Chapter 3
Air Dispersion and Deposition Modeling

What's Covered in Chapter 3:

- U.S. EPA-Recommended Air Dispersion and Deposition Model
- Air Model Development
- Site-Specific Characteristics Required for Air Modeling
- Use of Unit Emission Rate
- Partitioning of Emissions
- Meteorological Data Required for Air Modeling
- Meteorological Preprocessors and Interface Programs
- ISCST3 Model Input Files
- ISCST3 Model Execution
- Use of Modeled Output
- Modeling Fugitive Emissions
- Estimating Media Concentrations

Combustion of materials produces residual amounts of pollution that may be released to the environment. Estimation of potential ecological risks associated with these releases requires knowledge of atmospheric pollutant concentrations and annual deposition rates in the areas around the combustion facility at habitat-specific scenario locations. Air concentrations and deposition rates are usually estimated by using air dispersion models. Air dispersion models are mathematical constructs that approximate the physical processes occurring in the atmosphere that directly influence the dispersion of gaseous and particulate emissions from the stack of a combustion unit. These mathematical constructs are coded into computer programs to facilitate the computational process.

This chapter provides guidance on the development and use of the standard U.S. EPA air dispersion model that U.S. EPA expects to be used in most situations—the Industrial Source Complex Short-Term

Model (ISCST3). ISCST3 requires the use of the following information for input into the model, and consideration of output file development:

- Site-specific characteristics required for air modeling (Section 3.2)
    - Surrounding terrain (Section 3.2.1)
    - Surrounding land use (Section 3.2.2)
    - Facility building characteristics (Section 3.2.3)
- Unit emission rate (Section 3.3)
- Partitioning of emissions (Section 3.4)
- Meteorological data (Section 3.5)
- Source Characteristics (Section 3.7)

ISCST3 also requires the use of several preprocessing computer programs that prepare and organize data for use in the model. Section 3.6 describes these programs. Section 3.7 describes the structure and format of the input files. Section 3.8 describes limitations to be considered in executing ISCST3. Section 3.9 describes use of the air modeling output in the risk assessment computations. Section 3.10 discusses air modeling of fugitive emissions. Section 3.11 describes how to estimate the media concentrations of COPCs in media.

If applicable, readers are encouraged to consult the air dispersion modeling chapter (Chapter 3) of the U.S. EPA OSW guidance document *Human Health Risk Assessment Protocol* (HHRAP) (U.S. EPA 1998c) before beginning the air modeling process to ensure the consideration of specific issues related to human health risk assessment. Additionally, the *Guideline on Air Quality Models* (GAQM) (U.S. EPA 1996c) is a primary reference for all US EPA and state agencies on the use of air models for regulatory purposes. The GAQM is incorporated in 40 CFR Part 51 as Appendix W. The Office of Air Quality Planning and Support (OAQPS) provides the GAQM and extensive information on air dispersion models, meteorological data, data preprocessors, user’s guides, and model applicability on the Support Center for Regulatory Air Models (SCRAM) web site at address “http://www.epa.gov/scram001/index.htm”. General questions regarding air modeling or information on the web site should be addressed to “atkinson.dennis@epamail.epa.gov”. Specific questions on the use of this guidance should be addressed to the appropriate permitting authority.

3.1 DEVELOPMENT OF AIR MODELS

This section (1) briefly describes the history of air model development, (2) introduces some data preprocessing programs developed to aid in preparing air model input files (these preprocessing programs are described in more detail in Sections 3.2.4 and 3.6, and (3) introduces ExInter Version 1.0, a preprocessor to ISCST3.

3.1.1 History of Risk Assessment Air Dispersion Models

Before 1990, several air dispersion models were used by U.S. EPA and the regulated community. These models were inadequate for use in risk assessments because they considered only concentration, and not the deposition of contaminants to land. The original U.S. EPA guidance (1990a) on completing risk assessments identified two models that were explicitly formulated to account for the effects of deposition.

- COMPLEX terrain model, version 1 (COMPLEX I), from which a new model—COMPLEX terrain model with DEPosition (COMPDEP)—resulted
- Rough Terrain Diffusion Model (RTDM), from which a new model—RTDMDEP—resulted

COMPDEP was updated to include building wake effects from a version of the ISCST model in use at the time. Subsequent U.S. EPA guidance (1993h; 1994b) recommended the use of COMPDEP for air deposition modeling. U.S. EPA (1993h) specified COMPDEP Version 93252, and U.S. EPA (1994b) specified COMPDEP Version 93340. When these recommendations were made, a combined ISC-COMPDEP model (a merger of the ISCST2 and COMPLEX I model) was still under development. The merged model became known as ISCSTDFT. U.S. EPA guidance (1994l) recommended the use of the ISCSTDFT model. After reviews and adjustments, this model was released as ISCST3. The ISCST3 model contains algorithms for dispersion in simple, intermediate, and complex terrain; dry deposition; wet deposition; and plume depletion.

The use of the COMPDEP, RTDMDEP, and ISCST models is described in more detail in the following user's manuals; however, all models except the current version of ISCST3 are obsolete:

- Environmental Research and Technology (ERT). 1987. *User's Guide to the Rough Terrain Diffusion Model Revision 3.20*. ERT Document P-D535-585. Concord, Massachusetts.

- Turner, D.B. 1986. *Fortran Computer Code/User's Guide for COMPLEX I Version 86064: An Air Quality Dispersion Model in Section 4. Additional Models for Regulatory Use.* Source File 31 Contained in UNAMAP (Version 6). National Technical Information Service (NTIS) PB86-222361/AS.

- U.S. EPA. 1979. *Industrial Source Complex Dispersion Model User's Guide, Volume I.* Prepared by the H.E. Cramer Company. Salt Lake City, Utah. Prepared for the Office of Air Quality Planning and Standards. Research Triangle Park, North Carolina. EPA 450/4-79/030. NTIS PB80-133044.

- U.S. EPA. 1980b. *User's Guide for MPTER: A Multiple Point Gaussian Dispersion Algorithm with Optional Terrain Adjustment*. Environmental Sciences Research Laboratory. Research Triangle Park, North Carolina. EPA 600/8-80/016. NTIS PB80-197361.

- U.S. EPA. 1982a. *MPTER-DS: The MPTER Model Including Deposition and Sedimentation*. Prepared by the Atmospheric Turbulence and Diffusion Laboratory. National Oceanic and AtmosphericAdministration (NOAA). Oak Ridge, Tennessee. Prepared for the Environmental Sciences Research Laboratory. Research Triangle Park, North Carolina. EPA 600/8-82/024. NTIS PB83-114207.

- U.S. EPA. 1987b. *On-Site Meteorological Program Guidance for Regulatory Modeling Applications*. Office of Air Quality Planning and Standards. Research Triangle Park, North Carolina.

- U.S. EPA. 1995c. *User's Guide for the Industrial Source Complex (ISC3) Dispersion Models, Volumes I and II.* Office of Air Quality Planning and Standards. Emissions, Monitoring, and Analysis Division. Research Triangle Park, North Carolina. EPA 454/B-95/003a. September.

Users of this document are advised that a draft version of ISCST3 that includes algorithms for estimating the dry gas deposition (currently referred to as the “Draft Dry Gas Deposition Model: GDISCDFT, Version 96248") is available on the SCRAM web site. Use of this version to support site specific air modeling applications is not required, because many of the parameters needed to execute the model are not available in guidance or the technical literature. Therefore, until the draft version is reviewed and approved, and the data is provided by U.S. EPA or in the technical literature, U.S. EPA OSW recommends that the current version of ISCST3, in conjunction with the procedure presented in this guidance (Appendix B) for estimating dry gas deposition using deposition velocity and gas concentration, should be used for risk assessments.

3.1.2 Preprocessing Programs

ISCST3 requires the use of additional computer programs, referred to as "preprocessing" programs. These programs manipulate available information regarding surrounding buildings and meteorological data into a format that can be used by ISCST3. Currently, these programs include the following:

- PCRAMMET (Personal Computer Version of the Meteorological Preprocessor for the old RAM program) prepares meteorological data for use in ISCST3. The program organizes data—such as precipitation, wind speed, and wind direction—into rows and columns of information that are read by ISCST3. The PCRAMMET User's Guide contains detailed information for preparing the required meteorological input file for the ISCST3 model (U.S. EPA 1995b).

- Building Profile Input Program (BPIP) calculates the maximum crosswind widths of buildings, which ISCST3 then uses to estimate the effects on air dispersion. This effect on dispersion by surrounding buildings is typically known as building downwash or wake effects. The BPIP User's Guide contains detailed information for preparing the required building dimensions (length, height, and width) and locations for the ISCST3 model (U.S. EPA 1995d).

- Meteorological Processor for Regulatory Models (MPRM) prepares meteorological data for use in the ISCST3 by using on-site meteorological data rather than data from government sources (National Weather Service [NWS] or the Solar And Meteorological Surface Observational Network [SAMSON]). MPRM merges on-site measurements of precipitation, wind speed, and wind direction with off-site data from government sources into rows and columns of information that are read by ISCST3. The MPRM User's Guide contains information for preparing the required meteorological input file for the ISCST3 model (U.S. EPA 1996e).

Most air dispersion modeling performed to support risk assessments will use PCRAMMET and BPIP. MPRM will generally not be used unless on-site meteorological information is available. However, only MPRM is currently scheduled to be updated to include the meteorological parameters (solar radiation and leaf area index) required to execute the dry deposition of vapor algorithms included in the new version of ISCST3. The draft version of MPRM is available for review and comment on the SCRAM web site as GDMPRDFT (dated 96248).

3.1.3 Expert Interface (ExInter Version 1.0)

ExInter is an expert interface system enhanced by U.S. EPA Region 6 for the ISCST3 model. By enhancing ExInter, the goal of U.S. EPA Region 6 was to support the in-house performance of air dispersion modeling by regional U.S. EPA and state agency personnel at hazardous waste combustion units necessary to support risk assessments conducted at these facilities. ExInter enables the user to build input files and run ISCST3 and its preprocessor programs in a Windows-based environment. Specific procedures for developing input files are stored in an available knowledge database. The underlying premise of the ExInter system is that the knowledge of an "expert" modeler is available to "nonexpert" modeling personnel at all times. However, some air modeling experience is required to use ExInter and its components as recommended in this guidance. The ExInter program has been written in Microsoft Visual C++ in a Microsoft Windows environment.

ExInter allows for a generic source category that comprises point, area, and volume sources. For each source type, the program queries the relevant variables for the user. In addition to asking about the inputs regarding the source types, ExInter also asks about control options, receptors, meteorology, and output formats. ExInter then creates an input file, as required by the ISCST3 dispersion model. ExInter also allows the user to run the ISCST3 model and browse the results file.

Version 1.0 of ExInter provides for input parameters to model dry gas deposition included in a draft version of ISCST3. However, the data required for dry gas deposition requires a literature search and prior regulatory approval. The procedure presented in this guidance (Appendix B) for estimating dry gas deposition using deposition velocity and gas concentration is appropriate without prior approval. More detailed information on how to use ExInter can be found in the following:

- U.S. EPA. 1996i. *User's Guide for ExInter 1.0. Draft Version.* U.S. EPA Region 6 Multimedia Planning and Permitting Division. Center for Combustion Science and Engineering. Dallas, Texas. EPA/R6-096-0004. October.

ExInter is available on the SCRAM web site at "http://www.epa.gov/scram001/index.htm" under the Modeling Support section "Topics for Review". Six self-extracting compressed files contain all components for installation and use. The user's guide is accessed interactively using the help command. Individual user's guides to ISCST3, BPIP, PCRAMMET, and MPRM also provide good references for using ExInter components. ExInter requires a minimum of 15 megabytes of free hard disk space, Windows 3.1, 8 megabytes of system memory, and a 486 processor.

3.2 SITE-SPECIFIC INFORMATION REQUIRED TO SUPPORT AIR MODELING

Site-specific information for the facility and surrounding area required to support air dispersion modeling includes (1) the elevation of the surrounding land surface or terrain, (2) surrounding land uses, and (3) characteristics of on-site buildings that may affect the dispersion of COPCs into the surrounding environment.

Often, site-specific information required to support air dispersion modeling can be obtained from review of available maps and other graphical data on the area surrounding the facility. The first step in the air modeling process is a review of available maps and other graphical data on the surrounding area. U.S. Geological Survey (USGS) 7.5-minute topographic maps (1:24,000) extending to 10 kilometers from the facility, and USGS 1:250,000 maps extending out to 50 kilometers, should be obtained to identify site location, nearby terrain features, waterbodies and watersheds, ecosystems, special ecological habitats, and land use. Aerial photographs are frequently available for supplemental depiction of the area. An accurate facility plot plan—showing buildings, stacks, property and fence lines—is also needed. Facility information including stack and fugitive source locations, building corners, plant property, and fence lines should be provided in Universal Transverse Mercator (UTM) grid coordinates in meters east and north in both USGS reference systems.

Most USGS paper 7.5-minute topographic maps are published in the North American Datum system established in 1927 (NAD 27). However, most digital elevation data (e.g., USGS Digital Elevation Mapping) is in the 1983 revised system (NAD 83). Special consideration should be given not to mix source data obtained from USGS maps based on NAD 27 with digital terrain elevation data based on NAD 83. Emission source information should be obtained in the original units from the facility data, and converted to metric units for air modeling, if necessary. Digital terrain data can be acquired from USGS or another documented source.

The specific information that must be collected is described in the following subsections. Entry of this information into the ISCST3 input files is described in Section 3.7.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- All site-specific maps, photographs, or figures used in developing the air modeling approach
- Mapped identification of facility information including stack and fugitive source locations, locations of facility buildings surrounding the emission sources, and property boundaries of the facility

3.2.1 Surrounding Terrain Information

Terrain is important to air modeling because air concentrations and deposition rates are greatly influenced by the height of the plume above local ground level. Terrain is characterized by elevation relative to stack height. For air modeling purposes, terrain is referred to as “complex” if the elevation of the surrounding land within the assessment area—typically defined as anywhere within 50 kilometers from the stack—is above the top of the stack evaluated in the air modeling analysis. Terrain at or below stack top is referred to as “simple.” ISCST3 implements U.S. EPA guidance on the proper application of air modeling methods in all terrain if the modeler includes terrain elevation for each receptor grid node and specifies the appropriate control parameters in the input file.

Even small terrain features may have a large impact on the air dispersion and deposition modeling results and, ultimately, on the risk estimates. U.S. EPA OSW recommends that most air modeling include terrain elevations for every receptor grid node. Some exceptions may be those sites characterized by very flat terrain where the permitting authority has sufficient experience to comfortably defer the use of terrain data because its historical effect on air modeling results has been shown to be minimal.

In addition to maps which are used to orient and facilitate air modeling decisions, the digital terrain data used to extract receptor grid node elevations should be provided in electronic form. One method of obtaining receptor grid node elevations is using digital terrain data available from the USGS on the Internet at web site “http://www.usgs.gov”. An acceptable degree of accuracy is provided by the USGS “One Degree” (e.g., 90 meter data) data available as “DEM 250" 1:250,000 scale for the entire United States free of charge. USGS 30-meter data is available for a fee. Either 90-meter or 30-meter data is sufficient for most risk assessments which utilize 100 meter or greater grid spacing. Digital terrain data may also be purchased from a variety of commercial vendors which may require vendor-provided programs to extract the data. The elevations may also be extracted manually at each receptor grid node from USGS topographic maps.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Description of the terrain data used for air dispersion modeling
- Summary of any assumptions made regarding terrain data
- Description of the source of any terrain data used, including any procedures used to manipulate terrain data for use in air dispersion modeling

3.2.2 Surrounding Land Use Information

Land use information in the risk assessment is used for purposes of air dispersion modeling and the identification or selection of exposure scenario locations (see Chapter 4) in the risk assessment. Land use analysis for purposes of selecting exposure scenario locations usually occurs out to a radius of 50 kilometers from the centroid of the stacks to ensure identification of all receptors that may be impacted. However, in most cases, air modeling performed out to a radius of 10 kilometers allows adequate characterization for the evaluation of exposure scenario locations. If a facility with multiple stacks or emission sources is being evaluated, the radius should be extended from the centroid of a polygon drawn from the various stack coordinates.

Land use information is also important to air dispersion modeling, but at a radius closer (3 kilometers) to the emission source(s). Certain land uses, as defined by air modeling guidance, effect the selection of air dispersion modeling variables. These variables are known as dispersion coefficients and surface roughness. USGS 7.5-minute topographic maps, aerial photographs, or visual surveys of the area typically are used to define the air dispersion modeling land uses (www.usgs.gov).

3.2.2.1 Land Use for Dispersion Coefficients

The Auer method specified in the Guideline on Air Quality Models (40 CFR Part 51, Appendix W) is used to define land use for purposes of specifying the appropriate dispersion coefficients built into ISCST3.

Land use categories of “rural” or “urban” are taken from the methods of Auer (Auer 1978). Areas typically defined as rural include residences with grass lawns and trees, large estates, metropolitan parks and golf courses, agricultural areas, undeveloped land, and water surfaces. Auer typically defines an area as “urban” if it has less than 35 percent vegetation coverage or the area falls into one of the following use types:

Urban Land Use		
Type	**Use and Structures**	**Vegetation**
I1	Heavy industrial	Less than 5 percent
I2	Light/moderate industrial	Less than 5 percent
C1	Commercial	Less than 15 percent
R2	Dense single/multi-family	Less than 30 percent
R3	Multi-family, two-story	Less than 35 percent

In general, the Auer method is described as follows:

Step 1 Draw a radius of 3 kilometers from the center of the stack(s) on the site map.

Step 2 Inspect the maps, and define in broad terms whether the area within the radius is rural or urban, according to Auer’s definition.

Step 3 Classify smaller areas within the radius as either rural or urban, based on Auer’s definition. (It may be prudent to overlay a grid [for example, 100 by 100 meters] and identify each square as primarily rural or urban)

Step 4 Count the total of rural squares; if more than 50 percent of the total squares are rural, the area is rural; otherwise, the area is urban.

Alternatively, digital land use databases may be used in a computer-aided drafting system to perform this analysis.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Description of the methods used to determine land use surrounding the facility
- Copies of any maps, photographs, or figures used to determine land use
- Description of the source of any computer-based maps used to determine land use

3.2.2.2 Land Use for Surface Roughness Height (Length)

Surface roughness height—also referred to as (aerodynamic) surface roughness length—is the height above the ground at which the wind speed goes to zero. Surface roughness affects the height above local ground level that a particle moves from the ambient air flow above the ground (for example in the plume) into a "captured" deposition region near the ground. That is, ISCST3 causes particles to be "thrown" to the ground at some point above the actual land surface, based on surface roughness height. Surface roughness height is defined by individual elements on the landscape, such as trees and buildings.

U.S. EPA (1995b) recommended that land use within 5 kilometers of the stack be used to define the average surface roughness height. For consistency with the method for determining land use for dispersion coefficients (Section 3.2.2.1), the land use within 3 kilometers generally is acceptable for determination of surface roughness. Surface roughness height values for various land use types are as follows:

Surface Roughness Heights for Land Use Types and Seasons (meters)

Land Use Type	Spring	Summer	Autumn	Winter
Water surface	0.0001	0.0001	0.0001	0.0001
Deciduous forest	1.00	1.30	0.80	0.50
Coniferous forest	1.30	1.30	1.30	1.30
Swamp	0.20	0.20	0.20	0.05
Cultivated land	0.03	0.20	0.05	0.01
Grassland	0.05	0.10	0.01	0.001
Urban	1.00	1.00	1.00	1.00
Desert shrubland	0.30	0.30	0.30	0.15

Source: Sheih, Wesley, and Hicks (1979)

If a significant number of buildings are located in the area, higher surface roughness heights (such as those for trees) may be appropriate (U.S. EPA 1995b). A specific methodology for determining average surface roughness height has not been proposed in prior guidance documents. For facilities using National Weather Service surface meteorological data, the surface roughness height for the measurement site may be set to 0.10 meters (grassland, summer) without prior approval. If a different value is proposed for the measurement site, the value should be determined applying the following procedure to land use at the measurement site. For the application site, the following method should be used to determine surface roughness height:

Step 1 Draw a radius of 3 kilometers from the center of the stack(s) on the site map.

Step 2 Inspect the maps, and use professional judgment to classify the areas within the radius according to the PCRAMMET categories (for example water, grassland, cultivated land, and forest); a site visit may be necessary to verify some classifications.

Step 3 Calculate the wind rose directions from the 5 years of meteorological data to be used for the study (see Section 3.4.1.1); a wind rose can be prepared and plotted by using the U.S. EPA WRPLOT program from the U.S. EPA's Support Center for Regulatory Air Models bulletin board system (SCRAM BBS).

Step 4 Divide the circular area into 16 sectors of 22.5 degrees, corresponding to the wind rose directions (for example, north, north-northeast, northeast, and east-northeast) to be used for the study.

Step 5 Identify a representative surface roughness height for each sector, based on an area-weighted average of the land use within the sector, by using the land use categories identified above.

Step 6 Calculate the site surface roughness height by computing an average surface roughness height weighted with the frequency of wind direction occurrence for each sector.

Alternative methods of determining surface roughness height may be proposed for agency approval prior to use in an air modeling analysis.

3.2.3 Information on Facility Building Characteristics

Building wake effects have a significant impact on the concentration and deposition of COPCs near the stack. Building wake effects are flow lines that cause plumes to be forced down to the ground much sooner than they would if the building was not there. Therefore, the ISCST3 model contains algorithms for evaluating this phenomenon, which is also referred to as "building downwash." The downwash analysis should consider all nearby structures with heights at least 40 percent of the height of the shortest stack to be modeled. The 40 percent value is based on Good Engineering Practice (GEP) stack height of 2.5 times the height of nearby structures or buildings (stack height divided by 2.5 is equal to 0.40 multiplied by the stack height [40 CFR Part 51 Appendix W]). Building dimensions and locations are used with stack heights and locations in BPIP to identify the potential for building downwash. BPIP and the BPIP user's guide can be downloaded from the SCRAM web site and should be referred to when addressing specific questions. The BPIP output file is in a format that can be copied and pasted into the source (SO) pathway of the ISCST3 input file. The following procedure should be used to identify buildings for input to BPIP:

Step 1 Lay out facility plot plan, with buildings and stack locations clearly identified (building heights must be identified for each building); for buildings with more than one height or roof line, identify each height (BPIP refers to each height as a tier).

Step 2 Identify the buildings required to be included in the BPIP analysis by comparing building heights to stack heights. The building height test requires that only buildings at least 40 percent of the height of a potentially affected stack be included in the BPIP input file. For example, if a combustion unit stack is 50 feet high, only buildings at least 20 feet (0.40 multiplied by 50 feet) tall will affect air flow at stack top. Any buildings shorter than 20 feet should not be included in the BPIP analysis. The building height test is performed for each stack and each building.

Step 3 Use the building distance test to check each building required to be included in BPIP from the building height test. For the building distance test, only buildings "nearby" the stack will affect air flow at stack top. "Nearby" is defined as "five times the lesser of building height or crosswind width" (U.S. EPA 1995d). A simplified distance test may be used by considering only the building height rather than the crosswind width. While some buildings with more height than width will be included unnecessarily using this simplification, BPIP will identify correctly only the building dimensions required for ISCST3.

As an example, if a plot plan identifies a 25-foot tall building that is 115 feet from the 50-foot tall combustion unit stack center to the closest building corner. The building distance test, for this building only, is five times the building height, or 125 feet (five multiplied by the building height, 25 feet). This building would be included in the BPIP analysis, because it passes the building height test and building distance test.

Step 4 Repeat steps 2 and 3 for each building and each stack, identifying all buildings to be included in the BPIP. If the number of buildings exceeds the BPIP limit of eight buildings, consider combining buildings, modifying BPIP code for more buildings, or using third-party commercial software which implements BPIP. If two buildings are closer than the height of the taller building, the two buildings may be combined. For example, two buildings are 40 feet apart at their closest points. One building is 25 feet high, and the other building is 50 feet high. The buildings could be combined into one building for input to BPIP. For input to BPIP, the corners of the combined building are the outer corners of the two buildings. For unusually shaped buildings with more than the eight corners allowed by BPIP, approximate the building by using the eight corners that best represent the extreme corners of the building. The BPIP User's Guide contains additional description and illustrations on combining buildings, and BPIP model limitations (U.S. EPA 1995d).

