. A cloud that exhibits $Ri > 10$ should be modeled with a dense gas model (Trinity 1996).

Contaminants emitted from Subpart X units may include NO_x, SO_x, particulates (including metals), VOCs, and SVOCs. Most of the preferred models listed in this document are capable of simulating transport of both particulate matter and vapor-phase emissions.

Table 5.3 and the model descriptions of models provided in this document should be helpful to a permit writer in determining whether a permit applicant has selected the appropriate model.

Meteorological Parameters

It is important that the permit writer ensure that appropriate meteorological data have been included in a modeling analysis. For screening analyses, the information usually is straightforward because most screening models use generic, worst-case meteorological conditions. Usually, the meteorological conditions that produce the highest modeled concentrations are low wind speeds and stable atmospheric conditions. For models that require the entry of a single set of conditions, such as dense-gas models, the permit writer should verify that reasonable worst-case conditions have been entered. Reasonable worst-case conditions may be modified to reflect proposed operating restrictions. For example, OB/OD operations may be confined to daylight hours; therefore, worst-case stability might be the worst-case daylight stability conditions, since the atmosphere tends to become more stable at night.

If a refined modeling analysis requires entry of real meteorological data, either on-site meteorological data for one year, or off-site data for five years are needed for a refined analysis. If on-site data for five years are available, all those data should be used. Off-site data can be obtained from nearby National Weather Service stations, military facilities, or industrial facilities. The permit writer should examine the location from which any off-site data were collected to ensure that location resembles the site being modeled. Parameters to review include distance of the station from the site, unique features of the terrain that may change the wind flow patterns, and the exact location of the monitoring equipment. National Weather Service data from many stations nationwide are available on the SCRAM Bulletin Board System or from NTIS. Of the models listed in Table 5.3, those that use detailed meteorological data include ISC3, RAM, CTDMPLUS, INPUFF, CALPUFF, and

Tip:
Procedures for creating multi-year files can be found in the User's Guide for the air dispersion model. Procedures for the ISCST3 model are also presented in Section 3.7.4 of the Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilitis (HHRAP).

OBODM. The dense-gas models (DEGADIS, HGSYSTEM, and SLAB) accept only one set of ambient conditions.

If existing representative data are not available, a permit applicant must collect data from the site. Those data should be collected in accordance with the guidelines set forth in *Meteorological Monitoring Guidance for Regulatory Modeling Applications* (EPA 2000). More information about the collection of on-site meteorological data is presented below in the discussion of monitoring.

Locations of Receptors

Any modeling analysis must define the locations of receptors for which concentrations of contaminants will be calculated. For Subpart X permitting, the point of compliance (POC) receptors must be evaluated in a modeling analysis. POC receptors must be chosen to evaluate both direct exposure and indirect exposure from an air release (indirect exposure may result when hazardous constituents are present in soil or water through deposition of particulates or gases). Permit applicants should identify locations of potentially exposed individuals; the potentially maximum exposed individual (MEI); potential ecological receptors, such as local plants and animals; and other sensitive environments and endangered species.

Dispersion models vary in the amount of detail they require in information about receptors. Some screening models (for example, SCREEN3 and TSCREEN) do not require entry of an exact location, but only the distance to a receptor. For such models, the direction is not important because the models conservatively assume that meteorological conditions will be such that dispersion is in the exact direction of the chosen receptor.

Other models allow a user to enter discrete locations of receptors or a gridded receptor field. Models that evaluate considerations related to terrain also require entry of elevations for receptors. Modeling analyses for Subpart X permitting should include receptor points at all POC locations. In some cases, when POC locations are uncertain or when the maximum concentration must be determined for a given region, a full receptor grid may be necessary. The permit writer should evaluate, on a case-by-case basis, whether the modeled receptor locations are adequate to characterize potential effects to human health and the environment.

Features of the Terrain

Incorporation of features of the terrain is an important factor in modeling analyses, especially when buoyant plumes are being modeled. When there are significant terrain features in the vicinity of a site, a model should be used that can simulate a plume's transport over or around such features. For modeling a point source in complex terrain, CTSCREEN (for screening analyses) and CTDMPLUS (for refined analyses) are preferred. The two models require extensive information and significant sophistication on the part of the person operating the model. If the permit writer wishes to rerun the model to check results, he or she may require assistance from staff experienced in operating the models. The ISC3 model includes the complex terrain algorithm from the Valley model and can be applied in areas of complex terrain. When using a model that cannot address complex terrain an applicant may also choose to apply conservative assumptions to account for such terrain. Modeling analyses that make assumptions to account for features of the terrain should be considered screening analyses. In any case, the permit writer should verify that a modeling analysis has addressed problems related to complex terrain and that permit applicant has used the best model practicable under the circumstances.

