3 AIR DISPERSION AND DEPOSITION MODELING

The first step in assessing potential human health risks associated with releases of COPCs to the environment is calculating the dispersion of emitted COPCs to quantify atmospheric concentrations and deposition rates in the areas around the facility. Air concentrations and deposition rates are calculated using air dispersion models. Air dispersion models are mathematical computer programs that attempt to describe the effects of physical processes that occur in the atmosphere on rates of dispersion of emissions from a source.

3.1 MODELING OVERVIEW

The USEPA maintains a *Guideline on Air Quality Models* (USEPA, 2005b), which is published as Appendix W to Title 40 of the Code of Federal Regulations (CFR) Part 51. On December 9, 2005, the guidelines were revised and the American Meteorological Society/Environmental Protection Agency Regulatory Model (AERMOD) dispersion model became the recommended model for a wide range of regulatory applications in all types of terrain. Therefore, the latest version (Julian date 07026) of the AERMOD model was used to conduct the air dispersion and deposition modeling for this MPHRA.

AERMOD is a multi-source model that simulates dispersion of vapor and particulate matter. The model uses emission source characteristic data, meteorological data, and receptor locations (i.e., calculation points) to determine air concentrations and wet and dry deposition rates, while conserving mass through plume depletion. The model is applicable for use in all types of terrain, including the terrain associated with the PCAPP.

3.1.1 Averaging Times

AERMOD was used to calculate the maximum COPC air concentrations and dry and wet deposition rates at an array of receptors. The AERMOD results used in this MPHRA included the maximum annual COPC air concentrations and maximum annual dry and wet deposition rates for the chronic risk assessment and maximum 1-hour COPC air concentrations for the acute risk assessment.

The annual COPC air concentrations were calculated as an average over the 3 years of meteorological data. The 1-hour COPC concentrations were calculated as the highest 1-hour average concentration from the entire 3-year meteorological data set. The annual COPC deposition rates were calculated as the highest total deposition rate for each COPC occurring over one of the 3 years of meteorological data (i.e., the calendar year producing the highest total deposition rate).

3.1.2 Unit Response

A linear relationship exists between emission rate and modeled air parameter values. Specifically, the air concentration and deposition rates calculated by AERMOD for each receptor are directly proportional to the emission rate (i.e., when one doubles the emission rate, the calculated atmospheric concentration and depositions rates also double). Therefore, a unit emission rate (i.e., 1 gram per second [g/s]) can be input to the model for each modeled source, and the resulting concentration and deposition rates calculated by the model (referred to as a unit response) can be adjusted using chemical-specific emission rates to obtain chemical-specific concentrations and deposition rates. This precludes the need to run the model for each individual COPC (e.g., each of the 38 COPCs with toxicity data) in this MPHRA.

When modeling with unit emission rates, the unit response must be adjusted to perform chemical-specific exposure and risk assessments. This adjustment is performed using the following relationship:

$$C_{(air)} = Q \cdot Cy \qquad \text{Eq. 3-1}$$

where

$C_{(air)}$ = calculated chemical-specific concentration in air (micrograms per cubic meter, $\mu g/m^3$)
Q = estimated chemical-specific stack emission rate (g/s)
Cy = maximum ground-level unit response concentration ($\mu g/m^3$ per g/s).

Similarly, the chemical-specific wet and dry deposition rate adjustments are performed using the following relationship:

$$D_R = Q \cdot Dy \qquad \text{Eq. 3-2}$$

where

D_R = calculated chemical-specific deposition rate (grams per square meter-year [g/m^2-yr])
Q = estimated chemical-specific stack emission rate (g/s)
Dy = maximum ground-level unit response deposition rate (g/m^2-yr per g/s).

For this MPHRA, AERMOD provided a unit response for each modeled source. The long-term and short-term COPC-specific emission rates presented in Tables 2-2 and 2-3, respectively, were used to adjust the AERMOD unit response. The resulting COPC-specific adjusted air concentrations and deposition rates were then used to estimate media concentrations.

3.1.3 Overview of Model Inputs

One of the inputs to AERMOD is the runstream setup file that contains the selected modeling options, as well as source location and parameter data, receptor locations, meteorological data file specifications, and output options. Another input data need is the meteorological data files. AERMOD requires two types of meteorological data files, both of which are provided by the AERMET meteorological preprocessor program. One file consists of surface scalar parameters, and the other consists of vertical profiles of meteorological data. For applications involving elevated terrain effects, the AERMOD terrain preprocessor program (AERMAP) provides the required receptor terrain data for input to the AERMOD model. AERMAP requires a terrain data input file, as described in subsection 3.2.3.3.