Step 5 Mark off the facility plot plan with UTM grid lines. Extract the UTM coordinates of each building corner and each stack center to be included in BPIP input file. Although BPIP allows the use of "plant coordinates," U.S. EPA OSW requires that all inputs to the air modeling be prepared using UTM coordinates (meters) for consistency. UTM coordinates are rectilinear, oriented to true north, and in metric units required for ISCST3 modeling. Almost all air modeling will require the use of USGS topographic data (digital and maps) for receptor elevations, terrain grid files, location of plant property, and identification of surrounding site features. Therefore, using an absolute coordinate system will enable the modeler to check inputs at each step of the analysis. Also, the meteorological data are oriented to true north. Significant errors will result from ISCST3 if incorrect stack or building locations are used, plant north is incorrectly rotated to true north, or incorrect base elevations are used. With computer run times of multiple years of meteorological data requiring many hours (up to 40 hours for one deposition run with depletion), verification of locations at each step of preparing model inputs will prevent the need to remodel.

Several precautions and guidelines should be observed in preparing input files for BPIP:

- Before BPIP is run, the correct locations should be graphically confirmed. One method is to plot the buildings and stack locations by using a graphics program. Several commercial programs incorporating BPIP provide graphic displays of BPIP inputs.

- U.S. EPA OSW recommends, in addition to using UTM coordinates for stack locations and building corners, using meters as the units for height.

- Carefully include the stack base elevation and building base elevations by using the BPIP User's Guide instructions.

- Note that the BPIP User's Guide (revised February 8, 1995) has an error on page 3-5, Table 3-1, under the "TIER(i,j)" description, which incorrectly identifies tier height as base elevation.

- BPIP mixes the use of "real" and "integer" values in the input file. To prevent possible errors in the input file, note that integers are used where a count is requested (for example, the number of buildings, number of tiers, number of corners, or number of stacks).

- The stack identifications (up to eight characters) in BPIP must be identical to those used in the ISCST3 input file, or ISCST3 will report errors.

For most sites, BPIP executes in less than 1 minute. The array of 36 building heights and 36 building widths (one for each of 36 10-degree direction sectors) are input into the ISCST3 input file by cutting and pasting from the BPIP output file. The five blank spaces preceding "SO" in the BPIP output file must be deleted so that the "SO" begins in the first column of the ISCST3 input file.

One use of BPIP is to design stack heights for new facilities or determine stack height increases required to avoid the building influence on air flow, which may cause high concentrations and deposition near the facility. The output for BPIP provides the GEP heights for stacks. Significant decreases in concentrations and deposition rates will begin at stack heights at least 1.2 times the building height, and further decreases occur at 1.5 times building height, with continual decreases of up to 2.5 times building height (GEP stack height) where the building no longer influences stack gas.

3.3 USE OF UNIT EMISSION RATE

The ISCST3 model is usually run with a unit emission rate of 1.0 g/s in order to preclude having to run the model for each specific COPC. The unitized concentration and deposition output from ISCST3, using a unit emission rate, are adjusted to the COPC-specific air concentrations and deposition rates in the estimating media concentration equations (see Section 3-11) by using COPC-specific emission rates obtained during the trial burn (see Chapter 2). Concentration and deposition are directly proportional to a unit emission rate used in the ISCST3 modeling.

For facilities with multiple stacks or emission sources, each source must be modeled separately. The key to not allowing more than one stack in a single run is the inability to estimate stack-specific risks, which limits the ability of a permitting agency to evaluate which stack is responsible for the resulting risks. Such ambiguity would make it impossible for the agency to specify protective, combustion unit-specific permit limits. If a facility has two or more stacks with identical characteristics (emissions, stack parameters, and nearby locations), agency approval may be requested to represent the stacks with a single set of model runs.

3.4 PARTITIONING OF EMISSIONS

COPC emissions to the environment occur in either vapor or particle phase. In general, most metals and organic COPCs with very low volatility (refer to fraction of COPC in vapor phase [*Fv*] less than 0.05, as presented in Appendix A-2) are assumed to occur only in the particle phase. Organic COPCs occur as either only vapor phase (refer to *Fv* of 1.0, as presented in Appendix A-2) or with a portion of the vapor condensed onto the surface of particulates (e.g., particle-bound). COPCs released only as particulates are modeled with different mass fractions allocated to each particle size than the mass fractions for the organics released in both the vapor and particle-bound phases. Due to the limitations of the ISCST3 model, estimates of vapor phase COPCs, particle phase COPCs, and particle-bound COPCs cannot be provided in a single pass (run) of the model. Multiple runs are required. An example of this requirement is the risk assessment for the WTI incinerator located in East Liverpool, Ohio. The study used three runs; a vapor phase run for organic COPCs, a particle run with mass weighting of the particle phase metals and organic COPCs with very low volatility, and a particle run with surface area weighting of the particle-bound organic COPCs .

3.4.1 Vapor Phase Modeling

ISCST3 output for vapor phase air modeling runs are vapor phase ambient air concentration and wet vapor deposition at receptor grid nodes based on the unit emission rate. Vapor phase runs do not require a particle size distribution in the ISCST3 input file. One vapor phase run is required for each receptor grid that is modeled (see Section 3.7).

3.4.2 Particle Phase Modeling (Mass Weighting)

ISCST3 uses algorithms to compute the rate at which dry and wet removal processes deposit particulate-phase COPCs emitted from a combustion unit stack to the Earth’s surface. Particle size is the main determinant of the fate of particles in air flow, whether dry or wet. The key to dry particle deposition rate is the terminal, or falling, velocity of a particle. Particle terminal velocity is calculated mainly from the particle size and particle density. Large particles fall more rapidly than small particles and are deposited closer to the stack. Small particles have low terminal velocities, with very small particles remaining suspended in the air flow. Wet particle deposition also depends on particle size as larger particles are more easily removed, or scavenged, by falling liquid (rain) or frozen (snow or sleet) precipitation. An ISCST3 modeling analysis of particle phase emissions for deposition rate requires an initial estimate of the particle size distribution, distinguished on the basis of particle diameter.

The diameters of small particulates contained in stack emissions are usually measured in micrometers. The distribution of particulate by particle diameter will differ from one combustion process to another, and is greatly dependent on (1) the type of furnace, (2) the design of the combustion chamber, (3) the composition of the feed fuel, (4) the particulate removal efficiency, (5) the design of the APCS, (6) the amount of air, in excess of stoichiometric amounts, that is used to sustain combustion, and (7) the temperature of combustion. However, based on these variables, the particle size distribution cannot be calculated, but only directly measured or inferred from prior data. Unfortunately, few studies have been performed to directly measure particle size distributions from a variety of stationary combustion sources (U.S. EPA 1986a).

U.S. EPA OSW recommends that existing facilities perform stack tests to identify particle size distribution. These data should represent actual operating conditions for the combustion unit and air pollution control device (APCD) that remove particulate from the stack gas. A table of particle size distribution data should be prepared using stack test data in the format in Table 3-1.

U.S. EPA OSW expects that stack test data will be different from the values presented in Table 3-1 because of the use of particle "cut size" for the different cascade impactor filters (or Coulter counter-based distributions) used during actual stack sampling. The test method will drive the range of particle sizes that are presented in the results of the stack test. However, because ISCST3 requires mean particle diameter for each particle size distribution, and the stack test data identifies only the mass ("weight") of particles in a range bounded by two specific diameters, stack test data must be converted into a mean particle diameter which approximates the diameter of all the particles within a defined range. Consistent with U.S. EPA 1993h, the mean particle diameter is calculated by using the following equation:

$$D_{mean} = [0.25 \cdot (D_1^3 + D_1^2 D_2 + D_1 D_2^2 + D_2^3)]^{0.33} \qquad \text{Equation 3-1}$$

where

D_{mean} = Mean particle diameter for the particle size category (μm)
D_1 = Lower bound cut of the particle size category (μm)
D_2 = Upper bound cut of the particle size category (μm)

For example, the mean particle diameter of 5.5 μm in Table 3-1 is calculated from a lower bound cut size (assuming a cascade impactor is used to collect the sample) of 5.0 μm to an upper bound cut size of 6.15 μm. In this example, the mean particle diameter is calculated as:

$$D_{mean} = \left[0.25\ (5.0^3 + (5.0)^2(6.15) + (5.0)(6.15)^2 + 6.15^3)\right]^{0.33} = 5.5\ \mu m$$

TABLE 3-1

GENERALIZED PARTICLE SIZE DISTRIBUTION, AND PROPORTION OF AVAILABLE SURFACE AREA, TO BE USED AS A DEFAULT IN DEPOSITION MODELING IF SITE-SPECIFIC DATA ARE UNAVAILABLE

1	2	3	4	5	6
Mean Particle Diameter [a] (μm)	**Particle Radius (μm)**	**Surface Area/ Volume (μm^{-1})**	**Fraction of Total Mass[b]**	**Proportion Available Surface Area**	**Fraction of Total Surface Area**
> 15.0	7.50	0.400	0.128	0.0512	0.0149
12.5	6.25	0.480	0.105	0.0504	0.0146
8.1	4.05	0.741	0.104	0.0771	0.0224
5.5	2.75	1.091	0.073	0.0796	0.0231
3.6	1.80	1.667	0.103	0.1717	0.0499
2.0	1.00	3.000	0.105	0.3150	0.0915
1.1	0.55	5.455	0.082	0.4473	0.1290
0.7	0.40	7.500	0.076	0.5700	0.1656
< 0.7	0.40	7.500	0.224	1.6800	0.4880

Notes:

a Geometric mean diameter in a distribution from U.S. EPA (1980a), as presented in U.S. EPA (1993h)
b The terms mass and weight are used interchangeably when using stack test data

From Table 3-1, the mean particle diameter is 5.5 μm. The mass of particulate from the 5.0 μm stack test data is then assigned to the 5.5 μm mean particle diameter for the purpose of computing the "fraction of total mass."

Typically, eight to ten mean particle diameters are available from stack test results. As determined from a sensitivity analysis conducted by The Air Group-Dallas under contract to U.S. EPA Region 6 (www.epa.gov/region06), a minimum of three particle size categories (> 10 microns, 2-10 microns, and < 2 microns) detected during stack testing are generally the most sensitive to air modeling with ISCST-3 (U.S. EPA 1997). For facilities with stack test results which indicate mass amounts lower than the detectable limit (or the filter weight is less after sampling than before), a single mean particle size diameter of 1.0 microns should be used to represent all mass (e.g., particle diameter of 1.0 microns or a particle mass fraction of 1.0) in the particle and particle-bound model runs. Because rudimentary methods for stack testing may not detect the very small size or amounts of COPCs in the particle phase, the use of a 1.0 micron particle size will allow these small particles to be included properly as particles in the risk assessment exposure pathways while dispersing and depositing in the air model similar in behavior to a vapor.

After calculating the mean particle diameter (Column 1), the fraction of total mass (Column 4) per mean particle size diameter must be computed from the stack test results. For each mean particle diameter, the stack test data provides an associated mass of particulate. The fraction of total mass for each mean particle diameter is calculated by dividing the associated mass of particulate for that diameter by the total mass of particulate in the sample. In many cases, the fractions of total mass will not sum to 1.0 due to rounding errors. In these instances, U.S. EPA OSW advocates that the remaining mass fraction be added into the largest mean particle diameter mass fraction to force the total mass to 1.0.

Direct measurements of particle-size distributions at a proposed new facility may be unavailable, so it will be necessary to provide assumed particle distributions for use in ISCST3. In such instances, a representative distribution may be used. The unit on which the representative distribution is based should be as similar as practicable to the proposed unit. For example, the default distribution provided in Table 3-1 is not appropriate for a hazardous waste burning boiler with no APCD or a wet scrubber, because it is based on data from different type of unit. However, the generalized particle size (diameter) distribution in Table 3-1 may be used as a default for some combustion facilities equipped with either ESPs or fabric filters, because the distribution is relatively typical of particle size arrays that have been measured at the outlet to advanced equipment designs (Buonicore and Davis 1992; U.S. EPA 1986a; U.S. EPA 1987a).

After developing the particulate size distribution based on mass, this distribution is used in ISCST3 to apportion the mass of particle phase COPCs (metals and organics with F_v values less than 0.05) based on particle size. Column 4 of Table 3-1 (as developed from actual stack test data) is used in the ISCST3 input file to perform a particulate run with the particle phase COPCs apportioned based on mass weighting.

3.4.3 Particle-Bound Modeling (Surface Area Weighting)

A surface area weighting, instead of mass weighting, of the particles is used in separate particle runs of ISCST3. Surface area weighting approximates the situation where a semivolatile organic contaminant that has been volatilized in the high temperature environment of a combustion system and then condensed to the surface of particles entrained in the combustion gas after it cools in the stack. Thus, the apportionment of emissions by particle diameter becomes a function of the surface area of the particle that is available for chemical adsorption (U.S. EPA 1993h).

The first step in apportioning COPC emissions by surface area is to calculate the proportion of available surface area of the particles. If particle density is held constant (such as 1 g/m^3), the proportion of available surface area of aerodynamic spherical particles is the ratio of surface area (*S*) to volume (*V*), as follows:

- Assume aerodynamic spherical particles.
- Specific surface area of a spherical particle with a radius, r—$S = 4\ \pi r^2$
- Volume of a spherical particle with a radius, r—$V = 4/3\ \pi r^3$
- Ratio of S to V—$S/V = 4\ \pi r^2 / (4/3\ \pi r^3) = 3/r$

The following uses the particle size distribution in Table 3-1 as an example of apportioning the emission rate of the particle-bound portion of the COPC based on surface area. This procedure can be followed for apportioning actual emissions to the actual particle size distribution measured at the stack. In Table 3-1, a spherical particle having a diameter of 15 μm (Column 1) has a radius of 7.5 μm (Column 2). The proportion of available surface area (assuming particle density is constant) is 0.400 (S/V = 3/7.5), which is the value in Column 3. Column 4 shows that particles with a mean diameter of 15 μm, constitute 12.8 percent of the total mass. Multiplication of Column 3 by Column 4 yields a value in Column 5 of 0.0512. This value is an approximation of the relative proportion of total surface area, based on the percent of particles that are 15 μm in diameter. The sum of Column 5 yields the total surface area of all particles in the particle size distribution. In this example, the sum is 3.4423. Column 6 is the fraction of total surface area represented by the specific particle diameter in the distribution, and is calculated by dividing the relative proportion of surface area (Column 5) for a specific diameter by the total relative proportion of surface area (3.4423 square micrometers [μm^2]). In the example of the 15 μm-diameter particle, the fraction of total surface area available for adsorption is 0.0149 (0.0512/3.4423). This procedure is then repeated for all particle sizes in the array.

After developing the particulate size distribution based on surface area, this distribution is used in ISCST3 to apportion mass of particle-bound COPCs (most organics) based on particle size. Column 6 of Table 3-1 (as developed from actual stack test data) is used in the ISCST3 input file to perform a particulate run for the particle-bound COPCs apportioned based on surface area weighting.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Copies of all stack test data used to determine particle size distribution
- Copies of all calculations made to determine particle size distribution, fraction of total mass, and fraction of total surface area

3.5 METEOROLOGICAL DATA

To model air concentration and deposition, the ISCST3 model requires a variety of meteorological information:

1. Air concentration
    a. Hourly values

        (1) Wind direction (degrees from true north)
        (2) Wind speed (m/s)
        (3) Dry bulb (ambient air) temperature (K)
        (4) Opaque cloud cover (tenths)
        (5) Cloud ceiling height (m)

    b. Daily values

        (1) Morning mixing height (m)
        (2) Afternoon mixing height (m)

2. Deposition

    a. Dry particle deposition—hourly values for surface pressure (millibars)

    b. Wet particle deposition—hourly values
        (1) Precipitation amount (inches)
        (2) Precipitation type (liquid or frozen)

    c. Dry vapor deposition (when available)—hourly values for solar radiation (watts/m^2)

As shown in Figure 3-1, these data are available from several different sources. For most air modeling, five years of data from a representative National Weather Service station is recommended. However, in some instances where the closest NWS data is clearly not representative of site specific meteorlogical conditions, and there is insufficient time to collect 5 years of onsite data, 1 year of onsite meteorological data (consistent with GAQM) may be used to complete the risk assessment. The permitting authority should approve the representative meteorological data prior to performing air modeling.

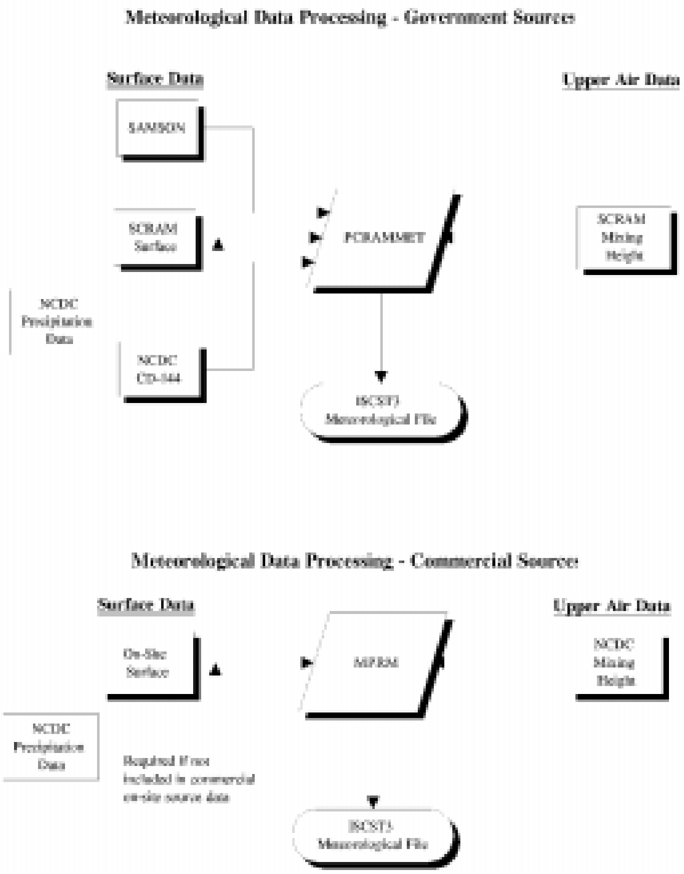
The following subsections describe how to select the surface and upper air data that will be used in conjunction with the ISCST3 model. Section 3.7 describes the computer programs used to process the meteorological data for input to the ISCST3 model.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Identification of all sources of meteorological data

FIGURE 3-1

SOURCES OF METEOROLOGICAL DATA



3.5.1 Surface Data

Surface data can be obtained from SAMSON in CD-ROM format. SAMSON data are available for 239 airports across the U.S. for the period of 1961 through 1990. The National Climate Data Center (NCDC) recently released the update to SAMSON through 1995 surface data. However, since the upper air (mixing height) data available from the U.S. EPA SCRAM web site has not been updated to cover this recent data period, it is acceptable to select the representative 5 years of meteorological data from the period up through 1990. SAMSON data contain all of the required input parameters for concentration, dry and wet particle deposition, and wet vapor deposition. SAMSON also includes the total solar radiation data required for dry vapor deposition, which may be added to ISCST3 in the future. Alternatively, some meteorological files necessary for running ISCST3 are also available on the SCRAM BBS for NWS stations located throughout the country (SCRAM BBS is part of the Office of Air Quality and Planning and Standards Technology Transfer Network [OAQPS TTN]). The meteorological data, preprocessors, and user's guides are also located on the SCRAM web site at "http://www.epa.gov/scram001/index.htm". However, these files do not contain surface pressure, types of precipitation (present weather), or precipitation amount. Although the ISCST3 model is not very sensitive to surface pressure variations, and a default value may be used, precipitation types and amounts are necessary for air modeling wet deposition. Precipitation data are available from the National Climatic Data Center (NCDC), and are processed by PCRAMMET to supplement the SCRAM BBS surface data. NCDC also has surface data in CD-144 format, which contains all of the surface data, including precipitation.

The SAMSON CD-ROM for the eastern, central, or western (Volumes I, II, and III) United States may be purchased from NCDC in Asheville, North Carolina.

National Climatic Data Center
Federal Building
37 Battery Park Avenue
Asheville, NC 28801-2733

Customer Service: (704) 271-4871

File type:	File name:
Hourly precipitation amounts	NCDC TC-3240
Hourly surface observations with precipitation type	NCDC TD-3280
Hourly surface observations with precipitation type	NCDC SAMSON CD-ROM (Vol. I, II, and/or III)
Twice daily mixing heights from nearest station	NCDC TD-9689 (also available on SCRAM web site for 1984 through 1991)

PCRAMMET and MPRM are the U.S. EPA meteorological preprocessor programs for preparing the surface and upper air data into a meteorlogical file of hourly parameters for input into the ISCST3 model. Most air modeling analyses will use PCRAMMET to process the National Weather Service data. However, both preprocessors require the modeler to replace any missing data. Before running PCRAMMET or MPRM, the air modeler must fill in missing data to complete 1 full year of values. A procedure recommended by U.S. EPA for filling missing surface and mixing height data is documented on the SCRAM BBS under the meteorological data section. If long periods of data are missing, and these data are not addressed by the U.S. EPA procedures on the SCRAM BBS, then a method must be developed for filling in missing data. One option is to fill the time periods with "surrogate place holder" data in the correct format with correct sequential times to complete preparation of the meteorological file. Place holder data are typically considered the last valid hourly data of record. Then, when ISCST3 is running, the `MSGPRO` keyword in the COntrol pathway can be used to specify that data are missing. Note that the `DEFAULT` keyword must not be used with `MSGPRO`. Since the missing data keyword is not approved generally for regulatory air modeling, the appropriate agency must provide approval prior to use. All processing of meteorological data should be completely documented to include sources of data, decision criteria for selection, consideration for precipitation amounts, preprocessor options selected, and filled missing data.

The most recently available 5 years of complete meteorological data contained on SAMSON, or more recent sources, should be used for the air modeling. It is desirable, but not mandatory, that the 5 years are consecutive. The use of less than five years of meteorological data should be approved by appropriate authorities. The following subsections describe important characteristics of the surface data.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Electronic copy of the ISCST3 input code used to enter meteorological information
- Description of the selection criteria and process used to identify representative years used for meteorological data
- Identification of the 5 years of meteorological selected
- Summary of the procedures used to compensate for any missing data

3.5.1.1 Wind Speed and Wind Direction

Wind speed and direction are two of the most critical parameters in ISCST3. The wind direction promotes higher concentration and deposition if it persists from one direction for long periods during a year. A predominantly south wind, such as on the Gulf Coast, will contribute to high concentrations and depositions north of the facility. Wind speed is inversely proportional to concentration in the ISCST3 algorithms. The higher the wind speed, the lower will be the concentration. If wind speed doubles, the concentration and deposition will be reduced by one-half. ISCST3 needs wind speed and wind direction at the stack top. Most air modeling is performed using government sources of surface data. Wind data are typically measured at 10 meters height at NWS stations. However, since some stations have wind speed recorded at a different height, the anemometer height must always be verified so that the correct value can be input into the PCRAMMET meteorological data preprocessing program. ISCST3 assumes that wind direction at stack height is the same as measured at the NWS station height. ISCST3 uses a wind speed profile to calculate wind speed at stack top. This calculation exponentially increases the measured wind speed from the measured height to a calculated wind speed at stack height (U.S. EPA 1995d).

3.5.1.2 Dry Bulb Temperature

Dry bulb temperature, or ambient air temperature, is the same temperature reported on the television and radio stations across the country each day. It is measured at 2 meters above ground level. Air temperature is used in ISCST3 in the buoyant plume rise equations developed by Briggs (U.S. EPA 1995c). The model results are not very sensitive to air temperature, except at extremes. However, buoyant plume rise is very sensitive to the stack gas temperature. Buoyant plume rise is mainly a result of the difference between stack gas temperature and ambient air temperature. Conceptually, it is similar to a hot air balloon. The higher the stack gas temperature, the higher will be the plume rise. High plume heights result in low concentrations and depositions as the COPCs travel further and are diluted in a larger volume of ambient air before reaching the surface. The temperature is measured in K, so a stack gas temperature of 450°F is equal to 505 K. Ambient temperature of 90°F is equal to 305 K, and 32°F is 273 K. A large variation in ambient temperature will affect buoyant plume rise, but not as much as variations in stack gas temperature.