If a facility is near a coastline or next to a large body of water, dispersion differs from that over land, and a model particularly suited for dispersion and transport over water may be necessary. The CALPUFF model incorporates algorithms for offshore and coastal dispersion. Other models that address offshore or coastal dispersion that are not listed in Table 5.3 include the Offshore and Coastal Dispersion Model (OCD) and the Shoreline Dispersion Model (SDM).

Deposition

Deposition of contaminants onto land or water surfaces may result in indirect exposure and risk to human and environmental receptors. Deposition may increase risk by exposure pathways other than air. A refined model with deposition capabilities can be used to model deposition, or modeled concentrations can be multiplied by calculated deposition velocities to estimate deposition. A third option, which the permit writer must consider at operating facilities on a case-by-case basis, is to estimate deposition by taking soil samples.

Chemical Transformation

Chemical transformation of contaminants after they have been released into the air is difficult to quantify; and most dispersion models do not address it, except in a limited fashion. Chemical reactions in the atmosphere from releases of contaminants depend on many different factors and cannot be incorporated easily into a modeling analysis. However, chemical transformations take time to occur in the atmosphere, so the processes generally are not considered significant when travel times are limited to a few hours (EPA 1995a). One exception is in urban areas, where photochemical models are applied to address complex chemical mechanisms. The models typically do not evaluate individual sources, but are used for regional modeling analyses.

Some of the models listed in Table 5.3 are capable of limited calculations of chemical transformations. ISC3 and RAM allow the user to enter an exponential decay factor to address breakdown of chemicals. CALPUFF is able to model pseudo-first-order chemical reactions and is based on algorithms from the MESOPUFF II model, which is a long-range puff model (EPA 1995b). Last, HGSYSTEM can calculate chemical transformation for releases of hydrogen fluoride.

Transformation of NO_x to NO_2 can be estimated by postmodeling calculations. Usually, a conservative assumption is made that all the NO_x converts to NO_2 in the atmosphere. If a permit applicant has included a transformation calculation from NO_x to NO_2 in the modeling analysis, the permit writer should refer to *Guidelines On Air Quality Models* for details on review of this process.

Other available dispersion models estimate chemical reactions in the plume (EPA 1995a) and may be used as determined appropriate on a case-by-case basis. Modeling calculations that include chemical transformations should be reserved for refined analyses. Screening analyses should use worst-case assumptions for chemical transformation.

Background Concentrations

Under the Subpart X permitting requirements listed in 40 CFR §264.601(c)(5), a permit applicant must provide information about existing air quality in the area. The information must include the effects of other sources of contamination. Other sources of contamination may be natural sources, nearby sources, or unidentified sources. The information is important in understanding the overall air quality at the site and in its vicinity. When an air dispersion modeling analysis is conducted, the existing concentrations of air contaminants (or background) must be determined so that total effects on air quality can be evaluated. Modeled effects from individual sources are added to the background concentration to obtain the total concentration of a contaminant at a given receptor location. In many cases, existing background concentrations measured in the vicinity of a Subpart X source may be obtained from local regulatory agencies, universities, or nearby industrial facilities. If the Subpart X unit is an isolated, single source and no data exist for the area, a regional background site may be used that is not nearby, but that is affected by similar natural and distant sources. However, if the site at which regional background data were collected is not affected by similar sources, those data should not be used. In general, the permit writer should evaluate the background data submitted by an applicant carefully to determine whether they adequately characterize the air quality in the vicinity of the unit. In cases in which Subpart X units are located near other sources that are expected to have a significant concentration gradient in the area, the nearby sources should be modeled explicitly. The effect expected from all other sources (natural and distant sources) then should be added to the results of modeling.

It is important that the background concentrations that are added to the results of modeling have the same averaging period as those results. For example, if the eight-hour average concentration of a contaminant is modeled, an eight-hour average background concentration should be added to determine the total eight-hour concentration.