To effectively model the emissions from the PCAPP, each emitted chemical must be characterized as occurring either in the vapor or particulate phase. In general, most chemicals with very low volatility are modeled in the particle phase. Organic chemicals occur as either vapor or as vapor condensed onto the surface of particulates (i.e., particle-bound). Based on their vapor pressures, all COPCs emitted from PCAPP are expected to be found solely in the vapor phase and were modeled in a single vapor-phase model run to determine both the air concentrations and deposition rates. Section 3.2 provides detailed descriptions of the input data.

3.2 DETAILED AERMOD INPUT DATA

AERMOD requires an array of data to characterize the emission sources, terrain features, receptor locations, and meteorology. The AERMOD runstream file contains the identification of the required data in the following input categories:

- control options
- source information
- receptor information
- meteorology data file specifications
- output options

The following subsections describe the data included in each of the five input categories for this MPHRA.

3.2.1 Control Options

The input requirements for the Control Option category include identification of the dispersion options, averaging times, and gas dry deposition inputs. Table 3-1 lists the Control Option specifications used in this MPHRA.

Table 3-1. Control Option Specifications

Control Option	Specification	Basis
Stack-tip downwash (except for Schulman-Scire downwash)	Use	Regulatory default
Elevated terrain	Incorporate	Regulatory default
Calms processing routines	Use	Regulatory default
Missing data processing routine	Use	Regulatory default
Air concentration	Calculate and output	MPHRA calculation input requirements
Dry deposition	Calculate and output	MPHRA calculation input requirements
Wet deposition	Calculate and output	MPHRA calculation input requirements
Averaging times	Annual and 1-hr	For lifetime and acute assessments
Dispersion coefficient	Rural	Land use analysis (Section 3.2.2.3)
Dry gas deposition parameters		
pollutant reactivity factor	0	AERMOD default
fraction of maximum green leaf area index during autumn	0.5	AERMOD default
fraction of maximum green leaf area index during transitional spring	0.25	AERMOD default
land use categories	Barren land, mostly desert for all 36 wind sectors	Surrounding land use
seasonal categories		
midsummer	June through August	Temperature and growing season
autumn	September through October	Temperature and growing season
late autumn	November through December	Temperature and growing season
winter	January through February	Temperature and growing season
transitional spring	March through May	Temperature and growing season

3.2.2 Source Information

The Source Information category contains information that defines the emission sources for a particular model run. The Source Information category requires the identification of the following information:

- source types, locations, and release parameters
- building downwash information
- land use type (rural or urban coefficients)
- deposition parameters
- source groups

The following subsections describe the information that was identified in this input category.

3.2.2.1 Source Types, Locations, and Release Parameters

The input parameters that define the emission source information for a particular model run vary depending on the source type. All of the emission points used in this MPHRA are considered "point" sources, or stacks. For point sources, which include releases from stacks and isolated vents, the following input parameters must be identified:

- source ID
- source type
- source location in Universal Transverse Mercator (UTM) coordinates
- emission rate (g/s)
- release height above ground (m)
- stack gas exit temperature (Kelvin [K])
- stack gas exit velocity (m/s)
- stack inside diameter (m)

The MPHRA included the most current (August 2007) stack design parameters as inputs to the AERMOD model. This design includes a total of 10 emission sources associated with hazardous waste operations. Table 3-2 summarizes the source locations and stack design parameters for these 10 future emission sources.

3.2.2.2 Building Downwash Information

The Source Information inputs must include direction-specific information for each source when the effects of structure-induced downwash influences on emissions from nearby or adjacent point sources are a consideration. Plume dispersion can be affected by nearby structures when a stack is short enough to allow the plume to be significantly influenced by surrounding building turbulence. This phenomenon, known as structure-induced downwash, generally results in a higher ground-level concentration in the vicinity of a stack and influencing structure. The height needed to avoid this phenomenon is referred to as the Good Engineering Practice (GEP) stack height; a stack constructed at or above this height will not be impacted by building turbulence and need not be subjected to a downwash analysis.

All PCAPP structures in the current (August 2007) site configuration were analyzed to determine their potential to influence the dispersion of stacks emissions. USEPA's *Guideline for Determination of Good Engineering Practice Stack Height* (USEPA, 1985) was followed in this evaluation. If the physical stack heights were found to be less than GEP, it was necessary to incorporate downwash effects into the AERMOD modeling.