3.5.1.3 Opaque Cloud Cover

PCRAMMET uses opaque cloud cover to calculate the stability of the atmosphere. Stability determines the dispersion, or dilution, rate of the COPCs. Rapid dilution occurs in unstable air because of surface heating that overturns the air. With clear skies during the day, the sun heats the Earth’s surface, thereby causing unstable air and dilution of the stack gas emission stream. Stable air results in very little mixing, or dilution, of the emitted COPCs. A cool surface occurs at night because of radiative loss of heat on clear nights. With a cloud cover, surface heating during the day and heat loss at night are reduced, resulting in moderate mixing rates, or neutral stability. Opaque cloud cover is a measure of the transparency of the clouds. For example, a completely overcast sky with 10/10ths cloud cover may have only 1/10th opaque cloud cover if the clouds are high, translucent clouds that do not prevent sunlight from reaching the Earth’s surface. The opaque cloud cover is observed at NWS stations each hour.

3.5.1.4 Cloud Ceiling Height

Cloud height is required in PCRAMMET to calculate stability. Specifically, the height of the cloud cover affects the heat balance at the Earth’s surface. Cloud ceiling height is measured or observed at all NWS stations provided on the SAMSON CD-Roms and the U.S. EPA SCRAM web site.

3.5.1.5 Surface Pressure

Surface pressure is required by ISCST3 for calculating dry particle deposition. However, ISCST3 is not very sensitive to surface pressure. SAMSON and NCDC CD-144 data include surface pressure. SCRAM BBS surface data do not include surface pressure. U.S. EPA believes that, if SCRAM BBS surface data are used, a default value of 1,000 millibars can be assumed, with little impact on modeled results.

3.5.1.6 Precipitation Amount and Type

The importance of precipitation to ISCST3 results was discussed in the selection of the meteorological data period (see Section 3.5.1). Precipitation is measured at 3 feet (1 meter) above ground level. Precipitation amount and type are required to be processed by PCRAMMET or MPRM into the ISCST3 meteorological file to calculate wet deposition of vapor and particles. The amount of precipitation, or precipitation rate, will directly influence the amount of wet deposition at a specific location. Particles and vapor are both captured by falling precipitation, known as precipitation scavenging. Scavenging coefficients are required as inputs to ISCST3 for vapors with a rate specified for liquid and frozen precipitation. The precipitation type in a weather report in SAMSON or CD-144 data file will identify to ISCST3 which event is occurring for appropriate use of the scavenging coefficients entered (see Section 3.7.2.6). SCRAM BBS surface data do not include precipitation data. Supplemental precipitation files from NCDC may be read into PCRAMMET for integration into the ISCST3 meteorological file.

3.5.1.7 Solar Radiation (Future Use for Dry Vapor Deposition)

The current version of ISCST3 does not use solar radiation. Several U.S. EPA models, including the Acid Deposition and Oxidant Model (ADOM), incorporate algorithms for dry vapor deposition. At such time as U.S. EPA approves the draft version of ISCST3 which includes dry gas deposition, the hourly total solar radiation will be required. Solar radiation affects the respiratory activity of leaf surfaces, which affects the rate of vapor deposition. With a leaf area index identified in the ISCST3 input file in the future, the model will be able to calculate dry vapor deposition.

3.5.2 Upper Air Data

Upper air data, also referred to as mixing height data, are required to run the ISCST3 model. ISCST3 requires estimates of morning and afternoon (twice daily) mixing heights. PCRAMMET and MPRM use these estimates to calculate an hourly mixing height by using interpolation methods (U.S. EPA 1996e). The mixing height files are typically available for the years 1984 through 1991 on the U.S. EPA SCRAM web site. U.S. EPA OSW recommends that only years with complete mixing height data be used as input for air modeling. In some instances, data may need to be obtained from more than one station to complete five years of data. The selection of representative data should be discussed with appropriate authorities prior to performing air modeling.

Mixing height data for years prior to 1983, in addition to current mixing height data, may be purchased from NCDC as described in Section 3.5.1. The years selected for upper air data must match the years selected for surface data. If matching years of mixing height data are not available from a single upper air station, another upper air station should be used for completing the five years.

3.6 METEOROLOGICAL PREPROCESSORS AND INTERFACE PROGRAMS

After the appropriate surface and upper air data is selected following the procedures outlined in Section 3.5, additional data manipulation is necessary before the data is used with the ISCST3 model. The following subsections describe the meteorological preprocessors and interface programs used for these manipulation tasks. To eliminate any need to repeat air modeling activities, U.S. EPA OSW recommends that the selection of representative mixing height and surface data be approved by the appropriate regulatory agency before preprocessing or air modeling is conducted. Permitting authority approval also is recommended in the selection of site-specific parameter values required as input to the meteorological data preprocessors.

3.6.1 PCRAMMET

U.S. EPA OSW recommends preparing a meteorological file for ISCST3 that can be used to calculate any concentration or deposition. By preparing a file that PCRAMMET terms a “WET DEPOSITION” file, all required parameters will be available to ISCST3 for any subsequent concentration or deposition modeling.

For example, if only the concentration option is selected in ISCST3 for a specific run, ISCST3 will ignore the precipitation values in the meteorological file. For subsequent air deposition modeling, ISCST3 will access the precipitation data from the same preprocessed meteorological file.

PCRAMMET may use SAMSON, SCRAM web site, and NCDC CD-144 surface data files. U.S. EPA OSW recommends using the SAMSON option in PCRAMMET to process the SAMSON surface data and U.S. EPA SCRAM web site mixing height data. The PCRAMMET User's Guide in the table "Wet Deposition, SAMSON Data" (U.S. EPA 1995b) identifies the PCRAMMET input requirements for creating an ASCII meteorological file for running ISCST3 to calculate air concentration, and wet and dry deposition. The meteorological file created for ISCST3 will contain all of the parameters needed for air modeling of concentration and deposition.

PCRAMMET requires the following input parameters representative of the measurement site:

- Monin-Obukhov length
- Anemometer height
- Surface roughness height (at measurement site)
- Surface roughness height (at application site)
- Noon-time albedo
- Bowen ratio
- Anthropogenic heat flux
- Fraction of net radiation absorbed at surface

The PCRAMMET User's Guide contains detailed information for preparing the required meteorological input file for the ISCST3 model (U.S. EPA 1995b). The parameters listed are briefly described in the following subsections. These data are not included in the surface or mixing height data files obtained from the U.S. EPA or NCDC. Representative values specific to the site to be modeled should be carefully selected using the tables in the PCRAMMET User's Guide or reference literature. The selected values should be approved prior to processing the meteorological data.

3.6.1.1 Monin-Obukhov Length

The Monin-Obukhov length (*L*) is a measure of atmospheric stability. It is negative during the day, when surface heating causes unstable air. It is positive at night, when the surface is cooled with a stable atmosphere. In urban areas during stable conditions, the estimated value of *L* may not adequately reflect the less stable atmosphere associated with the mechanical mixing generated by buildings or structures. However, PCRAMMET requires an input for minimum urban Monin-Obukhov length, even if the area to be analyzed by ISCST3 is rural. A nonzero value for *L* must be entered to prevent PCRAMMET from generating an error message. A value of 2.0 meter for *L* should be used when the land use surrounding the site is rural (see Section 3.2.2.1). For urban areas, Hanna and Chang (1991) suggest that a minimum value of *L* be set for stable hours to simulate building-induced instability. The following are general examples of *L* values for various land use classifications:

Land Use Classification	Minimum *L*
Agricultural (open)	2 meters
Residential	25 meters
Compact residential/industrial	50 meters
Commercial (19 to 40-story buildings)	100 meters
Commercial (>40-story buildings)	150 meters

PCRAMMET will use the minimum *L* value for calculating urban stability parameters. These urban values will be ignored by ISCST3 during the air modeling analyses for rural sites.

3.6.1.2 Anemometer Height

The height of the wind speed measurements is required by ISCST3 to calculate wind speed at stack top. The wind sensor (anemometer) height is identified in the station history section of the Local Climatological Data Summary available from NCDC for every National Weather Service station. Since 1980, most National Weather Service stations measure wind speed at the height of 10 meters. However, some stations operate at other heights or have valid representative data during years of operation at more than one height. The modeler must verify the correct measurement height for each year of data prior to processing with

PCRAMMET and running the ISCST3 model. ISCST3 modeled results are very sensitive to small variations in wind speed.

3.6.1.3 Surface Roughness Height at Measurement Site

Surface roughness height is a measure of the height of obstacles to wind flow. It is important in ISCST3 because it determines how close a particle must be above the ground before it is “captured” for deposition on the ground. Dramatic differences in ISCST3 calculations may result from slight variations in surface roughness. For surface meteorological data from a National Weather Station, a value of 0.10 meters for the “measurement site” typically may be used without prior approval. Surface roughness is proportional, but not equal, to the physical height of the obstacles. The table in Section 3.2.2.2 lists the roughness heights that can be used as input values. These values are based on the general land use in the vicinity of the measurement site. These values should be considered in discussions with the appropriate agency modeler prior to air modeling.

3.6.1.4 Surface Roughness Height at Application Site

Determination of surface roughness height is also required at the facility (application site) for performing PCRAMMET processing to prepare an ISCST3 meteorological file. ISCST3 model results are very sensitive to the value used in PCRAMMET for this parameter. The table in Section 3.2.2.2 is applicable to the application site. A site-specific computation of a single surface roughness value representative of the site is required using the method described in Section 3.2.2.2. The computed value of surface roughness height for the application site, along with maps or photographs illustrating land use, must be approved by the appropriate agency prior to use.

3.6.1.5 Noon-Time Albedo

“Noon-time albedo” is the fraction of the incoming solar radiation that is reflected from the ground when the sun is directly overhead. Albedo is used in calculating the hourly net heat balance at the surface for calculating hourly values of Monin-Obukhov length. PCRAMMET automatically adjusts for the variation in albedo with solar elevation angle. Experience suggests that ISCST3 modeling results are not sensitive to the value selected for this parameter. Typical albedo values are presented in Table 3-2. As shown in Table

3-2, albedo values vary from 0.10 to 0.20 on water surfaces from summer to winter. The most variability is for cultivated farmland, which varies from 0.14 during spring when land is tilled to expose dark earth, to 0.60 in winter when areas are snow-covered.

Based on the information in Table 3-2, albedos are estimated to vary in rural areas from 0.14 to 0.20 for cultivated land, and from 0.18 to 0.20 for grassland. For urban areas, the variation without snow is from 0.14 to 0.18. For practical purposes, the selection of a single value for noon-time albedo to process a complete year of meteorological data is desirable. For example, the single value of 0.18 may be appropriate to process all meteorological data for an urban site. For rural sites, a single albedo value of 0.18 representative of grassland and cultivated land may be appropriate for areas without significant snow cover during winter months. For desert shrubland, a single value of 0.28 may be appropriate. A single value of 0.12 could be representative of forested areas. The permitting authority should review proposed values used in the processing of the meteorological data.

TABLE 3-2

ALBEDO OF NATURAL GROUND COVERS FOR LAND USE TYPES AND SEASONS

Land Use Type	Season[a]			
	Spring	Summer	Autumn	Winter
Water surface	0.12	0.10	0.14	0.20
Deciduous forest	0.12	0.12	0.12	0.50
Coniferous forest	0.12	0.12	0.12	0.35
Swamp	0.12	0.14	0.16	0.30
Cultivated land	0.14	0.20	0.18	0.60
Grassland	0.18	0.18	0.20	0.60
Urban	0.14	0.16	0.18	0.35
Desert shrubland	0.30	0.28	0.28	0.45

Notes:

Source—Iqbal (1983)

[a] The various seasons are defined by Iqbal (1983) as follows:

Spring:	Periods when vegetation is emerging or partially green; this is a transitional situation that applies for 1 to 2 months after the last killing frost in spring.
Summer:	Periods when vegetation is lush and healthy; this is typical of mid-summer, but also of other seasons in which frost is less common.
Autumn:	Periods when freezing conditions are common, deciduous trees are leafless, crops are not yet planted or are already harvested (bare soil exposed), grass surfaces are brown, and no snow is present.
Winter:	Periods when surfaces are covered by snow and temperatures are below freezing. Winter albedo depends on whether a snow cover is present continuously, intermittently, or seldom. Albedo ranges from about 0.30 for bare snow cover to about 0.65 for continuous cover.

3.6.1.6 Bowen Ratio

The Bowen ratio is a measure of the amount of moisture at the surface. The presence of moisture affects the heat balance resulting from evaporative cooling, which, in turn, affects the hourly Monin-Obukhov length calculated by PCRAMMET. Surface moisture is highly variable. Daytime Bowen ratios are presented in Table 3-3.

Bowen ratio values vary throughout the country. For example, in urban areas where annual rainfall is less than 20 inches, a single Bowen ratio value of 4.0 may be representative. For rural areas, a Bowen ratio value of 2.0 may be appropriate for grassland and cultivated land. For areas where annual rainfall is greater than 20 inches, U.S. EPA OSW recommends a single Bowen ratio value of 2.0 for urban areas; and 0.7 for rural forests, grasslands, and cultivated lands. The applicable permiting authority should review proposed values used in the processing of the meteorological data.

3.6.1.7 Anthropogenic Heat Flux

Anthropogenic heat is the surface heating caused by human activity, including automobiles and heating systems. It is used to calculate hourly L values (Monin-Obukhov lengths). Table 3-4 presents anthropogenic heat flux (Q_f) values that have been calculated for several urban areas around the world. In rural areas, U.S. EPA OSW recommends that a value of 0.0 Watts/m^2 be used for the Q_f. A value of 20.0 Watts/m^2 is appropriate for large urban areas based on the annual value from Table 3-4 for Los Angeles.

3.6.1.8 Fraction of Net Radiation Absorbed at the Ground

Also used for calculating hourly values of Monin-Obukhov length, fraction of net radiation absorbed at the ground is the last component of radiative heat balance. Based on the net radiation (Q_*) values presented in Table 3-4, and recommendations presented in the PCRAMMET User's Manual based on Oke (1982), U.S. EPA OSW recommends values of 0.15 for rural areas and 0.27 for urban areas (U.S. EPA 1995b).

TABLE 3-3

DAYTIME BOWEN RATIOS BY LAND USE, SEASON, AND PRECIPITATION CONDITIONS

Land Use	Season[a]			
	Spring	Summer	Autumn	Winter
Dry Conditions				
Water (fresh and salt)	0.1	0.1	0.1	2.0
Deciduous forest	1.5	0.6	2.0	2.0
Coniferous forest	1.5	0.6	1.5	2.0
Swamp	0.2	0.2	0.2	2.0
Cultivated land	1.0	1.5	2.0	2.0
Grassland	1.0	2.0	2.0	2.0
Urban	2.0	4.0	4.0	2.0
Desert shrubland	5.0	6.0	10.0	2.0
Average Conditions				
Water (fresh and salt)	0.1	0.1	0.1	1.5
Deciduous forest	0.7	0.3	1.0	1.5
Coniferous forest	0.7	0.3	0.8	1.5
Swamp	0.1	0.1	0.1	1.5
Cultivated land	0.3	0.5	0.7	1.5
Grassland	0.4	0.8	1.0	1.5
Urban	1.0	2.0	2.0	1.5
Desert shrubland	3.0	4.0	6.0	6.0

TABLE 3-3

DAYTIME BOWEN RATIO BY LAND USE, SEASON, AND PRECIPITATION CONDITIONS (Continued)

Land Use	Season[a]			
	Spring	Summer	Autumn	Winter
Wet Conditions				
Water (fresh and salt)	0.1	0.1	0.1	0.3
Deciduous forest	0.3	0.2	0.4	0.5
Coniferous forest	0.3	0.2	0.3	0.3
Swamp	0.1	0.1	0.1	0.5
Cultivated land	0.2	0.3	0.4	0.5
Grassland	0.3	0.4	0.5	0.5
Urban	0.5	1.0	1.0	0.5
Desert shrubland	1.0	5.0	2.0	2.0

Note:

Source—Paine (1987)

[a] The various seasons are defined by Iqbal (1983) as follows:

Spring:	Periods when vegetation is emerging or partially green; this is a transitional situation that applies for 1 to 2 months after the last killing frost in spring.
Summer:	Periods when vegetation is lush and healthy; this is typical of mid-summer, but also of other seasons in which frost is less common.
Autumn:	Periods when freezing conditions are common, deciduous trees are leafless, crops are not yet planted or are already harvested (bare soil exposed), grass surfaces are brown, and no snow is present
Winter:	Periods when surfaces are covered by snow and temperatures are below freezing.

TABLE 3-4

ANTHROPOGENIC HEAT FLUX (Q_f) AND NET RADIATION (Q_*) FOR SEVERAL URBAN AREAS

Urban Area (Latitude)	Population (Millions)	Population Density (Persons/km^2)	Per Capita Energy Use (MJ x 10^3/year)	Q_f (Watts/m^2) (Season)	Q_* (Watts/m^2)
Manhattan (40° North)	1.7	28,810	128	117 (Annual) 40 (Summer) 198 (Winter)	93 (Annual)
Montreal (45° North)	1.1	14,102	221	99 (Annual) 57 (Summer) 153 (Winter)	52 (Annual) 92 (Summer) 13 (Winter)
Budapest (47° North)	1.3	11,500	118	43 (Annual) 32 (Summer) 51 (Winter)	46 (Annual) 100 (Summer) -8 (Winter)
Sheffield (53° North)	0.5	10,420	58	19 (Annual)	56 (Annual)
West Berlin (52° North)	2.3	9,830	67	21 (Annual)	57 (Annual)
Vancouver (49° North)	0.6	5,360	112	19 (Annual) 15 (Summer) 23 (Winter)	57 (Annual) 107 (Summer) 6 (Winter)
Hong Kong (22° North)	3.9	3,730	34	4 (Annual)	110 (Annual)
Singapore (1° North)	2.1	3,700	25	3 (Annual)	110 (Annual)
Los Angeles (34° North)	7.0	2,000	331	21 (Annual)	108 (Annual)
Fairbanks (64° North)	0.03	810	740	19 (Annual)	18 (Annual)

Note:

Source—Oke (1978)

3.6.2 MPRM

For on-site data, a new version of MPRM is used to mesh on-site data with NWS data in the preparation of the meteorological input file. MPRM performs the same meteorological file preparation as PCRAMMET, except the source of the surface data in MPRM consists of on-site measurements (U.S. EPA 1996e). MPRM includes extensive QA/QC for values that are out of range. MPRM also checks for missing data and summarizes values that require editing to fill missing data. After a complete surface file passes the quality checks, it is processed with NCDC mixing height data. NCDC data are purchased to correspond to the collection period of the on-site surface data. Mixing height data available on SCRAM's web site ends in 1991. A delay of about 3 months can occur for obtaining mixing height data from NCDC to process with recent on-site surface data.

Inputs to MPRM for preparing an ISCST3 meteorological file for concentration and deposition are the same as for PCRAMMET. Section 3.6.1 provides methods for determining values for these parameters.

Draft versions of ISCST3 and MPRM are available for review which implement dry vapor deposition. These versions are GDISCDFT (dated 96248) and GDMPRDFT (dated 96248), respectively. They may be found on the U.S. EPA SCRAM web site under "Topics for Review". These draft models are not the current regulatory versions and should not be used without approval from the appropriate permitting authority.

3.7 ISCST3 MODEL INPUT FILES

A thorough instruction of how to prepare the input files for ISCST3 is presented in the ISC3 User's Guide, Volume I (U.S. EPA 1995c), which is available for downloading from the SCRAM BBS. The example ISCST3 input file is provided in Figure 3-2 from the air dispersion modeling chapter (Chapter 3) of the U.S. EPA HHRAP (U.S. EPA 1998). This example illustrates a single year run (1984), for particle phase COPC emissions from a single stack, to compute acute (1-hour average) and chronic (annual average) and provide single year results in one hour and annual average plot files for post-processing. For ecological risk assessments, only the annual average air parameters are required, not the 1-hour values. However, by modeling both the 1-hour and annual averages in a single set of runs, the ISCST3 air dispersion model will provide the necessary air parameters for use in both the human health and ecological risk assessments. The specification of a terrain grid file in the TG pathway is optional. Each air modeling analysis has unique issues and concerns that should be addressed in the risk assessment report. U.S. EPA OSW recommends that the air modeling methodology be consistent in data collection, model set-up, and model output. This consistency will assist both the modeler and U.S. EPA in communicating and interpreting model results. The risk assessment report should document each section of the ISCST3 input file to identify consistent methods.

Three sets of ISCST3 runs are required for each COPC emission source. As discussed in Section 3.4, separate ISCST3 runs are required to model vapor phase COPCs, particle phase COPCs, and particle-bound phase COPCs for each source (stack or fugitive) of COPCs. The ISCST3 "Control Secondary Keywords" used for these three runs are:

Vapor Phase:	`CONC`	`WDEP`		
Particle Phase:	`CONC`	`DDEP`	`WDEP`	`DEPOS`
Particle-Bound Phase:	`CONC`	`DDEP`	`WDEP`	`DEPOS`

For ISCST3 modeling to provide air parameters for ecological risk assessments, only the total deposition (DEPOS) of the particle and particle-bound phases are required. The control secondary keywords for concentration in the air (CONC) and the components of deposition to the ground, dry deposition (DDEP) and wet deposition (WDEP), are not required to be output separately by ISCST3. However, by specifying these control secondary keywords as illustrated, the ISCST3 model will compute the needed air parameters for both human health and ecological risk assessments. ISCST3 requires site-specific inputs for source parameters, receptor locations, meteorological data, and terrain features. The model is prepared for execution by creating an input file. The input file is structured in five (or six if a terrain grid file is used) sections, or pathways, designated by two-letter abbreviations:

ISCST3 INPUT FILE SECTIONS	
Section	**Abbreviation**
Control	`CO`
Source	`SO`
Receptor	`RE`
Meteorology	`ME`
Terrain Grid (Optional)	*`TG`*
Output	`OU`

The following subsections describe how to specify the parameters for each pathway in the ISCST3 input file.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Electronic and hard copies of ISCST3 input file for all air modeling runs

3.7.1 COntrol Pathway

Model options (MODELOPT) are specified in the COntrol pathway to direct ISCST3 in the types of computations to perform. U.S. EPA OSW recommends that air modeling specify the `DFAULT` parameter to use the following regulatory default options:

- Use stack-tip downwash (except for Schulman-Scire downwash).
- Use buoyancy-induced dispersion (except for Schulman-Scire downwash).
- Do not use final plume rise (except for building downwash).
- Use the calms processing routines.

- Use upper-bound concentration estimates for sources influenced by building downwash from super-squat buildings.
- Use default wind speed profile exponents.
- Use default vertical potential temperature gradients.

The `CONC` parameter specifies calculation of air concentrations for vapor and particles. The `DDEP` and `WDEP` parameters specify dry and wet deposition. The `DEPOS` specifies computation of total (wet and dry) deposition flux. Since ISCST3 currently does not include an algorithm for the dry deposition of vapor phase COPCs, only wet deposition is specified for vapor phase runs. Note that dry deposition of vapor phase is addressed in the pathway equations during the risk assessment using the concentration of the vapor phase and a deposition velocity. `DRYDPLT` and `WETDPLT` are used for plume depletion resulting from dry and wet removal. U.S. EPA OSW recommends the following command lines for each of the three runs (these are for rural areas; substitute `URBAN` for urban areas):

Vapor:

```
CO MODELOPT DFAULT CONC WDEP WETDPLT RURAL
```

Particle Phase:

```
CO MODELOPT DFAULT CONC DDEP WDEP DEPOS DRYDPLT WETDPLT
RURAL
```

Particle-Bound:

```
CO MODELOPT DFAULT CONC DDEP WDEP DEPOS DRYDPLT WETDPLT
RURAL
```

Note that only the total deposition (DEPOS) air parameter values are required for the ecological risk assessment pathways. The modeler may elect not to include CONC, DDEP and WDEP as separate output components from ISCST3 if the air modeling results will not be used for a human health risk assessment. However, the control secondary keywords must always be specified for plume depletion through the dry deposition (DRYDPLT) and wet deposition (WETDPLT) processes.