If no representative background data are available, monitoring may need to be conducted to determine the existing air quality. Section 5.2.1.2 discusses collection of on-site air quality data.

Evaluation of Selection and Application of the Model

Selection and application of a suitable air dispersion model is to a great extent dependent on the application of site-specific criteria. Several of the principal criteria for selecting a model were discussed in preceding sections. They include type of source, meteorological data, locations of receptors, features of the terrain, deposition, chemical transformation, and background concentrations. Permit writers should evaluate the details about the site, the available data, and the process by which the applicant selected the site to determine whether the modeling analysis is appropriate.

In some cases, site-specific or source-specific characteristics of a Subpart X unit may be such that no screening models are capable of simulating their effects on the transport and dispersion of a contaminant. In such cases, a refined modeling analysis must be required. The permit writer should evaluate the capabilities of the screening model used in a permit applicant's screening analysis and compare those capabilities with the characteristics of the source and site to determine whether the model selected is appropriate. In cases in which the permit writer determines that the screening model selected is inadequate, he or she should issue a NOD to indicate the reasons for such inadequacy.

The permit writer should evaluate carefully any screening models that are not in Table 5.1 or in Appendix A or B of *Guidelines On Air Quality Models* to determine whether such models are suitable for the task at hand. In such cases, it is recommended that the permit writer seek the advice of modeling experts to determine whether the alternative model is suitable for the specified task.

If a permit applicant cannot demonstrate compliance with appropriate standards through the use of a screening model, or if the site-specific details require use of a more sophisticated model, the permit writer should issue a NOD to indicate that a refined modeling analysis must be conducted. Use of site-specific data will result in more accurate modeling results. Since refined models use more detailed data, the permit writer should verify that the model used in a refined analysis is appropriate for the special features of the site and the data available.

Of the refined models listed in Table 5.3, ISC3 is the most commonly used and accepted for regulatory applications. Other models in Table 5.3 can be applied for specific purposes. For example, releases from OB/OD units are usually intermittent or near instantaneous, and are not stack-type sources. In such cases, use of ISC3 would not be appropriate because it can simulate only continuous releases. The INPUFF model has been used for OB/OD operations and its results have been found acceptable. However, INPUFF has some limitations, and other models may be better suited for OB/OD applications. The limitations of INPUFF are discussed briefly in the model summary section of this guidance. The CALPUFF model can be used for OB/OD applications and has more extensive capabilities than INPUFF, but the model requires additional data and is more difficult to use. As discussed in the previous sections, OBODM was developed specifically to model OB/OD emissions. The OBODM algorithms address the unique dispersion characteristics associated with open burn and detonation operations.

Evaluation of Results of Modeling

A permit writer must consider several factors when evaluating results of modeling. Averaging time, background concentrations, and an overall perspective of the data entered and results produced must be taken into account in interpreting results to determine whether they make sense. The permit writer should compare the model results with the data entered to determine whether the results are realistic.

Often, model analyses must estimate maximum short-term as well as long-term effects. Some models calculate concentrations for only one averaging period (usually one hour), while others calculate concentrations for several averaging periods. If a model is limited to one averaging period, permit applicants may use modeled concentrations to estimate concentrations for other averaging periods. Adjustments may be made to reflect how long the unit emits hazardous constituents, and for variations in meteorological conditions. Any averaging time factors used by permit applicants should be well documented and justified.

Reviewing the Results of Air Modeling: Items to Check

- **Spot check source characterization data input files.**
- **Compare building down wash parameters to the output from BPIP.**
- **Spot check several modeled receptor elevation against USGS map.**
- **Review receptor lists or files to ensure that the elevation array contains non-zero values.**
- **Check the anemometer height to ensure that it is correct for the station and years used in the analysis.**
- **Ensure that the GEP stack height determined by BPIP was not used in the air modeling analysis.**

Additional guidance on reviewing air modeling results can be found in EPA Region 6's "Suggestions for Auditing Assessment Air Modeling Studies".

5.3.2 Groundwater Modeling

This section provides information regarding hydrogeological characterization and model selection to assist permit writers in evaluating modeling results submitted by Subpart X permit applicants.

Groundwater modeling can be used when monitoring is impractical or to supplement and verify monitoring data. Groundwater modeling has several applications in the permitting process for Subpart X units. The groundwater model can be used (1) to predict conservative, "worst-case" scenarios during a detailed groundwater assessment, (2) to assist in