Table 3-2. Summary of Source Parameters for Future Emission Sources

Source ID	Source Description	Location, UTM East	Location, UTM North	Base Elevation		Stack Height		Stack Temperature		Stack Velocity		Stack Diameter	
		(m)	(m)	(m)	(ft)	(m)	(ft)	(K)	(°F)	(m/s)	(ft/s)	(m)	(ft)
AFA	AFA stack	560515.3	4244440.6	1447.7	4749.5	26.2	86	305.2	90	18.1	59.3	2.0	6.7
30Day	Tanks Vent	560688.1	4244401.1	1446.6	4746.0	12.2	40	324.7	125	3.3	10.9	0.1	0.3
BTA1	Six BTA OTS stacks	560746.5	4244430.1	1446.6	4746.0	4.6	15	328.6	132	11.1	36.3	0.6	2.0
BTA2		560746.5	4244396.1	1446.6	4746.0	4.6	15	328.6	132	11.1	36.3	0.6	2.0
BTA3		560746.5	4244353.2	1446.6	4746.0	4.6	15	328.6	132	11.1	36.3	0.6	2.0
BTA4		560746.5	4244318.9	1446.6	4746.0	4.6	15	328.6	132	11.1	36.3	0.6	2.0
BTA5		560746.5	4244284.6	1446.6	4746.0	4.6	15	328.6	132	11.1	36.3	0.6	2.0
BTA6		560746.5	4244250.8	1446.6	4746.0	4.6	15	328.6	132	11.1	36.3	0.6	2.0
BRS_BC	Tank Vent	560817.4	4244431.8	1446.6	4746.0	16.8	55	321.9	120	17.7	58.0	0.2	0.7
BRS	BRS OTS	560759.2	4244480.3	1446.6	4746.0	16.8	55.0	394.1	250	12.1	39.5	0.6	2.0

USEPA's Building Profile Input Program for PRIME (BPIPPRM dated 04274) was used to produce an AERMOD input file with the proper direction-specific building downwash parameters. For each stack that is less than GEP height, BPIPPRM calculates the building heights, projected building widths, projected building lengths, and the along- and across-flow distances from the stack to the center of the upwind face of the projected building for each of the 36 wind flow vectors (i.e., one value for each 10-degree sector, beginning with the 10-degree flow vector [direction toward which the wind is blowing], and continuing clockwise). In order to calculate these direction-specific building downwash parameters, the individual stack parameters and structure dimensions were determined from facility design drawings and included in the BPIPPRM input file. Any structure located closer than five times the lesser of the structure height or projected building width to an emission point was included in the downwash analysis. Structures other than buildings that were included in this analysis included above-ground storage tanks, the AFA filter banks and associated duct work, and the bioreactor modules. Figure 3-1 graphically shows the structures and emission points included in the BPIPPRM analysis.

3.2.2.3 Land Use Type

The rural or urban coefficient is selected based on the methodology recommended in the *Guideline on Air Quality Models* (USEPA, 2005b). In this procedure, land circumscribed within a 3-km (1.9-mile) radius of the site is classified as rural or urban using the Auer land use classification method. Based on a visual inspection of the US Geological Survey (USGS) 7.5-minute topographical map of the future site location, the entire area within 3 km (1.9 miles) of the future is rural. Therefore, the rural land use coefficient was selected for use in the model input control pathway. Figure 3-2 presents an aerial photograph of the land use within 3 km of the PCAPP.

3.2.2.4 Gas Deposition Parameters

The deposition algorithms for dry and wet deposition of gaseous pollutants require the following inputs for each chemical included in the model:

- diffusivity in air (square centimeters per second [cm^2/s])
- diffusivity in water (cm^2/s)
- cuticular resistance to uptake by lipids for individual leaves (seconds per cm [s/cm])
- Henry's Law constant (pascal-cubic meter per mole [$Pa\text{-}m^3/mol$])

Table 3-3 presents the gas deposition parameter values for each COPC evaluated in this MPHRA. These gas deposition parameters are the only chemical-specific AERMOD inputs needed. To increase the efficiency of the AERMOD calculations and provide a conservative set of chemical-specific inputs, surrogate groups of COPCs were developed based on the magnitude of the Henry's Law constant. AERMOD runs were conducted for a COPC in each surrogate group to determine which chemical-specific gas deposition parameters resulted in an identifiable worst-case concentration and deposition rates. Table 3-4 presents the maximum unit response concentration and deposition rates for the AFA stack using the gas deposition parameter values from select chemicals within each surrogate group while keeping all other model inputs the same. As seen in Table 3-4, hexane resulted in the highest air concentration, 1,4-dioxane resulted in the highest dry deposition rate, and 4-methyl phenol resulted in the highest wet deposition rate. Therefore, the parameter values for these chemicals were used as surrogates for all other chemicals included in the MPHRA, thus yielding the highest possible media concentrations.