FIGURE 3-2

EXAMPLE INPUT FILE FOR "PARTICLE PHASE"

```
CO STARTING
CO TITLEONE Example input file, particle phase run
CO TITLETWO 1984 met data, Baton Rouge Surface, Boothville Upper Air
CO MODELOPT DFAULT CONC DDEP WDEP DEPOS DRYDPLT WETDPLT RURAL
CO AVERTIME 1 ANNUAL
CO POLLUTID UNITY
CO TERRHGTS ELEV
CO RUNORNOT RUN
CO SAVEFILE 84SAVE1 5 84SAVE2
** Restart incomplete runs with INITFILE, changing '**' to 'CO'
** INITFILE 84SAVE1
CO FINISHED

SO STARTING
SO LOCATION STACK1 POINT 637524. 567789. 347.
SO SRCPARAM STACK1 1.0 23.0 447.0 14.7 1.9
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29
SO BUILDWID STACK1 14.02 15.51 16.53 17.05 17.05 16.53 15.51 14.03
SO BUILDWID STACK1 12.10 14.02 15.51 16.53 17.05 17.05 16.53 15.51
SO BUILDWID STACK1 14.02 12.10 14.02 15.51 16.53 17.05 17.05 16.53
SO BUILDWID STACK1 15.51 14.02 12.10 14.02 15.51 16.53 17.05 17.05
SO BUILDWID STACK1 16.53 15.51 14.02 12.10
SO PARTDIAM STACK1 0.35 0.70 1.10 2.00 3.60 5.50 8.10 12.5 15.0
SO MASSFRAX STACK1 0.22 0.08 0.08 0.11 0.10 0.07 0.10 0.11 0.13
SO PARTDENS STACK1 1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
SO PARTSLIQ STACK1 7E-5 5E-5 6E-5 1.3E-4 2.6E-4 3.9E-4 5.2E-4 6.7E-4 6.7E-4
SO PARTSICE STACK1 2E-5 2E-5 2E-5   4E-5   9E-5 1.3E-4 1.7E-4 2.2E-4 2.2E-4
SO SRCGROUP ALL
SO FINISHED

RE STARTING
RE ELEVUNIT METERS
RE DISCCART 630000. 565000. 352.
RE DISCCART 630500. 565000. 365.
RE DISCCART 631000. 565000. 402.
      ...
      (ARRAY OF DISCRETE RECEPTORS)
      ...
RE DISCCART 635000. 570000. 387.
RE FINISHED

ME STARTING
ME INPUTFIL 84BTR.WET
ME ANEMHGHT 10.0
ME SURFDATA 13970 1984 BATON_ROUGE
ME UAIRDATA 12884 1984 BOOTHVILLE
ME FINISHED

TG STARTING
TG INPUTFIL TERRAIN.TER
TG LOCATION 0.0 0.0
TG ELEVUNIT METERS
TG FINISHED

OU STARTING
OU RECTABLE ALLAVE FIRST
OU PLOTFILE 1 ALL FIRST BTR841.PLT
OU PLOTFILE ANNUAL ALL BTR84A.PLT
OU FINISHED
```

For each of the three runs for each emission source, 5 years of off-site (e.g., National Weather Service from SAMSON) meteorological data are completed. For sites with meteorological data collected on-site, the appropriate permitting authority should be notified for the data period required for a risk assessment. The averaging times (`AVERTIME`) should be specified as `‘ANNUAL’` to compute long-term (annual average) ecological risk. Optionally, the ‘1' may be specified for convenience in modeling for the maximum 1-hour averages used in computing acute human health risks. Each phase run may be repeated five times (one for each year, or a total of 15 ISCST3 runs) to complete a set of 15 runs for the full five years of meteorological data.

Alternatively, the modeler may combine the 5 years of meteorological data into a single meteorological data file and complete only 3 runs for each emission source (one run for each phase). Section 3.5.1.1 of the ISC3 User’s Guide (U.S. EPA 1995c), includes a complete discussion of combining multiple years of meteorological data into a single file prior to running ISCST3. The modeler should select the ‘ANNUAL’ averaging time for all risk assessment runs, regardless of the number of years in the meteorological data file. The incorrect selection of ‘PERIOD’ will not compute the correct deposition rates required by the risk assessment equations (refer to Section 3.2.3 of the ISC3 User Guide, Volume I). No additional ISCST3 model execution time is required to obtain 1-year or 5-year air modeling values.

In addition, ISCST3 allows the specification of COPC half-life and decay coefficients. Unless approved by the permitting authority with documentation of COPC-specific data, these keywords should not be used when conducting air modeling to support risk assessments. The `TERRHGTS` keyword with the `ELEV` parameter typically should be used to model terrain elevations at receptor grid nodes. The `FLAGPOLE` keyword specifies receptor grid nodes above local ground level and is not typically used for most air modeling to perform impacts at ground level.

U.S. EPA OSW also recommends that `SAVEFIL` be used to restart ISCST3 in the event of a computer or power failure during long runs. `SAVEFIL` is best used by specifying two save files, each with a different name. The save interval should be no longer than 5 days for large runs. If two save files are used, and a failure occurs during writing to the savefile, no more than 10 days will be lost. The `INITFILE` command should be used to restart the runs after the failure, as shown in the following example:

```
CO SAVEFILE SAVE1 5 SAVE2
** INITFILE SAVE1
```

ISCST3 will save the results alternately to `SAVE1` and `SAVE2` every 5 days. If the run fails after successfully writing to `SAVE1`, the ISCST3 run can be restarted by replacing the two asterisks (*) in the `INITFILE` line with `CO` and running ISCST3 again. The run will begin after the last day in `SAVE1`. The modeler should change the names of the save files (e.g., SAVE3 and SAVE4) in the 'CO SAVEFILE' command line prior to restarting ISCST3 to avoid overwriting the SAVE1 and SAVE2 files containing valid data from the interrupted run. Note that the `MULTYEAR` keyword is not used for computing long-term averages and should not be specified.

The following is an example of the COntrol pathway computer code for a single-year ISCST3 particle run:

```
CO STARTING
CO TITLEONE Example input file, particle pahse run, 1 year
CO TITLETWO 1984 met data, Baton Rouge Surface, Boothville Upper Air
CO MODELOPT DFAULT CONC DDEP WDEP DEPOS DRYDPLT WETDPLT RURAL
CO AVERTIME 1 ANNUAL
CO POLLUTID UNITY
CO TERRHGTS ELEV
CO RUNORRUN RUN
CO SAVEFILE 84SAVE1 5 84SAVE2
** Restart incomplete runs with INITFILE, changing '**' to 'CO'
** INITFILE SAVE1
CO FINISHED
```

Additional runs for the other 4 years are set up with the same COntrol pathway, except for the title description and `SAVEFILE` filenames.

3.7.2 SOurce Pathway

As discussed in Section 3.3, ISCST3 normally uses a unit emission rate of 1.0 g/s. Additional source characteristics required by the model (typically obtained from the Part B permit application and trial burn report) include the following:

- Source type (point source for stack emissions; area or volume for fugitive emissions)
- Source location (UTM coordinates, m)
- Source base elevation
- Emission rate (1.0 g/s)
- Stack height (m)
- Stack gas temperature (K)
- Stack gas exit velocity (m/s)
- Stack inside diameter (m)
- Building heights and widths (m)
- Particle size distribution (percent)
- Particle density (g/cm^3)
- Particle and gas scavenging coefficients (unitless)

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Input values with supporting documentation for each parameter identified in Section 3.7.2

3.7.2.1 Source Location

The location keyword of the SOurce pathway (`SO LOCATION`) identifies source type, location, and base elevation. The source type for any stack is referred to as a point source in ISCST3. Fugitive source emissions are discussed in section 3.10. The source location must be entered into ISCST3. Locations should be entered in UTM coordinates. The easterly coordinate is entered to the nearest meter; for example, 637524 meters UTM-E (no commas are used). The northerly coordinate is entered to the nearest meter; for example, a northerly coordinate of 4,567,789 meters UTM-N is entered as 4567789. The base elevation of each stack must be entered in meters. Base elevation may be obtained from a USGS topographic map, facility plot plans or USGS digital data base.

An example input for the location keyword on the SOurce pathway includes source type, location, and base elevation in the following format:

```
SO LOCATION STACK1 POINT 637524. 4567789. 347.
```

3.7.2.2 Source Parameters

The source parameters keyword of the SOurce pathway `(SO SRCPARAM)` identifies the emission rate, stack height, stack temperature, stack velocity, and stack diameter. The unit emission rate is entered as 1.0 g/s. Stack height is the height above plant base elevation on the `SO LOCATION` keyword. Stack exit temperature is the most critical stack parameter for influencing concentration and deposition. High stack temperatures result in high buoyant plume rise, which, in turn, lowers concentration and deposition rates. Stack temperatures should be based on stack sampling tests for existing stacks. For new or undefined stacks, manufacturer's data for similar equipment should be used. Stack exit velocity should be calculated from actual stack gas flow rates and stack diameter. Actual stack gas flow rates should be determined for existing stacks during stack sampling. Representative values for new or undefined sources should be obtained from manufacturer's data on similar equipment. Stack diameter is the inside diameter of the stack at exit.

Following is an example of the source parameter input in the SOurce pathway for emission rate (grams per second), stack height (meters), stack temperature (K), stack velocity (meters per second), and stack diameter (meters):

```
SO SRCPARAM STACK1 1.0 23.0 447.0 14.7 1.9
```

3.7.2.3 Building Parameters

The building height and width keywords of the SOurce pathway `(SO BUILDHGT; SO BUILDWID)` identify the building dimensions that most influence the air flow for each of the 36 10-degree directions surrounding a stack. The dimensions are calculated by using the U.S. EPA program BPIP, as described in Section 3.2.4.

The BPIP output file is input as follows:

```
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29

SO BUILDWID STACK1 14.02 15.51 16.53 17.05 17.05 16.53 15.51 14.03
SO BUILDWID STACK1 12.10 14.02 15.51 16.53 17.05 17.05 16.53 15.51
SO BUILDWID STACK1 14.02 12.10 14.02 15.51 16.53 17.05 17.05 16.53
SO BUILDWID STACK1 15.51 14.02 12.10 14.02 15.51 16.53 17.05 17.05
SO BUILDWID STACK1 16.53 15.51 14.02 12.10
```

3.7.2.4 Particle Size Distribution

ISCST3 requires particle size distribution for determining deposition velocities. U.S. EPA OSW recommends site-specific stack test data for existing sources. New or undefined sources may use the particle size distribution presented in Table 3-1.

The following example is the ISCST3 input for particle phase run. From Table 3-1, the distribution for 9 mean diameter sizes includes the data required for the keywords of the SOurce pathway (`SO PARTDIAM; SO MASSFRAX`). The `PARTDIAM` is taken from Column 1 (Mean Particle Diameter). The `MASSFRAX` is taken from Column 4 (Fraction of Total Mass).

```
SO PARTDIAM STACK1 0.35 0.70 1.10 2.00 3.60 5.50 8.10 12.5 15.0
SO MASSFRAX STACK1 0.22 0.08 0.08 0.11 0.10 0.07 0.10 0.11 0.13
```

The example for the ISCST3 input for the particle-bound run is described below. From Table 3-1, the `PARTDIAM` is the same. The `MASSFRAX` is taken from Column 6 (Fraction of Total Surface Area).

```
SO PARTDIAM STACK1 0.35 0.70 1.10 2.00 3.60 5.50 8.10 12.5 15.0
SO MASSFRAX STACK1 0.49 0.17 0.13 0.09 0.05 0.02 0.02 0.01 0.02
```

3.7.2.5 Particle Density

Particle density is also required for modeling the air concentration and deposition rates of particles. Site-specific measured data on particle density should be determined for all existing sources when possible. For new or undefined sources requiring air modeling, a default value for particle density of 1.0 g/cm^3 may be used. Particles from combustion sources, however, may have densities that are less than 1.0 g/cm^3 (U.S. EPA 1994a), which would reduce the modeled deposition flux.

Following is an example of the particle density input in the SOurce pathway `(SO PARTDENS)` for the 9 mean particle size diameters of the previous example:

```
      SO PARTDENS STACK1 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
```

3.7.2.6 Scavenging Coefficients

Wet deposition flux is calculated within ISCST3 by multiplying a scavenging ratio by the vertically integrated concentration. The scavenging ratio is the product of a scavenging coefficient and a precipitation rate. Studies have shown that best fit values for the scavenging coefficients vary with particle size. For vapors, wet scavenging depends on the properties of the COPCs involved. However, not enough data are now available to adequately develop COPC-specific scavenging coefficients. Therefore, vapors are assumed to be scavenged at the rate of the smallest particles with behavior in the atmosphere that is assumed to be influenced more by the molecular processes that affect vapors than by the physical processes that may dominate the behavior of larger particles (U.S. EPA 1995c).

To use the wet deposition option in ISCST3, users must input scavenging coefficients for each particle size and a file that has hourly precipitation data. For wet deposition of vapors, a scavenging coefficient for a 0.1-μm particle may be input to simulate wet scavenging of very small (molecular) particles. Alternatively, site-specific measured washout data or a calculation based on Henry's Law constant may be approved by the appropriate permitting authority prior to analysis. Wet deposition results only during precipitation. Scavenging coefficients should be determined for each particle size from the best fit curve based on the work of Jindal and Heinhold (1991) presented in the ISC3 User's Guide (U.S. EPA 1995c). The curves are limited to a maximum particle size of 10-μm, so all scavenging coefficients for particle sizes greater than or equal to 10-μm are assumed to be equal. This assumption follows research on wet scavenging of particles (Jindal and Heinhold 1991).

The ISCST3 model input also differentiates between frozen and liquid scavenging coefficients. As a conservative estimate, the frozen scavenging coefficients are assumed to be equal to the liquid scavenging coefficients (PEI and Cramer 1986). If desired, the user may input separate scavenging coefficients for frozen precipitation. Research on sulfate and nitrate data has shown that frozen precipitation scavenging coefficients are about one-third of the values of liquid precipitation (Scire, Strimaitis, and Yamartino 1990; Witby 1978).

Following is an example of the particle liquid (rain) and frozen (sleet or snow) scavenging coefficients input in the SOurce pathway for 9 mean particle size diameters assuming particles are scavenged by frozen precipitation at 1/3 the rate of liquid precipitation:

```
SO PARTSLIQ STACK1 7E-5 5E-5 6E-5 1.3E-4 2.6E-4 3.9E-4 5.2E-4 6.7E-4 6.7E-4
SO PARTSICE STACK1 2E-5 2E-5 2E-5   4E-5   9E-5 1.3E-4 1.7E-4 2.2E-4 2.2E-4
```

The complete SOurce pathway for the example particle phase input file is as follows:

```
SO STARTING
SO LOCATION STACK1 POINT 637524. 4567789. 347.
SO SRCPARAM STACK1 1.0 23.0 447.0 14.7 1.9
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29
SO BUILDWID STACK1 14.02 15.51 16.53 17.05 17.05 16.53 15.51 14.03
SO BUILDWID STACK1 12.10 14.02 15.51 16.53 17.05 17.05 16.53 15.51
SO BUILDWID STACK1 14.02 12.10 14.02 15.51 16.53 17.05 17.05 16.53
SO BUILDWID STACK1 15.51 14.02 12.10 14.02 15.51 16.53 17.05 17.05
SO BUILDWID STACK1 16.53 15.51 14.02 12.10
SO PARTDIAM STACK1 0.35 0.70 1.10 2.00 3.60 5.50 8.10 12.5 15.0
SO MASSFRAX STACK1 0.22 0.08 0.08 0.11 0.10 0.07 0.10 0.11 0.13
SO PARTDENS STACK1 1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
SO PARTSLIQ STACK1 7E-5 5E-5 6E-5 1.3E-4 2.6E-4 3.9E-4 5.2E-4 6.7E-4 6.7E-4
SO PARTSICE STACK1 2E-5 2E-5 2E-5   4E-5   9E-5 1.3E-4 1.7E-4 2.2E-4 2.2E-4
SO SRCGROUP ALL
SO FINISHED
```

When modeling air vapors using ISCST3, the following is an example of the SOurce pathway input for wet vapor scavenging coefficients that replaces the PARTDIAM, MASSFRAX, PARTDENS, PARTSLIQ and PARTSICE lines in the above example:

```
SO GAS-SCAV STACK1 LIQ 1.7E-4
SO GAS-SCAV STACK1 ICE 0.6E-4
```

3.7.3 REceptor Pathway

The REceptor pathway identifies sets or arrays of receptor grid nodes identified by UTM coordinates for which ISCST3 generates estimates of air parameters including air concentration, dry and wet deposition, and total deposition. Previous U.S. EPA guidance (U.S. EPA 1994a) recommended using a polar receptor grid to identify maximum values, because polar grids provide coverage over large areas with a reduced number of receptor grid nodes, thereby reducing computer run times. However, U.S. EPA Region 6 experience indicates that, although the use of polar grids may reduce computer run times, air modelers typically choose a different option, because the benefit of reduced run time is offset by difficulties in identifying polar grid locations in absolute UTM coordinates for (1) extracting terrain values from digital terrain files, and (2) selecting receptor grid node locations for evaluation of ecosystems and special ecological habitats (see Chapter 4).

Receptor grid node arrays may be generated by using ISCST3 grid generation. However, assigning terrain elevations for each receptor grid node in an array associated with the generated grid can result in errors. One method of obtaining a Cartesian grid with terrain elevations is to open the USGS DEM file in a graphics program (e.g., SURFER®). Selection of the grid option samples the DEM file, at the user-specified spacing, over a range of east (x) and north (y) values. The specified x and y locations extract terrain elevation (z) from the DEM file at the desired receptor grid node for air modeling with the appropriate terrain elevations at each receptor grid node. These x, y, and z values are saved as a text file with one receptor grid node per line. A text editor is used to prefix each line with “`RE DISCCART`” to specify a discrete receptor grid node in ISCST3 format. Commercial receptor grid generators are also available. One commercial program (Lakes Environmental Software) generates the recommended receptor grid node array and extracts terrain elevations from the USGS DEM downloaded files, or any terrain file in x-y-z format.

The following is an example of the REceptor pathway for discrete receptor grid nodes at 500-meter spacing and including terrain elevations (in meters):

```
RE STARTING
RE ELEVUNIT METERS
RE DISCCART 630000. 565000. 352.
RE DISCCART 630500. 565000. 365.
RE DISCCART 631000. 565000. 402.
       ↓
RE DISCCART 635000. 570000. 387.
RE FINISHED
```

U.S. EPA OSW recommends that air modeling for each risk assessment include, at a minimum, an array of receptor grid nodes covering the area within 10 kilometers of the facility with the origin at the centroid of a polygon formed by the locations of the stack emission sources. This receptor grid node array should consist of a Cartesian grid with grid nodes spaced 100 meters apart extending from the centroid of the emission sources out to 3 kilometers from the centroid. For the distances from 3 kilometers out to 10 kilometers, the receptor grid node spacing can be increased to 500 meters. The single grid node array contains both grid node spacings. This same receptor grid node array is included in the REceptor pathway for all ISCST3 runs for all years of meteorological data and for all emission sources.

Terrain elevations should be specified for all receptor grid nodes. Several methods are available for assigning terrain elevations to grid nodes using digital terrain data. The 1:250,000 scale DEM digital data are available for download at the USGS Internet site:

Worldwide Web:	http://edcwww.cr.usgs.gov/pub/data/dem/250
FTP (two options):	ftp://edcwww.cr.usgs.gov/pub/data/dem/250 ftp://edcftp.cr.usgs.gov/pub/data/dem/250

This data has horizontal spacing between digital terrain values of approximately 90 meters which provides sufficient accuracy for air modeling.

In addition to the receptor grid node array evaluated for each facility out to 10 kilometers, other grid node arrays may be considered for evaluation of water bodies and their watersheds, ecosystems and special ecological habitats located beyond 10 kilometers. Grid node spacing of 500 meters between nodes is recommended for grid node arrays positioned at distances greater than 10 kilometers from the emission source. An equally spaced grid node array facilitates subsequent computation of area averages for deposition rates.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Summary of all information regarding the coordinates and placement of the receptor grid node array used in air modeling
- Copies of any maps, figures, or aerial photographs used to develop the receptor grid node array
- Map presenting UTM locations of receptor grid nodes, along with other facility information.

3.7.4 MEteorological Pathway

The file containing meteorological data is specified in the MEteorological pathway. PCRAMMET creates individual files for each of 5 years, as ASCII files, to be read into ISCST3 for computing hourly concentrations and deposition rates. The modeler may specify a single year of meteorological data in each ISCST3 run, or combine the total period of meteorological data into a single meteorological file for processing by ISCST3 in a single 5-year run. When combining meteorological files, the modeler is cautioned to consider the following:

- Preprocess each year separately using PCRAMMET or MPRM into an ASCII format
- Combine the years into a single file (using a text editor or DOS COPY command)
- The first line (header) of the combined file is read by ISCST3 for comparison to the Surface and Upper Air Station ID numbers specified in the input file ME pathway
- The header for subsequent years is read by ISCST3 only if not deleted in the combined file. If subsequent year headers are included in the combined file, ISCST3 will compare the station IDs to the input file station ID. For air modeling analysis which use meteorological data from more than one surface station or upper air station (e.g., the upper air station is moved after the third year of the period and assigned a new station ID by the National Weather Service), the modeler should delete the headers for subsequent years in the combined file.

- For sites where the anemometer height is changed during the 5 year period (e.g., for the period 1984-1988, the anemometer was relocated from 20 feet to 10 meters on December 15, 1985), the modeler should run each year separately to specify the correct anemometer height in the ISCST3 input file ME pathway which corresponds to the correct height for that year of meteorological data.

Details of specifying the meteorological data file are in the ISC3 User's Guide (Section 3.5.1.1). Each year within the file must be complete with a full year of data (365 days, or 366 days for leap years). The anemometer height must be verified for the surface station from Local Climate Data Summary records, or other sources, such as the state climatologist office. U.S. EPA OSW recommends that the anemometer height `ANEMHGHT` for the wind speed measurements at the surface station be correctly identified before air modeling.

The following is an example input section for the MEteorological pathway, using the 1984 Baton Rouge file, with an anemometer height of 10 meters and station identification numbers:

```
ME STARTING
ME INPUTFIL 84BR.WET
ME ANEMHGHT 10.0
ME SURFDATA 13970 1984 BATON_ROUGE
ME UAIRDATA 12884 1984 BOOTHVILLE
ME FINISHED
```

3.7.5 Terrain Grid (TG) Pathway

The computation of dry plume depletion is sensitive to terrain elevation. In the absence of a terrain grid file, ISCST3 automatically assumes that the terrain slope between the stack base and the receptor grid node elevation is linear. In concept, this assumption may underestimate plume deposition. However, based on experience, the magnitude of the differences in computed concentrations and deposition rates is nominal. Since the inclusion of a terrain grid file in the TG pathway significantly increases model execution time, U.S. EPA OSW recommends that a terrain grid file is not necessary for all sites. If a terrain grid file is desired for a specific site based on highly variable terrain over short distances, the format of the TG file is described in the ISC3 User's Guide.

The location keyword of the TG pathway (`TG LOCATION`) identifies the x and y values to be added to the source and receptor grid to align with the terrain file coordinates. If the source and receptor grid nodes are in relative units such that the source is at location 0,0, the location keywords in the TG pathway would be the UTM coordinates of the source. U.S. EPA OSW requires that all emission sources and receptor grid nodes be specified in UTM coordinates (NAD27 or NAD83 format), and that the TG file, if used, be in UTM coordinates. Therefore, the location of the origin of the TG file relative to the source location will be 0,0. Also, U.S. EPA OSW recommends that the terrain elevations in the TG file be presented in meters. Following is an example of the TG pathway:

```
TG STARTING
TG INPUTFIL TERRAIN.TER
TG LOCATION 0.0 0.0
TG ELEVUNIT METERS
TG FINISHED
```

3.7.6 OUtput Pathway

ISCST3 provides numerous output file options in addition to the results in the output summary file specified in receptor tables (RECTABLE). The plot file is most useful for facilitating post-processing of the air parameter values in the model output. The plot file lists the x and y coordinates and the concentration or deposition rate values for each averaging period in a format that can be easily pulled into a post-processing program (or spreadsheet). Note that the ISCST3 generated ‘plot’ file is not the same format as the ISCST3 generated ‘post’ file. U.S. EPA OSW recommends using the plot file, not the post file.

Following is an example OUtput file specification for single-year run of 1-hour and annual average plot files:

```
OU STARTING
OU RECTABLE ALLAVE FIRST
OU PLOTFILE 1 ALL FIRST BTR841.PLT
OU PLOTFILE ANNUAL ALL BTR84A.PLT
OU FINISHED
```

For ecological risk assessments, the 1-hour average plot file is not needed. If the modeler has directed in the ISCST3 control pathway for 1-hour averages to be computed for use in a human health acute risk assessment, then the 1-hour average plot file also should be specified (U.S. EPA 1998). The second line in the example directs ISCST3 to create a table of values for each receptor grid node for all averaging periods in the model run (annual and optionally 1-hour). The third line directs ISCST3 to create a separate plot file of the 1-hour average results, if desired by the modeler. The fourth line directs ISCST3 to create another separate plot file of the annual average results for all sources in the run for each receptor grid node.

3.8 ISCST3 MODEL EXECUTION

Model execution time should be considered for each analysis. A complete air modeling run—including air concentration, wet and dry deposition, and plume depletion—may require 10 times the run time for the same source and receptor grid nodes for air concentration only. Even if only the total deposition is specified, ISCST3 must compute air concentration and the dry and wet deposition components in order to compute the total deposition air parameter values required for the ecological risk assessment. For example, an ISCST3 particle run of one source with 800 receptor grid nodes, on 1 year of meteorological data, with the options for air concentration, wet and dry deposition, and plume depletion required about 40 hours on a personal computer with a 486 processor running at 66 megahertz (486/66). The same run can be completed in about 10 hours on a 586/120 personal computer. Five years of meteorological data and an additional 1,600 receptor grid nodes result in total run times of 120 hours for 1 year, and 600 hours for a 5-year analysis on a 486/66 personal computer. Run time on a 586/120 personal computer is estimated at about 150 hours. A significant loss of modeling effort and analysis time can be prevented by verifying input parameters and conducting test runs prior to executing the ISCST3 runs.

Long run times result mainly from two algorithms—plume depletion and terrain grid file. ISCST3 run times are increased as much as tenfold for runs applying plume depletion. U.S. EPA OSW believes that constituent mass must be conserved between suspended concentration and deposition rate by allowing for depletion of deposited mass from the plume concentration in ISCST3. The overestimate of plume concentration, and the subsequent overestimate of deposition, which results when plume depletion is not allowed, is too conservative. However, the nominal benefits of including a terrain grid file do not justify the added run times. Therefore, plume depletion should always be included, but terrain grid files are not recommended.

3.9 USE OF MODELED OUTPUT

The ISCST3 modeled output (air concentrations and deposition rates) are provided on a unit emission rate (1.0 g/s) basis from the combustion unit or emission source, and are not COPC-specific. The estimating media equations presented in Section 3.11 and Appendix B require the model output (air parameters, see Table 3-5) directly without converting the unit based output to COPC-specific output. However, there may be some instances where the risk assessor will need to convert modeled output to COPC-specific output for the risk assessment. For example, the risk assessor may want to compare modeled COPC concentrations in ambient media to concentrations actually measured in the field.

3.9.1 Unit Rate Output vs. COPC-Specific Output

The relationship between the unit emission rate and the unit air parameter values (air concentrations and deposition rates) is linear. Similarly, the relationship between the COPC-specific emission rate (Q) and the COPC-specific air parameter values (air concentrations and deposition rates) would also be linear if the COPC-specific emission rate was used in the air model. Section 3.3 discussed the use of the unit emission rate and advanced the theory that a unit emission rate should be used instead of the COPC-specific emission rate in order to preclude having to run the ISCST3 model separately for each individual COPC. The use of a unit emission rate in the air modeling is advocated because a common ratio relationship can be developed between the unit emission rate and the COPC-specific emission rate based on the fact that in the air model, both individual relationships are linear. This ratio relationship can be expressed by the following equation:

TABLE 3-5

AIR PARAMETERS FROM ISCST3 MODELED OUTPUT

Air Parameter	Description	Units
Cyv	Unitized yearly average air concentration from vapor phase	μg-s/g-m^3
Cyp	Unitized yearly average air concentration from particle phase	μg-s/g-m^3
Dywv	Unitized yearly average wet deposition from vapor phase	s/m^2-yr
Dydp	Unitized yearly average dry deposition from particle phase	s/m^2-yr
Dywp	Unitized yearly average wet deposition f rom particle phase	s/m^2-yr
Cywv	Unitized yearly (water body or watershed) average air concentration from vapor phase	μg-s/g-m^3
Dywwv	Unitized yearly (water body or watershed) average wet deposition from vapor phase	s/m^2-yr
Dytwp	Unitized yearly (water body or watershed) average total (wet and dry) deposition from particle phase	s/m^2-yr

$$\frac{\text{COPC-Specific Air Concentration}}{\text{COPC-Specific Emission Rate}} = \frac{\text{Modeled Output Air Concentration}}{\text{Unit Emission Rate}} \qquad \text{Equation 3-2}$$

Use of this equation requires that three of the variables be known. The modeled output air concentration (or deposition rate) is provided by the air model, the unit emission is 1.0 g/s, and the COPC-specific emission rate; which is obtained directly from stack or source test data.

3.9.1.1 Determination of the COPC-Specific Emission Rate (*Q*)

The COPC-specific emission rate can usually be determined with information obtained directly from the trial burn report. The COPC-specific emission rate from the stack is a function of the stack gas flow rate and the stack gas concentration of each COPC; which can be calculated from the following equation:

$$Q = SGF \cdot \frac{SGC \cdot CFO_2}{1 \times 10^6} \qquad \text{Equation 3-4}$$

where

Q = COPC-specific emission rate (g/s)
SGF = Stack gas flow rate at dry standard conditions (dscm/s)
SGC = COPC stack gas concentration at 7 percent O_2 as measured in the trial burn (µg/dscm)
CFO_2 = Correction factor for conversion to actual stack gas concentration O_2 (unitless)
1×10^6 = Unit conversion factor (µg/g)

Guidance for determining COPC-specific emission rates for fugitive emission sources can be found in Chapter 2. Also, it is sometimes necessary to derive the COPC-specific emission rate from surrogate data, such as for a new facility that has not yet been constructed and trial burned (see Chapter 2).

3.9.1.2 Converting Unit Output to COPC-Specific Output

Once the three of the four variables in Equation 3-1 are known, the COPC-specific air concentrations and deposition rates can be obtained directly by multiplication, as follows:

$$\begin{matrix}\text{COPC}-\text{Specific}\\ \text{Air Concentration}\end{matrix} = \frac{\text{Modeled Output Air Concentration} \cdot \text{COPC}-\text{Specific Emission Rate}}{\text{Unit Emission Rate}} \qquad \text{Equation 3-3}$$

For example, if COPC A is emitted at a rate of 0.25 g/s, and the ISCST3 modeled concentration at a specific receptor grid node is 0.2 $\mu g/m^3$ per the 1.0 g/s unit emission rate, the concentration of COPC A at that receptor grid node is 0.05 $\mu g/m^3$ (0.25 multiplied by 0.2). Deposition is calculated similarly, proportional to the emission rate of each COPC. Readers are reminded once again that this process of converting modeled unitized output into COPC-specific output is taken directly into account in the estimating media concentration equations in Section 3.11 and Appendix B.

3.9.2 Output from the ISCST3 Model

The ISCST3 output is structured and the risk assessor must understand how to read the output in order to ensure accurate use of modeled output in the risk assessment. The output from each ISCST3 model run is written to two separate file formats. The ‘output file’ is specified by name at run time in the execution command. Typical command line nomenclature is:

```
ISCST3 inputfile.INP outputfile.OUT
```

where

`ISCST3`: specifies execution of the ISCST3 model
`inputfile.INP`: is the input file name selected by the modeler
`outputfile.OUT`: is the output file name selected by the modeler, typically the same as the input file name

For example, the following ISCST3 input line would run the input file (PART84.INP) created by the modeler for particulate emissions using 1984 meteorological data. The output file (PART84.OUT) from the run will automatically be written by ISCST3 during model execution.

```
ISCST3 PART84.INP PART84.OUT
```

The output ‘plot file’ is specified by the modeler in the ISCST3 input file OUtput pathway and created by ISCST3 during the run (see Section 3.7.6). Figure 3-3 is an example of the first few lines in the particle phase plot file with single-year annual average concentration, total deposition, dry deposition and wet deposition values for each receptor grid node. The total deposition is the sum of the dry and wet components of deposition. The single-year values at each receptor grid node being evaluated must be averaged to a 5-year value. The 5-year averaged values at the receptor grid nodes selected for evaluation in the risk assessment (see Section 3.9.3), are used in the estimating media concentration equations. This file is usually imported into a post-processing program (or spreadsheet) before entry into the risk assessment computations.

Similar plot files are produced for the particle-bound and vapor phase runs. The output for the vapor phase runs will be average concentration and wet deposition. The output for the particle and particle-bound phase runs will be average concentration, dry deposition, wet deposition and total deposition. Again, the 1-year values at each receptor grid node must be averaged to a 5-year value at each node unless a single five-year ISCST3 run using a combined meteorological file is used. If the 5-year combined file is used, the results from the ISCST3 plot file may be used directly in the risk assessment without averaging over the five years.

All values are defined as used in the estimating media concentration equations (see Section 3.11).

3.9.3 Use of Model Output in Estimating Media Equations

Section 3.4 discussed how consideration of partitioning of the COPCs effects the development of ISCST3 modeling runs. The selection of which air modeled air parameter values (air concentrations and deposition rates) to use in the estimating media concentration equations is based on this same partitioning theory.

3.9.3.1 Vapor Phase COPCs

ISCST3 output generated from vapor phase air modeling runs are vapor phase air concentrations (unitized *Cyv* and unitized *Cywv*) and wet vapor depositions (unitized *Dywv* and unitized *Dywwv*) for organic COPCs at receptor grid nodes based on the unit emission rate. These values are used in the estimating media concentration equations for all COPC organics except the polycyclic aromatic hydrocarbons dibenzo(a,h)anthracene and indeno(1,2,3-cd)pyrene, which have vapor phase fractions, Fv, less than five percent. The air concentration (unitized *Cyv*) and wet vapor deposition (unitized *Dywv*) from the vapor phase run is also used in the estimating media concentration equations for mercury. Values for these COPCs are selected from the vapor phase run because the mass of the COPC emitted by the combustion unit is assumed to have either all or a portion of its mass in the vapor phase (see Appendix A-2).

3.9.3.2 Particle Phase COPCs

ISCST3 output generated from particle phase air modeling runs are air concentration (unitized *Cyp*), dry deposition (unitized *Dydp*), wet deposition (unitized *Dywp*), and combined deposition (unitized *Dytwp*) for inorganics and relatively non-volatile organic COPCs at receptor grid nodes based on the unit emission rate. These values are used in the estimating media concentration equations for all COPC inorganics (except mercury, see Chapter 2 and Appendix A-2) and polycyclic aromatic hydrocarbons with fraction of vapor phase, Fv , less than 0.05 (e.g., dibenzo(a,h)anthracene and indeno(1,2,3-cd)pyrene). Values for inorganic and relatively non-volative COPCs are selected from the particle phase run because the mass of the COPC emitted by the combustion unit is assumed to have all of its mass in the particulate phase (see Appendix A-2), apportioned across the particle size distribution based on mass weighting.

3.9.3.3 Particle-Bound COPCs

ISCST3 output generated from particle-bound air modeling runs are air concentration (unitized *Cyp*), dry deposition (unitized *Dydp*), wet deposition (unitized *Dywp*), and combined deposition (unitized *Dytwp*) for organic COPCs and mercury (see Chapter 2 and Appendix A-2) at receptor grid nodes based on the unit emission rate. These values are used in the estimating media concentration equations for all COPC organics and mercury to account for a portion of the vapor condensed onto the surface of particulates. Values for these COPCs are selected from the particle-bound run because the mass of the COPC emitted by the combustion unit is assumed to have a portion of its mass condensed on particulates (see Appendix A-2), apportioned across the particle size distribution based on surface area weighting.

3.10 MODELING OF FUGITIVE EMISSIONS

Fugitive source emissions, as defined in Chapter 2, should be modeled using the procedures presented throughout this chapter for stack source emissions. However, the fugitive emissions should be represented in the ISCST3 input file SOurce pathway as either “area” or “volume” source types. Fugitive emissions of volatile organics are modeled only in the vapor phase. Fugitive emissions of ash are modeled only in the particle and particle-bound phases, not vapor phase.

As discussed in Chapter 2, fugitive emissions of volatile organic vapors are associated with combustion units that include storage vessels, pipes, valves, seals and flanges. The horizontal area of the fugitive source (which can be obtained from the facility plot plan) is entered into the ISCST3 input file following the instructions presented in the ISC3 User's Guide, Volume I (U.S. EPA 1995c). The height of the fugitive source is defined as the top of the vertical extent of the equipment. If the vertical extent of the fugitive source is not known, a default height of ground level (release height of zero) may be input, providing a conservative estimate of potential impacts. The ISCST3 model run time is faster for volume source types than for area source types, and should be considered for most applications. The methods in the ISCST3 User's Guide should be followed in defining the input parameters to represent the fugitive source.

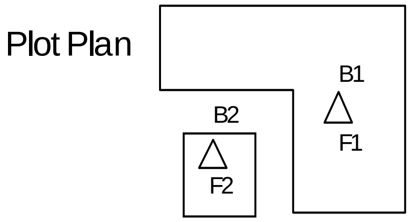
FIGURE 3-3

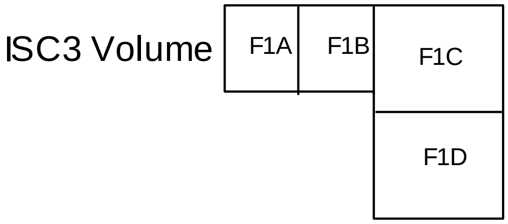
EXAMPLE PLOT FILE

```
*ISCST3 (96113):  Example Particle Phase Run, Single Year 1990
*MODELING OPTIONS USED:
* CONC   DEPOS  DDEP   WDEP   RURAL  ELEV          DFAULT                                         DRYDPL WETDPL

*        PLOT FILE OF ANNUAL VALUES FOR SOURCE GROUP: ALL
*        FOR A TOTAL OF    21 RECEPTORS.
*        FORMAT: (6(1X,F13.5),1X,F8.2,2X,A6,2X,A8,2X,I8,2X,A8)
*     X            Y        AVERAGE CONC  TOTAL DEPO    DRY DEPO      WET DEPO   ZELEV      AVE   GRP   NUM HRS   NET
ID
*___________ _____________  ___________    _________   ___________   _________   ______   ______  _____ _______
________
691600.00000 3342050.00000     0.29900     0.28658       0.20024      0.08634     4.00     ANNUAL  ALL    8760     NA
691700.00000 3342050.00000     0.30203     0.35416       0.23884      0.11532     5.00     ANNUAL  ALL    8760     NA

691800.00000 3342050.00000     0.25174     0.42461       0.25976      0.16485     5.00     ANNUAL  ALL    8760     NA

691900.00000 3342050.00000     0.13256     0.50524       0.23852      0.26672     5.00     ANNUAL  ALL    8760     NA

692000.00000 3342050.00000     0.00322     0.61790       0.05850      0.55940     5.00     ANNUAL  ALL    8760     NA

692100.00000 3342050.00000     0.00000     6.32022       0.00000      6.32022     6.00     ANNUAL  ALL    8760     NA

692200.00000 3342050.00000     0.00319     0.32218       0.06577      0.25641     6.00     ANNUAL  ALL    8760     NA

692300.00000 3342050.00000     0.13768     0.39938       0.21734      0.18204     6.00     ANNUAL  ALL    8760     NA

692400.00000 3342050.00000     0.23546     0.33855       0.20975      0.12880     6.00     ANNUAL  ALL    8760     NA

692500.00000 3342050.00000     0.25673     0.27475       0.17903      0.09572     6.00     ANNUAL  ALL    8760     NA

692600.00000 3342050.00000     0.24706     0.22195       0.14812      0.07384     6.00     ANNUAL  ALL    8760     NA

691600.00000 3342150.00000     0.37348     0.40644       0.25958      0.14685     5.00     ANNUAL  ALL    8760     NA

691700.00000 3342150.00000     0.37166     0.51388       0.31119      0.20269     5.00     ANNUAL  ALL    8760     NA
```

```
691800.00000 3342150.00000     0.34332     0.68794      0.39582      0.29212     5.00     ANNUAL  ALL    8760     NA

691900.00000 3342150.00000     0.22930     0.98039      0.54883      0.43156     5.00     ANNUAL  ALL    8760     NA

692000.00000 3342150.00000     0.03473     0.90823      0.37421      0.53402     6.00     ANNUAL  ALL    8760     NA

692100.00000 3342150.00000     0.00098     0.62882      0.15736      0.47146     6.00     ANNUAL  ALL    8760     NA

692200.00000 3342150.00000     0.02605     0.48160      0.15582      0.32578     7.00     ANNUAL  ALL    8760     NA

692300.00000 3342150.00000     0.17300     0.49313      0.22998      0.26315     7.00     ANNUAL  ALL    8760     NA

692400.00000 3342150.00000     0.24520     0.29443      0.19715      0.09729     7.00     ANNUAL  ALL    8760     NA

692500.00000 3342150.00000     0.25561     0.23482      0.16744      0.06738     7.00     ANNUAL  ALL    8760     NA
```

The following example is for organic fugitive emissions modeled as a volume source type. For a facility which may have two stack emission sources (B1, B2) and two fugitive emission sources (areas F1, F2); a total of four runs for each year (or 5-year combined file) of meteorological data is required. One run is required for each of the two stacks as point sources. One run is required for each of the two fugitive areas as volume sources (Note: modeler may alternatively model as an area source). Since the emissions are fugitive volatile organics, only the vapor phase is modeled. The vertical extent of the pipes, valves, tanks and flanges associated with each fugitive emission area is 15 feet (about 5 meters) above plant elevation. To define the sources for input to ISCST3, the release height is specified as 2.5 meters (½ of vertical extent of fugitive emissions). The initial vertical dimension is specified as 1.16 meters (vertical extent of 5 meters divided by 4.3 as described in the ISC3 User's Guide).





The initial horizontal dimension is the side length of the square fugitive area (footprint) divided by 4.3. If fugitive area F2 has a measured side of 30 meters, the initial horizontal dimension is 6.98 (30 meters divided by 4.3). For fugitive area F1, the area on the plot plan must be subdivided (ISC3 Volume) to create square areas for input to ISCST3. The four areas depicted represent subdivision into square areas. The resulting four square areas are input into a single ISCST3 run for Fugitive source F1 as four separate volume sources (F1A, F1B, F1C, F1D). The initial horizontal dimension for each volume source is the side of the square divided by 4.3. It is very important to allocate proportionately the unit emission rate (1.0 gram per second) among the subdivided areas. For example, if the areas of the subdivided squares in the ISC3 Volume figure results in F1A equal to F1B each with 1/8th the total area, the proportion of the unit emissions allocated to each of these volume sources is 0.125 grams per second. The remaining two areas are each 3/8ths of the total area of fugitive F1, so that 0.375 grams per second is specified for the emission rate from each source. The total emissions for the four volume sources sum to the unit emission rate for the F1 fugitive source (0.125 + 0.125 + 0.375 + 0.375 = 1.0 g/s). By specifying all sources to be included in the model results from ISCST3 (SO SRCGROUP ALL), the ISCST3 model will appropriately combine all four volume source subdivisions of fugitive source F1 into combined impact results for fugitive source F1. The resulting air parameter values in the plot files may be used directly in the risk assessment equations, the same as if a stack emission were modeled as a single point source. The initial vertical dimension is defined the same as F2, using the vertical extent of 5 meters divided by 4.3 and a release height of 2.5 meters (½ vertical extent). For volume sources, the location is specified by the x and y coordinates of the center of each square area.

The COntrol parameters should follow the recommendations for setting up a vapor phase computation.

```
CO CONC WDEP
```

Fugitive emissions of ash particles are from the storage piles associated with combustion units. The horizontal area of the storage pile is entered into the ISCST3 input file following the ISCST3 User's Guide, Volume I (U.S. EPA 1995c). The height of emissions is input as the top of the pile. If the vertical extent is not known, the height may be input as ground level (or zero height). Fugitive ash will typically be modeled as area source type. However, volume source type may be considered by the appropriate regulatory agency prior to air modeling. The methods in the ISCST3 User's Guide should be followed in defining the input parameters to represent the ash release as an area source.

The COntrol parameters should follow the recommendations for setting up a particulate phase computation.

```
CO CONC DDEP WDEP DEPOS
```

The emissions characterization and source type must be documented.

3.11 ESTIMATION OF COPC CONCENTRATIONS IN MEDIA

As discussed in Section 3.9 (see also Table 3-5), the ISCST3 modeled output of unitized air parameters (air concentrations and deposition rates) are provided on a unit emission (1.0 g/s) basis from the combustion unit, and are not COPC-specific. The estimating media concentration equations, presented in this section, accept these unitized output values directly to calculate COPC-specific media concentrations for use in characterizing ecological risk. Selection of the appropriate ISCST3 modeled output for use in the equations is discussed in Section 3.9.

This section presents the estimating media concentration equations used for calculating, from the appropriate ISCST3 unitized model output and COPC-specific emission rates, COPC-specific media concentrations in soil, surface water, and sediment. Determining COPC media concentrations is relevant to estimating risks to potentially impacted ecosystems through exposure of ecological receptors to COPCs in air (plant only), soil, surface water, and sediment. This section also includes equations for calculating COPC-specific concentrations in terrestrial plants resulting from foliar and root uptake.

Section 3.11.1 describes the equations for calculating COPC-specific concentration in soils. Section 3.11.2 describes the equations for calculating COPC-specific concentrations in surface water and sediment. Section 3.11.3 describes the equations for calculating COPC-specific plant concentrations from foliar and root uptake. In addition, Appendix B also provides in more detail the media concentration equations and default input variables recommended by U.S. EPA OSW.

3.11.1 CALCULATION OF COPC CONCENTRATIONS IN SOIL

As depicted in Figure 3-4, COPC concentrations in soil are calculated by summing the particle and vapor phase deposition of COPCs to the soil. Wet and dry deposition of particles and vapors are considered, with dry deposition of vapors calculated from the vapor air concentration and the dry deposition velocity. Soil concentrations may require many years to reach steady state. As a result, the equations used to calculate the soil concentration over the period of deposition were derived by integrating the instantaneous soil concentration equation over the period of deposition. U.S. EPA OSW recommends that the highest 1-year annual average COPC concentration in soil be used as the soil concentration for estimating ecological risk, which would typically occur at the end of the time period of combustion (see Section 3.11.1).

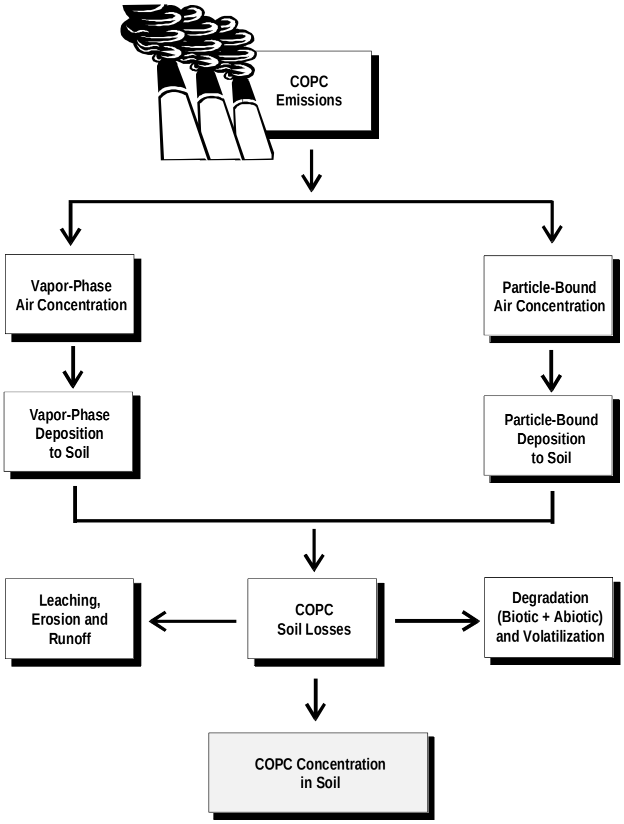


Figure 3-4 - COPC Concentration in Soil

Following deposition, the calculation of soil concentration also considers losses of COPCs by several mechanisms, including leaching, erosion, runoff, degradation (biotic and abiotic), and volatilization. All of these loss mechanisms may lower the soil concentration if included in the soil concentration calculation (see Section 3.11.1.2). Soil conditions—such as pH, structure, organic matter content, and moisture content—can also affect the distribution and mobility of COPCs in soil. Loss of COPCs from the soil is modeled using a combination of default and site-specific values to account for the physical and chemical characteristics of the soil.

COPCs may also be physically incorporated into the upper layers of soil through tilling. The concentration in the top 20 centimeters of soil should be computed for estimating a COPC concentration in soils that are physically disturbed or tilled. The COPC concentration in the top 1 centimeter of soil should be computed for estimating a COPC concentration in soils that are not tilled (see Section 3.11.1.4).

3.11.1.1 Calculating Highest Annual Average COPC Concentration in Soil

U.S. EPA OSW recommends the following equation for calculating the highest average annual COPC soil concentration.

Recommended Equations for Calculating:
Highest Annual Average COPC Concentration in Soil (*Cs*)

$$Cs = \frac{Ds \cdot [1 - \exp(-ks \cdot tD)]}{ks} \qquad \text{Equation 3-7}$$

where

Cs = COPC concentration in soil (mg COPC/kg soil)
Ds = Deposition term (mg/kg-yr)
ks = COPC soil loss constant due to all processes (yr^{-1})
tD = Total time period over which deposition occurs (time period of combustion) (yr)

This equation calculates the highest annual average soil concentration, which is typically expected to occur at the end of the time period of deposition (U.S. EPA 1994l; 1998c). Derivation of the equation is presented in U.S. EPA (1998c). Appendix B, Table B-1-1 also describes the equation, definitions of its terms, and default values for the variables.

3.11.1.2 Calculating the COPC Soil Loss Constant (*ks*)

COPCs may be lost from the soil by several processes that may or may not occur simultaneously. In Equation 3-8, the soil loss constant, *ks*, expresses the rate at which a COPC is lost from soil (U.S. EPA 1993h; 1998c). The constant *ks* is determined by using the soil's physical, chemical, and biological characteristics to consider the losses resulting from:

(1) biotic and abiotic degradation,

(2) erosion,

(3) surface runoff,

(4) leaching, and

(5) volatilization.

Consistent with earlier U.S. EPA guidance (U.S. EPA 1993h; 1994l; 1998c), U.S. EPA OSW recommends using Equation 3-8 to compute the soil loss constant.

Recommended Equation for Calculating:
COPC Soil Loss Constant (*ks*)

$$ks = ksg + kse + ksr + ksl + ksv \qquad \text{Equation 3-8}$$

where

ks = COPC soil loss constant due to all processes (yr^{-1})
ksg = COPC loss constant due to degradation (yr^{-1})
kse = COPC loss constant due to erosion (yr^{-1})
ksr = COPC loss constant due to runoff (yr^{-1})
ksl = COPC loss constant due to leaching (yr^{-1})
ksv = COPC loss constant due to volatilization (yr^{-1})

The use of Equation 3-8 assumes that COPC loss can be defined by using first-order reaction kinetics. First-order reaction rates depend on the concentration of one reactant (Bohn, McNeal, and O'Connor 1985). The loss of a COPC by a first-order process depends only on the concentration of the COPC in the soil, and a constant fraction of the COPC is removed from the soil over time. Those processes that apparently exhibit first-order reaction kinetics without implying a mechanistic dependence on a first-order loss rate are termed “apparent first-order” loss rates (Sparks 1989). The assumption that COPC loss follows first-order reaction kinetics may be an oversimplification because—at various concentrations or under various environmental conditions—the loss rates from soil systems will resemble different kinetic expressions. However, at low concentrations, a first-order loss constant may be adequate to describe the loss of the COPC from soil (U.S. EPA 1990a).

COPC loss in soil can also follow zero or second-order reaction kinetics. Zero-order reaction kinetics are independent of reactant concentrations (Bohn, McNeal, and O'Connor 1985). Zero-order loss rates describe processes in which the reactants are present at very high concentrations. Under zero-order kinetics, a constant amount of a COPC is lost from the soil over time, independent of its concentration. Processes that follow second-order reaction kinetics depend on the concentrations of two reactants or the concentration of one reactant squared (Bohn, McNeal, and O'Connor 1985). The loss constant of a COPC following a second-order process can be contingent on its own concentration, or on both its concentration and the concentration of another reactant, such as an enzyme or catalyst.

Because COPC loss from soil depends on many complex factors, it may be difficult to model the overall rate of loss. In addition, because the physical phenomena that cause COPC loss can occur simultaneously, the use of Equation 3-8 may also overestimate loss rates for each process (Valentine 1986). When possible, the common occurrence of all loss processes should be taken into account.

The following subsections discuss issues associated with the calculation of the *ksl*, *kse*, *ksr*, *ksg*, and *ksv* variables. Appendix B, Tables B-1-2 through B-1-6 present the equations for computing the overall and individual soil loss constant, except for loss due to degradation, which is discussed below.

COPC Loss Constant Due to Biotic and Abiotic Degradation *(ksg)*

Soil losses resulting from biotic and abiotic degradation (*ksg*) are determined empirically from field studies and should be addressed in the literature (U.S. EPA 1990a). Lyman et al. (1982) states that degradation rates can be assumed to follow first order kinetics in a homogenous media. Therefore, the half-life of a compound can be related to the degradation rate constant. Ideally, *ksg* is the sum of all biotic and abiotic rate constants in the soil media. Therefore, if the half-life of a compound (for all of the mechanisms of transformation) is known, the degradation rate can be calculated. However, literature sources do not provide sufficient data for all such mechanisms, especially for soil. Therefore, Appendix A-2 presents U.S. EPA OSW recommended values for this COPC specific variable.

Recommended Values for: COPC Loss Constant Due to Biotic and Abiotic Degradation (*ksg*)

See Appendix A-2

The rate of biological degradation in soils depends on the concentration and activity of the microbial populations in the soil, the soil conditions, and the COPC concentration (Jury and Valentine 1986). First-order loss rates often fail to account for the high variability of these variables in a single soil system. However, the use of simple rate expressions may be appropriate at low chemical concentrations (e.g., nanogram per kilogram soil) at which a first-order dependence on chemical concentration may be reasonable. The rate of biological degradation is COPC-specific, depending on the complexity of the COPC and the usefulness of the COPC to the microorganisms. Some substrates, rather than being used by the organisms as a nutrient or energy source, are simply degraded with other similar COPCs, which can be further utilized. Environmental and COPC-specific factors that may limit the biodegradation of COPCs in the soil environment (Valentine and Schnoor 1986) include:

(1) availability of the COPC,

(2) nutrient limitations,

(3) toxicity of the COPC, and

(4) inactivation or nonexistence of enzymes capable of degrading the COPC.

Chemical degradation of organic compounds can be a significant mechanism for removal of COPCs in soil (U.S. EPA 1990a). Hydrolysis and oxidation-reduction reactions are the primary chemical transformation processes occurring in the upper layers of soils (Valentine 1986). General rate expressions describing the transformation of some COPCs by all non-biological processes are available, and these expressions are helpful when division into component reactions is not possible.

Hydrolysis in aqueous systems is characterized by three processes: acid-catalyzed, base-catalyzed, and neutral reactions. The overall rate of hydrolysis is the sum of the first-order rates of these processes (Valentine 1986). In soil systems, sorption of the COPC can increase, decrease, or not affect the rate of hydrolysis, as numerous studies cited in Valentine (1986) have shown. The total rate of hydrolysis in soil can be predicted by adding the rates in the soil and water phases, which are assumed to be first-order reactions at a fixed pH (Valentine 1986). Methods for estimating these hydrolysis constants are described by Lyman et al. (1982).

Organic and inorganic compounds also undergo oxidation-reduction (redox) reactions in the soil (Valentine 1986). Organic redox reactions involve the exchange of oxygen and hydrogen atoms by the reacting molecules. Inorganic redox reactions may involve the exchange of atoms or electrons by the reactants. In soil systems where the identities of oxidant and reductant species are not specified, a first-order rate constant can be obtained for describing loss by redox reactions (Valentine 1986). Redox reactions involving metals may promote losses from surface soils by making metals more mobile (e.g., leaching to subsurface soils).

COPC Loss Constant Due to Soil Erosion (*kse*)

U.S. EPA (1993h) recommended the use of Equation 3-8A to calculate the constant for soil loss resulting from erosion (*kse*).

$$kse = \frac{0.1 \cdot X_e \cdot SD \cdot ER}{BD \cdot Z_s} \cdot \frac{Kd_s \cdot BD}{\theta_{sw} + (Kd_s \cdot BD)} \qquad \text{Equation 3-8A}$$

where:

kse = COPC soil loss constant due to soil erosion
0.1 = Units conversion factor (1,000 g-kg/10,000 cm^2-m^2)
X_e = Unit soil loss (kg/m^2-yr)
SD = Sediment delivery ratio (unitless)
ER = Soil enrichment ratio (unitless)
Kd_s = Soil-water partition coefficient (mL/g)
BD = Soil bulk density (g/cm^3 soil)
Z_s = Soil mixing zone depth (cm)
θ_{sw} = Soil volumetric water content (mL/cm^3 soil)

Unit soil loss (X_e) is calculated by using the Universal Soil Loss Equation (USLE), as described in Section 3.11.2. Variables associated with Equation 3-8A are further discussed in Appendix B, Table B-1-3.

U.S. EPA guidance (1994b and 1994l) have stated that all *kse* values are equal to zero. U.S. EPA (1994l) stated that *kse* is equal to zero because of contaminated soil eroding onto and off of the site.

Consistent with earlier U.S. EPA guidance (1994b and 1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends that the constant for the loss of soil resulting from erosion (*kse)* should be set equal to zero.

Recommended Value for: **COPC Loss Constant Due to Erosion (*kse*)**
0

For additional information on addressing *kse*, U.S. EPA OSW recommends consulting the methodologies described in U.S. EPA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S. EPA In Press). The use of *kse* values is also further described in Appendix B, Table B-1-3.

COPC Loss Constant Due to Runoff (*ksr*)

Consistent with earlier U.S. EPA guidance (1993h; 1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends that Equation 3-8B be used to calculate the constant for the loss of soil resulting from surface runoff (*ksr*). The use of this equation is further described in Appendix B, Table B-1-4.

Recommended Equation for Calculating:
COPC Loss Constant Due to Runoff (*ksr*)

$$ksr = \frac{RO}{\theta_{sw} \cdot Z_s} \cdot \left(\frac{1}{1 + \left(Kd_s \cdot BD / \theta_{sw} \right)} \right) \qquad \text{Equation 3-8B}$$

where

ksr = COPC loss constant due to runoff (yr^{-1})
RO = Average annual surface runoff from pervious areas (cm/yr)
θ_{sw} = Soil volumetric water content ($\mathrm{mL/cm^3}$ soil)

Z_s = Soil mixing zone depth (cm)
Kd_s = Soil-water partition coefficient (mL/g)
BD = Soil bulk density (g/cm^3 soil)

COPC Loss Constant Due to Leaching (*ksl*)

Consistent with earlier U.S. EPA guidance (1993h and 1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends that Equation 3-8C be used to calculate the COPC loss constant due to leaching (*ksl)*. The use of this equation is further described in Appendix B, Table B-1-5.

Recommended Equation for Calculating:
COPC Loss Constant Due to Leaching (*ksl*)

$$ksl = \frac{P + I - RO - E_v}{\theta_{sw} \cdot Z_s \cdot [1.0 + (BD \cdot Kd_s / \theta_{sw})]} \qquad \text{Equation 3-8C}$$

where
ksl = COPC loss constant due to leaching (yr^{-1})
P = Average annual precipitation (cm/yr)
I = Average annual irrigation (cm/yr)
RO = Average annual surface runoff from pervious areas (cm/yr)
E_v = Average annual evapotranspiration (cm/yr)
θ_{sw} = Soil volumetric water content (mL/cm^3 soil)
Z_s = Soil mixing zone depth (cm)
Kd_s = Soil-water partition coefficient (mL/g)
BD = Soil bulk density (g/cm^3 soil)

Appendix B, Table B-1-5 further describes the variables associated with Equation 3-8C. The average annual volume of water ($P + I - RO - E_v$) available to generate leachate is the mass balance of all water inputs and outputs from the area under consideration.

COPC Loss Constant Due to Volatilization (*ksv*)

Semi-volatile and volatile COPCs emitted in high concentrations may become adsorbed to soil particles and exhibit volatilization losses from soil. The loss of a COPC from the soil by volatilization depends on the rate of movement of the COPC to the soil surface, the chemical vapor concentration at the soil surface, and the rate at which vapor is carried away by the atmosphere (Jury 1986).

Consistent with U.S. EPA (In Press), U.S. EPA OSW recommends that Equation 3-8D be used to calculate the constant for the loss of soil resulting from volatilization (*ksv)*. The soil loss constant due to volatilization (*ksv*) is based on gas equilibrium coefficients and gas phase mass transfer. The first order decay constant, *ksv*, is obtained by adapting the Hwang and Falco equation for soil vapor phase diffusion (Hwang and Falco 1986). The use of this equation is further described in Appendix B, Table B-1-6.

Recommended Equation for Calculating:
COPC Loss Constant Due to Volatilization (*ksv*)

$$ksv = \left(\frac{3.1536 \times 10^7 \cdot H}{Z_s \cdot Kd_s \cdot R \cdot T_a \cdot BD} \right) \cdot \left(\frac{D_a}{Z_s} \right) \cdot \left[1 - \left(\frac{BD}{\rho_s} \right) - \Theta_{sw} \right] \qquad \text{Equation 3-8D}$$

where

ksv = COPC loss constant due to volatization (yr^{-1})
3.1536×10^7 = Units conversion factor (s/yr)
H = Henry’s Law constant (atm-m^3/mol)
Z_s = Soil mixing zone depth (cm)
Kd_s = Soil-water partition coefficient (mL/g)
R = Universal gas constant (atm-m^3/mol-K)
T_a = Ambient air temperature (K) = 298.1 K
BD = Soil bulk density (g/cm^3 soil)
D_a = Diffusivity of COPC in air (cm^2/s)
θ_{sw} = Soil volumetric water content (mL/cm^3 soil)
ρ_s = Solids particle density (g/cm^3)

Appendix B, Table B-1-5 further describes the variables associated with Equation 3-8C. In cases where high concentrations of volatile organic compounds are expected to be present in the soil, U.S. EPA OSW recommends consulting the methodologies described in U.S. EPA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S. EPA In Press). The use of *ksv* values is also further described in Appendix B, Table B-1-6.

3.11.1.3 Deposition Term (*Ds*)

U.S. EPA OSW recommends that Equation 3-9 be used to calculate the deposition term *(Ds)*. This equation is further described in Appendix B, Table B-1-1. The use of Equation 3-11 to calculate the deposition term is consistent with earlier U.S. EPA guidance (1994l) and U.S. EPA (1998c), which both incorporate a deposition term (*Ds*) into Equation 3-7 for the calculation of the COPC concentration in soil (*Cs*) (see also Section 3.11.1.1).

Recommended Equation for Calculating:
Deposition Term (*Ds*)

$$Ds = \left[\frac{100 \cdot Q}{Z_s \cdot BD}\right] \cdot [F_v(0.31536 \cdot Vdv \cdot Cyv + Dywv) + (Dywp + Dydp) \cdot (1 - F_v)] \quad \text{Equation 3-9}$$

where

Ds = Deposition term (mg COPC/kg soil-yr)
100 = Units conversion factor (m^2-mg/cm^2-kg)
Q = COPC-specific emission rate (g/s)
Z_s = Soil mixing zone depth (cm)
BD = Soil bulk density (g/cm^3 soil)
F_v = Fraction of COPC air concentration in vapor phase (unitless)
0.31536 = Units conversion factor (m-g-s/cm-μg-yr)
Vdv = Dry deposition velocity (cm/s)
Cyv = Unitized yearly average air concentration from vapor phase (μg-s/g-m^3)
$Dywv$ = Unitized yearly average wet deposition from vapor phase (s/m^2 year)
$Dydp$ = Unitized yearly average dry deposition from particle phase (s/m^2 year)
$Dywp$ = Unitized yearly average wet deposition from particle phase (s/m^2 year)

Section 3.9 further describes the ISCST3 unitized air parameters (*Cyv*, *Dywv*, *Dydp*, and *Dywp*) obtained as output from the air dispersion modeling. Appendix B describes the determination of other variables associated with Equation 3-9. The proper use of this equation is also further described in Appendix B, Table B-1-1.

3.11.1.4 Site-Specific Parameters for Calculating Soil Concentration

As discussed in the previous sections, calculating the COPC concentration in soil (*Cs*) requires some site-specific parameter values, which must be calculated or derived from available literature or site-specific data. These site-specific parameters include the following:

- Soil mixing zone depth (Z_s)
- Soil bulk density (*BD*)
- Available water ($P + I - RO - E_v$)
- Soil volumetric water content (θ_{sw})

Determination of values for these parameters is further described in the following subsections, and in Appendix B.

Soil Mixing Zone Depth (Z_s)

When exposures to COPCs in soils are modeled, the depth of contamination is important in calculating the appropriate soil concentration. Due to leaching and physical disturbance (e.g., tilling) COPCs may migrate deeper in the soil in for some areas. Therefore, the value for the depth of soil contamination, or soil mixing zone depth (Z_s), used in modeling ecological risk should be considered specific to tilled (e.g., large plowed field) or untilled soil areas.

In general, previous U.S. EPA combustion risk assessment guidance (1990a) has estimated that if the area under consideration is tilled or mechanically disturbed, the soil mixing zone depth is about 10 to 20 centimeters depending on local conditions and the equipment used. If soil is not moved, COPCs are assumed to be retained in the shallower, upper soil layer. In this case, earlier U.S. EPA guidances (U.S. EPA 1990a; U.S. EPA 1993h) have typically recommended a value of 1 centimeter.

Consistent with earlier U.S. EPA guidance (1990a) and U.S. EPA (1998c), U.S. EPA OSW recommends the following values for the soil mixing zone depth (Z_s).

Recommended Values for: **Soil Mixing Zone Depth (Z_s)**
1 cm - untilled 20 cm - tilled

Soil Bulk Density (*BD*)

BD is the ratio of the mass of soil to its total volume. This variable is affected by the soil structure, type, and moisture content (Hillel 1980). Consistent with U.S. EPA (1990a; 1994b) and information presented in Hoffman and Baes (1979), U.S. EPA OSW recommends the following value for the soil dry bulk density (*BD*).

Recommended Value for: **Soil Dry Bulk Density (*BD*)**
1.50 g/cm^3 soil

For determination of actual field values specific to a specified location at a site, U.S. EPA (1994l) recommended that wet soil bulk density be determined by weighing a thin-walled, tube soil sample (e.g., a Shelby tube) of known volume and subtracting the tube weight (ASTM Method D2937). Moisture content can then be calculated (ASTM Method 2216) to convert wet soil bulk density to dry soil bulk density.

Available Water ($P + I - RO - E_v$)

The average annual volume of water available ($P + I - RO - E_v$) for generating leachate is the mass balance of all water inputs and outputs from the area under consideration. A wide range of values for these variables may apply in the various U.S. EPA regions.

The average annual precipitation (P), irrigation (I), runoff (RO), and evapotranspiration (E_v) rates and other climatological data may be obtained from either data recorded on site or from the Station Climatic Summary for a nearby airport.

Meteorological parameters—such as the evapotranspiration rate and the runoff rate—may also be found in resources such as Geraghty, Miller, van der Leeden, and Troise (1973). Surface runoff may also be estimated by using the curve number equation developed by the U.S. Soil Conservation Service (U.S. EPA 1990a). U.S. EPA (1985b) cites isopleths of mean annual cropland runoff corresponding to various curve numbers developed by Stewart, Woolhiser, Wischmeier, Caro, and Frere (1975). Curve numbers are assigned to an area on the basis of soil type, land use or cover, and the hydrologic condition of the soil (U.S. EPA 1990a).

Using these different references may introduce uncertainties and limitations. For example, Geraghty, van der Leeden, and Troise (1973) present isopleths for annual surface water contributions that include interflow and ground water recharge; these values should be adjusted downward to reflect surface runoff only. U.S. EPA (1994b) recommends that these values be reduced by 50 percent.

Soil Volumetric Water Content (θ_{sw})

The soil volumetric water content θ_{sw} depends on the available water and the soil structure. A wide range of values for these variables may apply in the various U.S. EPA regions. Consistent with earlier guidance documents (U.S. EPA 1994b), U.S. EPA OSW recommends the following value for θ_{sw}.

Recommended Value for: **Soil Volumetric Water Content (θ_{sw})**
0.2 ml/cm^3 soil

Additional information on soil water content is presented in Appendix B, specific to the equations in which it is used.

3.11.2 CALCULATION OF COPC CONCENTRATIONS IN SURFACE WATER AND SEDIMENTS

COPC concentrations in surface water and sediments are calculated for all water bodies selected for evaluation in the risk assessment. Mechanisms considered for determination of COPC loading of the water column are:

(1) Direct deposition,

(2) Runoff from impervious surfaces within the watershed,

(3) Runoff from pervious surfaces within the watershed,

(4) Soil erosion over the total watershed,

(5) Direct diffusion of vapor phase COPCs into the surface water, and

(6) Internal transformation of compounds chemically or biologically.

Other potential mechanisms may require consideration on a case-by-case basis (e.g., tidal influences), however, contributions from other potential mechanisms are assumed to be negligible in comparison with those being evaluated.

The USLE and a sediment delivery ratio are used to estimate the rate of soil erosion from the watershed. To evaluate the COPC loading to a water body from its associated watershed, the COPC concentration in watershed soils should be calculated. As described in Section 3.11.1, the equation for COPC concentration in soil includes a loss term that considers the loss of contaminants from the soil after deposition. These loss mechanisms may all lower the soil concentration associated with a specific deposition rate.

Surface water concentration algorithms include a sediment mass balance, in which the amount of sediment assumed to be buried and lost from the water body is equal to the difference between the amount of soil introduced to the water body by erosion and the amount of suspended solids lost in downstream flow. As a result, the assumptions are made that sediments do not accumulate in the water body over time, and an equilibrium is maintained between the surficial layer of sediments and the water column. The total water column COPC concentration is the sum of the COPC concentration dissolved in water and the COPC concentration associated with suspended solids. Partitioning between water and sediment varies with the COPC. The total concentration of each COPC is partitioned between the sediment and the water column.

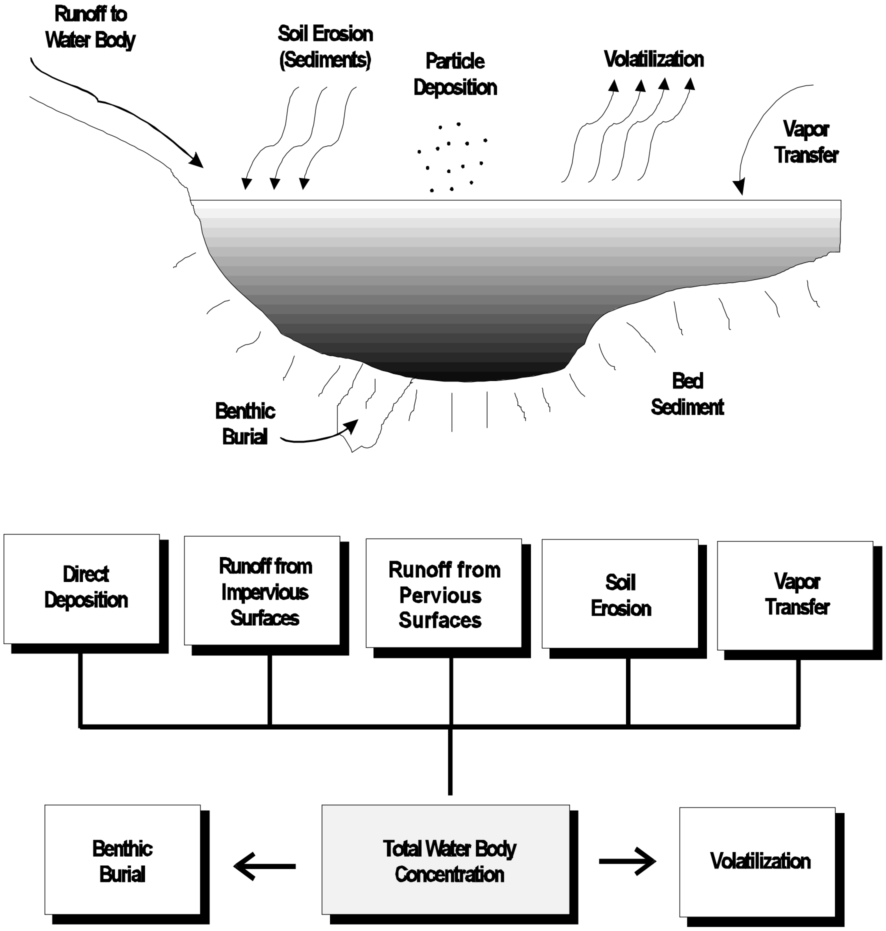


Figure 3-5 COPC Loading to the Water Body

Section 3.11.2.1 describes equations for computing COPC loading to a water body. Section 3.11.2.2 describes equations for computing total COPC concentration in a water body. Section 3.11.2.3 present the equations for computing COPC concentration in water column and in sediment. These equations are also presented and further defined in Appendix B.

3.11.2.1 Total COPC Loading to a Water Body (L_T)

Consistent with earlier U.S. EPA guidance (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-10 to calculate the total COPC load to a water body (L_T). This equation is also further described in Appendix B, Table B-2-1.

Recommended Equation for Calculating:
Total COPC Load to the Water Body (L_T)

$$L_T = L_{DEP} + L_{dif} + L_{RI} + L_R + L_E + L_I \qquad \text{Equation 3-10}$$

where

L_T = Total COPC load to the water body (including deposition, runoff, and erosion) (g/yr)
L_{DEP} = Total (wet and dry) particle phase and wet vapor phase COPC direct deposition load to water body (g/yr)
L_{dif} = Vapor phase COPC diffusion (dry deposition) load to water body (g/yr)
L_{RI} = Runoff load from impervious surfaces (g/yr)
L_R = Runoff load from pervious surfaces (g/yr)
L_E = Soil erosion load (g/yr)
L_I = Internal transfer (g/yr)

Due to the limited data and uncertainty associated with the chemical or biological internal transfer, L_I, of compounds into daughter products, U.S. EPA OSW recommends a default value for this variable of zero. However, if a permitting authority determines that site-specific conditions indicate calculation of internal transfer should be considered, U.S. EPA OSW recommends following the methodologies described in U.S. EPA NCEA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S EPA In Press). Calculation of each of the remaining variables (L_{DEP}, L_{dif}, L_{RI}, L_R, and L_E) is discussed in the following subsections.

Total (Wet and Dry) Particle Phase and Wet Vapor Phase Contaminant Direct Deposition Load to Water Body (L_{DEP})

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends Equation 3-11 to calculate the load to the water body from the direct deposition of wet and dry particles and wet vapors onto the surface of the water body (L_{DEP}). The equation is also further described in Appendix B, Table B-2-2.

Recommended Equation for Calculating:
Total Particle Phase and Wet Vapor Phase Direct Deposition Load to Water Body (L_{DEP})

$$L_{DEP} = Q \cdot [\ F_v \cdot Dywwv + (1 - F_v\ ) \cdot Dytwp\ ] \cdot A_W \qquad \text{Equation 3-11}$$

where

L_{DEP} = Total (wet and dry) particle phase and wet vapor phase COPC direct deposition load to water body (g/yr)
Q = COPC emission rate (g/s)
F_v = Fraction of COPC air concentration in vapor phase (unitless)
$Dywwv$ = Unitized yearly (water body and watershed) average wet deposition from vapor phase (s/m^2-yr)
$Dytwp$ = Unitized yearly (water body and watershed) average total (wet and dry) deposition from vapor phase (s/m^2-yr)
A_W = Water body surface area (m^2)

Section 3.9 describes the unitized air parameters, *Dywwv* and *Dywwv*, obtained as output from the ISCST3 air dispersion modeling. The determination of water body surface area, A_w, is described in Chapter 4. Appendix A-2 describes determination of the compound-specific parameter, F_v.

Diffusion Load to Water Body (L_{dif})

Consistent with earlier U.S. EPA guidance (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends using Equation 3-12 to calculate the dry vapor phase COPC diffusion load to the water body (L_{dif}). The equation is described in detail in Appendix B, Table B-2-3.

Recommended Equation for Calculating:
Vapor Phase COPC Diffusion (Dry Deposition) Load to Water Body (L_{Dif})

$$L_{dif} = \frac{K_v \cdot Q \cdot F_v \cdot Cywv \cdot A_W \cdot 1 \times 10^{-6}}{\dfrac{H}{R \cdot T_{wk}}} \qquad \text{Equation 3-12}$$

where

L_{dif} = Vapor phase COPC diffusion (dry deposition) load to water body (g/yr)
K_v = Overall COPC transfer rate coefficient (m/yr)
Q = COPC emission rate (g/s)
F_v = Fraction of COPC air concentration in vapor phase (unitless)
$Cywv$ = Unitized yearly (water body and watershed) average air concentration from vapor phase (μg-s/g-m^3)
A_W = Water body surface area (m^2)
10^{-6} = Units conversion factor (g/μg)
H = Henry's Law constant (atm-m^3/mol)
R = Universal gas constant (atm-m^3/mol-K)
T_{wk} = Water body temperature (K)

The overall COPC transfer rate coefficient (K_v) is calculated by using the equation in Appendix B, Table B-2-13. Consistent with previous U.S. EPA guidance (1994l; 1993h) and U.S. EPA (1998c), U.S. EPA OSW recommends a water body temperature (T_{wk}) of 298 K (or 25°C). Section 3.9 describes the determination of the modeled air parameter, *Cywv*. The determination of water body surface area, A_w, is described in Chapter 4. Appendix A-2 describes determination of compound-specific parameters, F_v and *H*.

Runoff Load from Impervious Surfaces (L_{RI})

In some watershed soils, a fraction of the wet and dry deposition in the watershed will be to impervious surfaces. Dry deposition may accumulate and be washed off during rain events. Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-13 to calculate impervious runoff load to a water body (L_{RI}). The equation is also presented in Appendix B, Table B-2-4.

Recommended Equation for Calculating:
Runoff Load from Impervious Surfaces (L_{RI})

$$L_{RI} = Q \cdot [\ F_v \cdot Dywwv + (1.0 - F_v\ ) \cdot Dytwp\ ] \cdot A_I \qquad \text{Equation 3-13}$$

where

L_{RI} = Runoff load from impervious surfaces (g/yr)
Q = COPC emission rate (g/s)
F_v = Fraction of COPC air concentration in vapor phase (unitless)
$Dywwv$ = Unitized yearly (water body and watershed) average wet deposition from vapor phase (s/m^2-yr)
$Dytwp$ = Unitized yearly (water body and watershed) average total (wet and dry) deposition from vapor phase (s/m^2-yr)
A_I = Impervious watershed area receiving COPC deposition (m^2)

Impervious watershed area receiving COPC deposition (A_I) is the portion of the total effective watershed area that is impervious to rainfall (i.e., roofs, driveways, streets, and parking lots) and drains to the water body.

Runoff Load from Pervious Surfaces (L_R)

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-14 to calculate the runoff dissolved COPC load to the water body from pervious soil surfaces in the watershed (L_R). The equation is also presented in Appendix B, Table B-2-5.

Recommended Equation for Calculating: Runoff Load from Pervious Surfaces (L_R)

$$L_R = RO \cdot (A_L - A_I) \cdot \frac{Cs \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.01 \qquad \text{Equation 3-14}$$

where

L_R = Runoff load from pervious surfaces (g/yr)
RO = Average annual surface runoff from pervious areas (cm/yr)
A_L = Total watershed area receiving COPC deposition (m^2)
A_I = Impervious watershed area receiving COPC deposition (m^2)
Cs = COPC concentration in soil (in watershed soils) (mg COPC/kg soil)
BD = Soil bulk density (g soil/cm^3 soil)
θ_{sw} = Soil volumetric water content (mL water/cm^3 soil)
Kd_s = Soil-water partition coefficient (cm^3 water/g soil)
0.01 = Units conversion factor (kg-cm^2/mg-m^2)

Appendix B describes the determination of site-specific parameters, RO, A_L, A_I, BD, and θ_{sw}. The calculation of the COPC concentration in soil (Cs) is discussed in Section 3.11.1 and Appendix B. Soil bulk density (BD) and soil water content (θ_{sw}) are described in Section 3.11.1.4.

Soil Erosion Load (L_E)

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-15 to calculate soil erosion load (L_E). The equation is also presented in Appendix B, Table B-2-6.

Recommended Equation for Calculating:
Soil Erosion Load (L_E)

$$L_E = X_e \cdot (A_L - A_I) \cdot SD \cdot ER \cdot \frac{Cs \cdot Kd_s \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.001 \qquad \text{Equation 3-15}$$

where

L_E = Soil erosion load (g/yr)
X_e = Unit soil loss (kg/m^2-yr)
A_L = Total watershed area (evaluated) receiving COPC deposition (m^2)
A_I = Impervious watershed area receiving COPC deposition (m^2)
SD = Sediment delivery ratio (watershed) (unitless)
ER = Soil enrichment ratio (unitless)
Cs = COPC concentration in soil (in watershed soils) (mg COPC/kg soil)
BD = Soil bulk density (g soil/cm^3 soil)
θ_{sw} = Soil volumetric water content (mL water/cm^3 soil)
Kd_s = Soil-water partition coefficient (mL water/g soil)
0.001 = Units conversion factor (k-cm^2/mg-m^2)

Unit soil loss (X_e) and watershed sediment delivery ratio (SD) are calculated as described in the following subsections and in Appendix B. COPC concentration in soil (Cs) is described in Section 3.11.1 and Appendix B, Table B-1-1. Soil bulk density (BD) and soil water content (θ_{sw}) are described in Section 3.11.1.4.

Universal Soil Loss Equation - USLE

U.S. EPA OSW recommends that the universal soil loss equation (USLE), Equation 3-16, be used to calculate the unit soil loss (X_e) specific to each watershed. This equation is further described in Appendix B, Table B-2-7. Appendix B also describes determination of the site- and watershed-specific values for each of the variables associated with Equation 3-16. The use of Equation 3-16 is consistent with U.S. EPA (1994b; 1994l) and U.S. EPA (1998c).

Recommended Equation for Calculating:
Unit Soil Loss (X_e)

$$X_e = RF \cdot K \cdot LS \cdot C \cdot PF \cdot \frac{907.18}{4047} \qquad \text{Equation 3-16}$$

where

X_e = Unit soil loss (kg/m^2-yr)
RF = USLE rainfall (or erosivity) factor (yr^{-1})
K = USLE erodibility factor (ton/acre)
LS = USLE length-slope factor (unitless)
C = USLE cover management factor (unitless)
PF = USLE supporting practice factor (unitless)
907.18 = Units conversion factor (kg/ton)
4047 = Units conversion factor (m^2/acre)

The USLE *RF* variable, which represents the influence of precipitation on erosion, is derived from data on the frequency and intensity of storms. This value is typically derived on a storm-by-storm basis, but average annual values have been compiled (U.S. Department of Agriculture 1982). Information on determining site-specific values for variables used in calculating X_e is provided in U.S. Department of Agriculture (U.S. Department of Agriculture 1997) and U.S. EPA guidance (U.S. EPA 1985b).
Refer to Appendix B, Table B-2-7 for additional discussion of the USLE.

Sediment Delivery Ratio (*SD*)

U.S. EPA OSW recommends the use of Equation 3-17 to calculate sediment delivery ratio (*SD*). The use of this equation is further described in Appendix B, Table B-2-8.

Recommended Equation for Calculating:
Sediment Delivery Ratio *(SD)*

$$SD = a \cdot (A_L)^{-b} \qquad \text{Equation 3-17}$$

where

SD = Sediment delivery ratio (watershed) (unitless)
a = Empirical intercept coefficient (unitless)
b = Empirical slope coefficient (unitless)
A_L = Total watershed area (evaluated) receiving COPC deposition (m^2)

The sediment delivery ratio (*SD*) for a large land area, a watershed or part of a watershed, can be calculated, on the basis of the area of the watershed, by using an approach proposed by Vanoni (1975). Accordingly, U.S. EPA (1993h) recommended the use of Equation 3-17 to calculate the sediment delivery ratio.

According to Vanoni (1975), sediment delivery ratios vary approximately with the -0.125 power of the drainage area. Therefore, the empirical slope coefficient is assumed to be equal to 0.125. An inspection of the data presented by Vanoni (1975) indicates that the empirical intercept coefficient varies with the size of the watershed, as illustrated in Appendix B, Table B-2-8.

A_L is the total watershed surface area affected by deposition that drains to the body of water. A watershed includes all of the land area that contributes water to a water body. In assigning values to the watershed surface area affected by deposition, consideration should be given to (1) the distance from the stack, (2) the location of the area affected by deposition fallout with respect to the water body, and (3) in the absence of any deposition considerations, watershed hydrology. Total sediment in a water body may have originated from watershed soils that are (or have the potential to be) both affected and unaffected by deposition of combustion emissions. If a combustor is depositing principally on a land area that feeds a tributary of a larger river system, consideration must be given to an "effective" area. An effective drainage area will almost always be less than the watershed.

3.11.2.2 Total Water Body COPC Concentration (C_{wtot})

U.S. EPA OSW recommends the use of Equation 3-18 to calculate total water body COPC concentration (C_{wtot}). The total water body concentration includes both the water column and the bed sediment. The equation is also presented in Appendix B, Table B-2-9.

Recommended Equation for Calculating:
Total Water Body COPC Concentration (C_{wtot})

$$C_{wtot} = \frac{L_T}{Vf_x \cdot f_{wc} + k_{wt} \cdot A_W \cdot (d_{wc} + d_{bs})} \qquad \text{Equation 3-18}$$

where

C_{wtot} = Total water body COPC concentration (including water column and bed sediment) (g COPC/m^3 water body)
L_T = Total COPC load to the water body (including deposition, runoff, and erosion) (g/yr)
Vf_x = Average volumetric flow rate through water body (m^3/yr)
f_{wc} = Fraction of total water body COPC concentration in the water column (unitless)
k_{wt} = Overall total water body COPC dissipation rate constant (yr^{-1})
A_W = Water body surface area (m^2)
d_{wc} = Depth of water column (m)
d_{bs} = Depth of upper benthic sediment layer (m)

The total COPC load to the water body (L_T)—including deposition, runoff, and erosion—is described in Section 3.11.2.1 and Appendix B, Table B-2-1. The depth of the upper benthic layer (d_{bs}), which represents the portion of the bed that is in equilibrium with the water column, cannot be precisely specified;

however, U.S. EPA (1993h) recommended values ranging from 0.01 to 0.05. Consistent with U.S. EPA (1994l; 1998c), U.S. EPA OSW recommends a default value of 0.03, which represents the midpoint of the specified range. Issues related to the remaining parameters are summarized in the following subsections.

Fraction of Total Water Body COPC Concentration in the Water Column (f_{wc}) and Benthic Sediment (f_{bs})

Consistent with U.S. EPA (1998c), U.S. EPA OSW recommends using Equation 3-19 to calculate fraction of total water body COPC concentration in the water column (f_{wc}), and Equation 3-20 to calculate fraction of total water body contaminant concentration in benthic sediment (f_{bs}). The equations are also presented in Appendix B, Table B-2-10.

Recommended Equation for Calculating:
Fraction of Total Water Body COPC Concentration in
the Water Column (f_{wc}) and Benthic Sediment (f_{bs})

$$f_{wc} = \frac{(1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}) \cdot d_{wc} / d_z}{(1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}) \cdot d_{wc} / d_z + (\theta_{bs} + Kd_{bs} \cdot BS) \cdot d_{bs} / d_z} \qquad \text{Equation 3-19}$$

$$f_{bs} = 1 - f_{wc} \qquad \text{Equation 3-20}$$

where

f_{wc} = Fraction of total water body COPC concentration in the water column (unitless)
f_{bs} = Fraction of total water body COPC concentration in benthic sediment (unitless)
Kd_{sw} = Suspended sediments/surface water partition coefficient (L water/kg suspended sediment)
TSS = Total suspended solids concentration (mg/L)
1×10^{-6} = Units conversion factor (kg/mg)
d_z = Total water body depth (m)
θ_{bs} = Bed sediment porosity ($L_{water}/L_{sediment}$)

Kd_{bs} = Bed sediment/sediment pore water partition coefficient (L water/kg bottom sediment)
BS = Benthic solids concentration (g/cm^3 [equivalent to kg/L])
d_{wc} = Depth of water column (m)
d_{bs} = Depth of upper benthic sediment layer (m)

U.S. EPA (1993h) and NC DEHNR (1997) recommended the use of Equations 3-19 and 3-20 to calculate the fraction of total water body concentration occurring in the water column (f_{wc}) and the bed sediments (f_{bs}). The partition coefficient Kd_{sw} describes the partitioning of a contaminant between sorbing material, such as soil, surface water, suspended solids, and bed sediments (see Appendix A-2). NC DEHNR (1997) also recommended adding the depth of the water column to the depth of the upper benthic layer (d_{wc} + d_{bs}) to calculate the total water body depth (d_z).

NC DEHNR (1997) recommended a default total suspended solids (*TSS*) concentration of 10 mg/L, which was adapted from U.S. EPA (1993h). However, due to variability in water body specific values for this variable, U.S. EPA OSW recommends the use of water body-specific measured *TSS* values representative of long-term average annual values for the water body of concern. Average annual values for *TSS* are generally expected to be in the range of 2 to 300 mg/L; with additional information on anticipated *TSS* values available in the U.S. EPA NCEA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S. EPA In Press).

If measured data is not available, or of unacceptable quality, a calculated *TSS* value can be obtained for non-flowing water bodies using Equation 3-21.

$$TSS = \frac{X_e \cdot (A_L - A_I) \cdot SD \cdot 1x10^3}{Vf_x + D_{ss} \cdot A_W} \qquad \text{Equation 3-21}$$

where

TSS = Total suspended solids concentration (mg/L)
X_e = Unit soil loss (kg/m^2-yr)
A_L = Total watershed area (evaluated) receiving COPC deposition (m^2)
A_I = Impervious watershed area receiving COPC deposition (m^2)

SD = Sediment delivery ratio (watershed) (unitless)
Vf_x = Average volumetric flow rate through water body (value should be 0 for quiescent lakes or ponds) (m^3/yr)
D_{ss} = Suspended solids deposition rate (a default value of 1,825 for quiescent lakes or ponds) (m/yr)
A_W = Water body surface area (m^2)

The default value of 1,825 m/yr provided for D_{ss} is characteristic of Stoke's settling velocity for an intermediate (fine to medium) silt.

Also, to evaluate the appropriateness of watershed-specific values (specific for non-flowing water bodies) used in calculating the unit soil loss (X_e), as described in Section 3.11.2.1 and Appendix B, the water-body specific measured *TSS* value should be compared to the calculated *TSS* value obtained using Equation 3-21. If the measured and calculated *TSS* values differ significantly, parameter values used in calculating X_e should be re-evaluated. This re-evaluation of *TSS* and X_e should also be conducted if the calculated *TSS* value is outside of the normal range expected for average annual measured values, as discussed above.

Bed sediment porosity (θ_{bs}) can be calculated from the benthic solids concentration by using the following equation (U.S. EPA 1993h):

$$\theta_{bs} = 1 - \frac{BS}{\rho_s}$$

where

θ_{bs} = Bed sediment porosity ($L_{water}/L_{sediment}$)
ρ_s = Bed sediment density (kg/L)
BS = Benthic solids concentration (kg/L)

U.S. EPA OSW recommends the following default value for bed sediment porosity (θ_{bs}), which was adapted from U.S. EPA (1993h) and U.S. EPA (1998c):

Recommended Value for:
Bed Sediment Porosity (θ_{bs})

$$\theta_{bs} = 0.6 \ \ L_{water}/L_{sediment}$$

(assuming ρ_s = 2.65 kg/L [bed sediment density] and BS = 1 kg/L [benthic solids concentration])

Values for the benthic solids concentration (*BS*) and depth of upper benthic sediment layer (d_{bs}) range from 0.5 to 1.5 kg/L and 0.01 to 0.05 meters, respectively. However, consistent with earlier U.S. EPA guidance (1993h; 1994l) and U.S. EPA (1998c), 1 kg/L is a reasonable default for most applications of the benthic solids concentration (*BS*), and 0.03 meter is the default depth of the upper benthic layer (d_{bs}). The default depth of 0.03 meters is based on the midpoint of the range presented above. The use of this equation is further described in Appendix B, Table B-2-10.

Overall Total Water Body COPC Dissipation Rate Constant (k_{wt})

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-22 to calculate the overall dissipation rate of COPCs in surface water, resulting from volatilization and benthic burial. The equation is also presented in Appendix B, Table B-2-11.

Recommended Equation for Calculating:
Overall Total Water Body COPC Dissipation Rate Constant (k_{wt})

$$k_{wt} = f_{wc} \cdot k_v + f_{bs} \cdot k_b \qquad \text{Equation 3-22}$$

where

k_{wt} = Overall total water body dissipation rate constant (yr^{-1})
f_{wc} = Fraction of total water body COPC concentration in the water column (unitless)
k_v = Water column volatilization rate constant (yr^{-1})
f_{bs} = Fraction of total water body COPC concentration in benthic sediment (unitless)
k_b = Benthic burial rate constant (yr^{-1})

The variables f_{wc} and f_{bs} are discussed in the previous section, Equations 3-19 and 3-20, and calculated by using the equations presented in Appendix B, Table B-2-10.

Water Column Volatilization Rate Constant (k_v)

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends using Equation 3-23 to calculate water column volatilization rate constant. The equation is also presented in Appendix B, Table B-2-12.

Recommended Equation for Calculating:
Water Column Volatilization Rate Constant (k_v)

$$k_v = \frac{K_v}{d_z \cdot (1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6})} \qquad \text{Equation 3-23}$$

---

where

k_v = Water column volatilization rate constant (yr^{-1})
K_v = Overall COPC transfer rate coefficient (m/yr)
d_z = Total water body depth (m)
Kd_{sw} = Suspended sediments/surface water partition coefficient (L water/kg suspended sediments)
TSS = Total suspended solids concentration (mg/L)
1×10^{-6} = Units conversion factor (kg/mg)

Total water body depth (d_z), suspended sediment and surface water partition coefficient (Kd_{sw}), and total suspended solids concentration (TSS), are previously described in this section. Kd_{sw} is discussed in Appendix A-2. The overall transfer rate coefficient (K_v) is described in the following subsection.

Overall COPC Transfer Rate Coefficient (K_v)

Volatile organic chemicals can move between the water column and the overlying air. The overall transfer rate K_v, or conductivity, is determined by a two-layer resistance model that assumes that two “stagnant films” are bounded on either side by well-mixed compartments. Concentration differences serve as the driving force for the water layer diffusion. Pressure differences drive the diffusion for the air layer. From balance considerations, the same mass must pass through both films; the two resistances thereby combine in series, so that the conductivity is the reciprocal of the total resistance.

Consistent with U.S. EPA (1993h) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-24 to calculate the overall transfer rate coefficient (K_v). The equation is also presented in Appendix B, Table B-2-13.

Recommended Equation for Calculating:
Overall COPC Transfer Rate Coefficient (K_v)

$$K_v = \left(K_L^{-1} + \left(K_G \cdot \frac{H}{R \cdot T_{wk}} \right)^{-1} \right)^{-1} \cdot \theta^{T_{wk} - 293} \qquad \text{Equation 3-24}$$

where

K_v = Overall COPC transfer rate coefficient (m/yr)
K_L = Liquid phase transfer coefficient (m/yr)
K_G = Gas phase transfer coefficient (m/yr)
H = Henry’s Law constant (atm-m^3/mol)
R = Universal gas constant (atm-m^3/mol-K)
T_{wk} = Water body temperature (K)
θ = Temperature correction factor (unitless)

The value of the conductivity K_v depends on the intensity of turbulence in the water body and the overlying atmosphere. As Henry’s Law constant increases, the conductivity tends to be increasingly influenced by the intensity of turbulence in water. Conversely, as Henry’s Law constant decreases, the value of the conductivity tends to be increasingly influenced by the intensity of atmospheric turbulence.

The liquid and gas phase transfer coefficients, K_L and K_G, respectively, vary with the type of water body. The liquid phase transfer coefficient (K_L) is calculated by using Equations 3-25 and 3-26. The gas phase transfer coefficient (K_G) is calculated by using Equations 3-27 and 3-28.

Henry's Law constants generally increase with increasing vapor pressure of a COPC and generally decrease with increasing solubility of a COPC. Henry's Law constants are compound-specific and are presented in Appendix A-2. The universal ideal gas constant, R, is 8.205×10^{-5} atm-m^3/mol-K, at 20°C. The temperature correction factor (θ), which is equal to 1.026, is used to adjust for the actual water temperature. Volatilization is assumed to occur much less readily in lakes and reservoirs than in moving water bodies.

Liquid Phase Transfer Coefficient (K_L)

Consistent with U.S. EPA (1998c), U.S. EPA OSW recommends using Equations 3-25 and 3-26 to calculate liquid phase transfer coefficient. (K_L). The use of these equations is further described in Appendix B, Table B-2-14.

Recommended Equation for Calculating:
Liquid Phase Transfer Coefficient (K_L)

For flowing streams or rivers:

$$K_L = \sqrt{\frac{(1 \times 10^{-4}) \cdot D_w \cdot u}{d_z}} \cdot 3.1536 \times 10^7 \qquad \text{Equation 3-25}$$

For quiescent lakes or ponds:

$$K_L = (C_d^{0.5} \cdot W) \cdot (\frac{\rho_a}{\rho_w})^{0.5} \cdot \frac{k^{0.33}}{\lambda_z} \cdot (\frac{\mu_w}{\rho_w \cdot D_w})^{-0.67} \cdot 3.1536 \times 10^7 \qquad \text{Equation 3-26}$$

where

K_L = Liquid phase transfer coefficient (m/yr)
D_w = Diffusivity of COPC in water (cm^2/s)
u = Current velocity (m/s)
1×10^{-4} = Units conversion factor (m^2/cm^2)
d_z = Total water body depth (m)
C_d = Drag coefficient (unitless)
W = Average annual wind speed (m/s)

ρ_a = Density of air (g/cm^3)
ρ_w = Density of water (g/cm^3)
k = von Karman's constant (unitless)
λ_z = Dimensionless viscous sublayer thickness (unitless)
μ_w = Viscosity of water corresponding to water temperature (g/cm-s)
3.1536×10^7 = Units conversion factor (s/yr)

For a flowing stream or river, the transfer coefficients are controlled by flow-induced turbulence. For these systems, the liquid phase transfer coefficient is calculated by using Equation 3-25, which is the O'Connor and Dobbins (1958) formula, as presented in U.S. EPA (1993h).

For a stagnant system (quiescent lake or pond), the transfer coefficient is controlled by wind-induced turbulence. For quiescent lakes or ponds, the liquid phase transfer coefficient can be calculated by using Equation 3-26 (O'Connor 1983; U.S. EPA 1993h).

The total water body depth (d_z) for liquid phase transfer coefficients is discussed previously in this section.

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of the following default values. These values are further described in Appendix A-2:

(1) a diffusivity of chemical in water ranging (D_w) from 1.0×10^{-5} to 8.5×10^{-2} cm^2/s,

(2) a dimensionless viscous sublayer thickness (λ_z) of 4,

(3) a von Karman's constant (k) of 0.4,

(4) a drag coefficient (C_d) of 0.0011 which was adapted from U.S. EPA (1993h),

(5) a density of air (ρ_a) of 0.0012 g/cm^3 at standard conditions (temperature = 20°C or 293 K, pressure = 1 atm or 760 millimeters of mercury) (Weast 1986),

(6) a density of water (ρ_w) of 1 g/cm^3 (Weast 1986),

(7) a viscosity of water (μ_w) of a 0.0169 g/cm-s corresponding to water temperature (Weast 1986).

Gas Phase Transfer Coefficient (K_G)

U.S. EPA OSW recommends using Equations 3-27 and 3-28 to calculate gas phase transfer coefficient (K_G). The equation is also discussed in Appendix B, Table B-2-15.

Recommended Equation for Calculating:
Gas Phase Transfer Coefficient (K_G)

For flowing streams or rivers:

$$K_G = 36500 \text{ m/yr} \qquad \text{Equation 3-27}$$

For quiescent lakes or ponds:

$$K_G = (C_d^{0.5} \cdot W) \cdot \frac{k^{0.33}}{\lambda_z} \cdot \left(\frac{\mu_a}{\rho_a \cdot D_a}\right)^{-0.67} \cdot 3.1536 \times 10^7 \qquad \text{Equation 3-28}$$

where

K_G = Gas phase transfer coefficient (m/yr)
C_d = Drag coefficient (unitless)
W = Average annual wind speed (m/s)
k = von Karman's constant (unitless)
λ_z = Dimensionless viscous sublayer thickness (unitless)
μ_a = Viscosity of air corresponding to air temperature (g/cm-s)
ρ_a = Density of air corresponding to water temperature (g/cm^3)
D_a = Diffusivity of COPC in air (cm^2/s)
3.1536×10^7 = Units conversion factor (s/yr)

U.S. EPA (1993h) indicated that the rate of transfer of a COPC from the gas phase for a flowing stream or river is assumed to be constant, in accordance with O'Connor and Dobbins (1958) (Equation 3-27).

For a stagnant system (quiescent lake or pond), the transfer coefficients are controlled by wind-induced turbulence. For quiescent lakes or ponds, U.S. EPA OSW recommends that the gas phase transfer coefficient be computed by using the equation presented in O'Connor (1983) (Equation 3-28).

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends 1.81 x 10^{-4} g/cm-s for the viscosity of air corresponding to air temperature.

Benthic Burial Rate Constant (k_b)

U.S. EPA OSW recommends using Equation 3-29 to calculate benthic burial rate (k_b). The equation is also discussed in Appendix B, Table B-2-16.

Recommended Equation for Calculating:
Benthic Burial Rate Constant (k_b)

$$k_b = \left(\frac{X_e \cdot A_L \cdot SD \cdot 1 \times 10^3 - Vf_x \cdot TSS}{A_W \cdot TSS} \right) \cdot \left(\frac{TSS \cdot 1 \times 10^{-6}}{BS \cdot d_{bs}} \right) \qquad \text{Equation 3-29}$$

where

k_b = Benthic burial rate constant (yr^{-1})
X_e = Unit soil loss ($\text{kg/m}^2\text{-yr}$)
A_L = Total watershed area (evaluated) receiving deposition (m^2)
SD = Sediment delivery ratio (watershed) (unitless)
Vf_x = Average volumetric flow rate through water body ($\text{m}^3\text{/yr}$)
TSS = Total suspended solids concentration (mg/L)
A_W = Water body surface area (m^2)
BS = Benthic solids concentration (g/cm^3)
d_{bs} = Depth of upper benthic sediment layer (m)
1 x 10^{-6} = Units conversion factor (kg/mg)
1 x 10^3 = Units conversion factor (g/kg)

The benthic burial rate constant (k_b), which is calculated in Equation 3-29, can also be expressed in terms of the rate of burial (Wb):

$$Wb = k_b \cdot d_{bs} \qquad \text{Equation 3-30}$$

where

Wb = Rate of burial (m/yr)
k_b = Benthic burial rate constant (yr^{-1})
d_{bs} = Depth of upper benthic sediment layer (m)

According to U.S. EPA (1994l) and U.S. EPA (1998c), COPC loss from the water column resulting from burial in benthic sediment can be calculated by using Equation 3-29. These guidance documents also recommend a benthic solids concentration (*BS*) value ranging from 0.5 to 1.5 kg/L, which was adapted from U.S. EPA (1993h). U.S. EPA OSW recommends the following default value for benthic solids concentration (*BS*).

Recommended Default Value for: **Benthic Solids Concentration (*BS*)**
1.0 kg/L

The calculated value for k_b should range from 0 to 1.0; with low k_b values expected for water bodies characteristic of no or limited sedimentation (rivers and fast flowing streams), and k_b values closer to 1.0 expected for water bodies characteristic of higher sedimentation (lakes). This range of values is based on the relation between the benthic burial rate and rate of burial expressed in Equation 3-30; with the depth of upper benthic sediment layer held constant. For k_b values calculated as a negative (water bodies with high average annual volumetric flow rates in comparison to watershed area evaluated), a k_b value of 0 should be assigned for use in calculating the total water body COPC concentration (C_{wtot}) in Equation 3-18. If the calculated k_b value exceeds 1.0, re-evaluation of the parameter values used in calculating X_e should be conducted.

3.11.2.3 Total COPC Concentration in Water Column (C_{wctot})

U.S. EPA OSW recommends using Equation 3-31 to calculate total COPC concentration in water column (C_{wctot}). The equation is also discussed in Appendix B, Table B-2-17.

Recommended Equation for Calculating:
Total COPC Concentration in Water Column (C_{wctot})

$$C_{wctot} = f_{wc} \cdot C_{wtot} \cdot \frac{d_{wc} + d_{bs}}{d_{wc}} \qquad \text{Equation 3-31}$$

where

C_{wctot} = Total COPC concentration in water column (mg COPC/L water column)
f_{wc} = Fraction of total water body COPC concentration in the water column (unitless)
C_{wtot} = Total water body COPC concentration, including water column and bed sediment (mg COPC/L water body)
d_{wc} = Depth of water column (m)
d_{bs} = Depth of upper benthic sediment layer (m)

The use of Equation 3-31 to calculate total COPC concentration in water column is consistent with U.S. EPA (1994l; 1998c).

Total water body COPC concentration—including water column and bed sediment (C_{wtot}) and fraction of total water body COPC concentration in the water column (f_{wc})—should be calculated by using Equation 3-18 and Equation 3-19, respectively. Depth of upper benthic sediment layer (d_{bs}) is discussed previously.

Dissolved Phase Water Concentration (C_{dw})

U.S. EPA OSW recommends the use of Equation 3-32 to calculate the concentration of COPC dissolved in the water column (C_{dw}). The equation is discussed in detail in Appendix B, Table B-2-18.

Recommended Equation for Calculating: Dissolved Phase Water Concentration (C_{dw})

$$C_{dw} = \frac{C_{wctot}}{1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}} \qquad \text{Equation 3-32}$$

where

C_{dw} = Dissolved phase water concentration (mg COPC/L water)
C_{wctot} = Total COPC concentration in water column (mg COPC/L water column)
Kd_{sw} = Suspended sediments/surface water partition coefficient (L water/kg suspended sediment)
TSS = Total suspended solids concentration (mg/L)
1×10^{-6} = Units conversion factor (kg/mg)

The use of Equation 3-32 to calculate the concentration of COPC dissolved in the water column is consistent with U.S. EPA (1994l; 1998c).

The total COPC concentration in water column (C_{wctot}) is calculated by using the Equation 3-31 (see also Appendix B, Table B-2-17). The surface water partition coefficient (Kd_{sw}) and total suspended solids concentration (*TSS*) are discussed previously.

COPC Concentration in Bed Sediment (*Csed*)

U.S. EPA OSW recommends the use of Equation 3-33 to calculate COPC concentration in bed sediment (*Csed*). The equation is also presented in Appendix B, Table B-2-19.

Recommended Equation for Calculating:
COPC Concentration in Bed Sediment (*Csed*)

$$C_{sed} = f_{bs} \cdot C_{wtot} \cdot \left(\frac{Kd_{bs}}{\theta_{bs} + Kd_{bs} \cdot BS} \right) \cdot \left(\frac{d_{wc} + d_{bs}}{d_{bs}} \right) \qquad \text{Equation 3-33}$$

where

C_{sed}	=	COPC concentration in bed sediment (mg COPC/kg sediment)
f_{bs}	=	Fraction of total water body COPC concentration in benthic sediment (unitless)
C_{wtot}	=	Total water body COPC concentration, including water column and bed sediment (mg COPC/L water body)
Kd_{bs}	=	Bed sediment/sediment pore water partition coefficient (L COPC/kg water body)
θ_{bs}	=	Bed sediment porosity ($L_{pore\ water}/L_{sediment}$)
BS	=	Benthic solids concentration (g/cm^3)
d_{wc}	=	Depth of water column (m)
d_{bs}	=	Depth of upper benthic sediment layer (m)

The use of Equation 3-33 to calculate the COPC concentration in bed sediment is consistent with U.S. EPA (1994l; 1998c).

The total water body COPC concentration—including water column and bed sediment (C_{wtot}) and the fraction of total water body COPC concentration that occurs in the benthic sediment (f_{bs})—is calculated by using Equations 3-18 and 3-20, respectively. The bed sediment and sediment pore water partition coefficient (Kd_{bs}) is discussed in Appendix A-2. Bed sediment porosity (θ_{bs}), benthic solids concentration (BS), depth of water column (d_{wc}), and depth of upper benthic layer (d_{bs}) are discussed previously.

3.11.3 CALCULATION OF COPC CONCENTRATIONS IN PLANTS

The concentration of COPCs in plants is assumed to occur by three possible mechanisms:

- **Direct deposition of particles—**wet and dry deposition of particle phase COPCs onto the exposed plant surfaces.
- **Vapor transfer—**uptake of vapor phase COPCs by plants through their foliage.

- **Root uptake—**root uptake of COPCs available from the soil and their transfer to the aboveground portions of the plant.

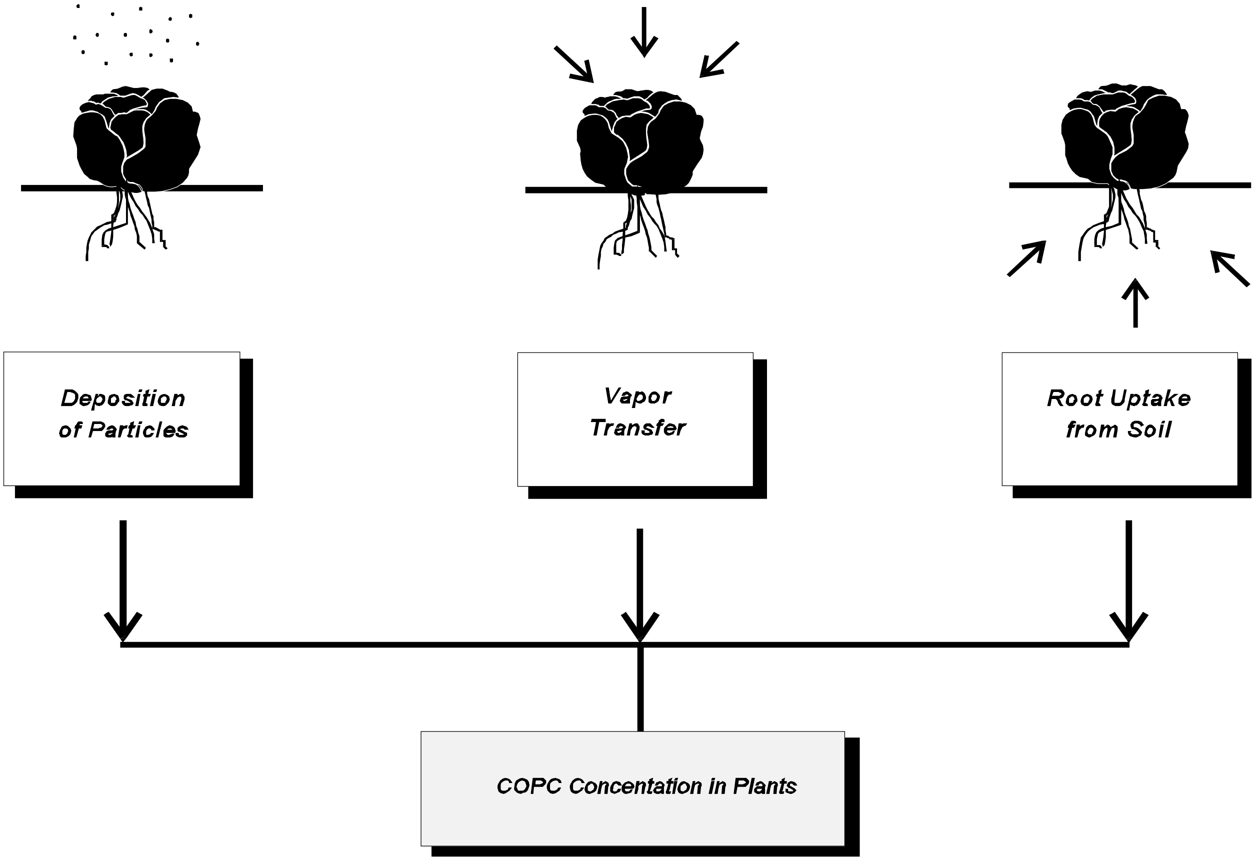


Figure 3-6 COPC Concentration in Plants

The total COPC concentration in terrestrial plants, C_{TP} is calculated as a sum of contamination occurring through all three of these mechanisms.

3.11.3.1 Calculating Plant Concentration Due to Direct Deposition (*Pd*)

Consitent with previous U.S. EPA guidance (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-34 to calculate COPC concentration in plants due to direct deposition. The use of this equation is further described in Appendix B, Table B-3-1.

Recommended Equation for Calculating:
Plant Concentration Due to Direct Deposition (*Pd*)

$$Pd = \frac{1{,}000 \cdot Q \cdot (1 - Fv) \cdot [Dydp + (Fw \cdot Dywp)] \cdot Rp \cdot [1.0 - \exp(-kp \cdot Tp)] \cdot 0.12}{Yp \cdot kp} \qquad \text{Equation 3-34}$$

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where

Pd = Plant concentration due to direct (wet and dry) deposition (mg COPC/kg WW)
1,000 = Units conversion factor (mg/g)
Q = COPC emission rate (g/s)
F_v = Fraction of COPC air concentration in vapor phase (unitless)
$Dydp$ = Unitized yearly average dry deposition from particle phase (s/m^2-yr)
Fw = Fraction of COPC wet deposition that adheres to plant surfaces (unitless)
$Dywp$ = Unitized yearly wet deposition from particle phase (s/m^2-yr)
Rp = Interception fraction of the edible portion of plant (unitless)
kp = Plant surface loss coefficient (yr^{-1})
Tp = Length of plant exposure to deposition per harvest of the edible portion of the *i*th plant group (yr)
012 = Dry weight to wet weight conversion factor (unitless)
Yp = Yield or standing crop biomass of the edible portion of the plant (productivity) (kg DW/m^2)

Section 3.9 describes the use of the unitized air parameters, *Dydp* and *Dywp*, obtained as output from the air dispersion modeling. Appendix A-3 describes determination of *Fv*. Appendix B describes determination of *Fw*, *Rp*, *kp*, *Tp*, and *Yp*. The dry weight to wet weight conversion factor of 0.12 is based on the average rounded value from the range of 80 to 95 percent water content in herbaceous plants and nonwoody plant parts (Taiz at al. 1991).

3.11.3.2 Calculating Plant Concentration Due to Air-to-Plant Transfer (*Pv*)

Consistent with U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-35 to calculate the plant concentration due to air-to-plant transfer (*Pv*). The use of this equation is further described in Appendix B, Table B-3-2.

Recommended Equation for Calculating:
Plant Concentration Due to Air-to-Plant Transfer (*Pv*)

$$Pv = Q \cdot F_v \cdot 0.12 \cdot \frac{Cyv \cdot Bv}{\rho_a}$$

Equation 3-35

where

Pv = Plant concentration due to air-to-plant transfer (mg COPC/kg WW)
Q = COPC emission rate (g/s)
F_v = Fraction of COPC air concentration in vapor phase (unitless)
Cyv = Unitized yearly average air concentration from vapor phase (μg-s/g-m^3)
Bv = Air-to-plant biotransfer factor ([mg COPC/g DW plant]/[mg COPC/g air]) (unitless)
012 = Dry weight to wet weight conversion factor (unitless)
ρ_a = Density of air (g/m^3)

Section 3.9 describes the use of the unitized air parameter, *Cyv*. Appendix A-3 describes determination of the COPC-specific parameters, *Fv* and *Bv*. The dry weight to wet weight conversion factor of 0.12 is based on the average rounded value from the range of 80 to 95 percent water content in herbaceous plants and nonwoody plant parts (Taiz at al. 1991). Appendix B further describes use of Equation 3-35, including determination of *Fw* and ρ_a.

3.11.3.3 Calculating Plant Concentration Due to Root Uptake (*Pr*)

Consistent with previous U.S. EPA guidance (1994g; 1994l; 1995h) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-36 to calculate the plant concentration due to root uptake (*Pr*). The use of this equation is further described in Appendix B, Table B-3-3.

Recommended Equation for Calculating:
Plant Concentration Due to Root Uptake (*Pr*)

$$Pr = Cs \cdot BCF_r \cdot 0.12$$ Equation 3-36

where

Pr	=	Plant concentration due to root uptake (mg COPC/kg WW)
BCF_r	=	Plant-soil biotransfer factor (unitless)
Cs	=	COPC concentration in soil (mg COPC/kg soil)
012	=	Dry weight to wet weight conversion factor (unitless)

Equation 3-36 is based on the soil-to-aboveground plant transfer approach developed by Travis and Arms (1988). The dry weight to wet weight conversion factor of 0.12 is based on the average rounded value from the range of 80 to 95 percent water content in herbaceous plants and nonwoody plant parts (Taiz at al. 1991). Appendix A-3 describes determination of the COPC-specific parameter BCF_r. Section 3.11.1 and Appendix B describe calculation of *Cs*.

3.12 REPLACING DEFAULT PARAMETER VALUES

As discussed in Chapter 1, default parameter values are provided in this guidance for numerous inputs to the fate and transport modeling. After completing a risk assessment based on the default parameter values recommended in this guidance, risk assessors may choose to investigate replacing default parameter values with measured or published values if a more representative estimate of site-specific risk can be obtained. Use of parameter values other than those specified in this guidance should always be clearly described in the risk assessment report and work plan, and approved by the permitting authority. U.S. EPA OSW recommends that requests to change default parameter values include the following information, as appropriate:

1. An explanation of why the use of a measured or published value other than the default value is warranted (e.g., the default parameter value is based on data or studies at sites in the northwestern U.S., but the facility is located in the southeast);

2. The supporting technical basis of the replacement parameter value, including readable copies (printed in English) of any relevant technical literature or studies;

3. The basis of the default parameter value, as understood by the requestor, including readable copies (printed in English) of the referenced literature or studies (if available);

4. A comparison of the weight-of-evidence between the competing studies (e.g., the proposed replacement parameter value is based on a study that is more representative of site conditions, a specific exposure setting being evaluated, or a more scientifically valid study than the default parameter value, the proposed replacement parameter is based on the analysis of 15 samples as opposed to 5 for the default parameter value, or the site-specific study used more stringent quality control/quality assurance procedures than the study upon which the default parameter value is based);

5. A description of other risk assessments or projects where the proposed replacement parameter value has been used, and how such risk assessments or projects are similar to the risk assessment in consideration.