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 November 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 14134) 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 and accounting for building wake effects (i.e., plume downwash). The model is applicable for use in all types of terrain, including the terrain associated with the PCD.

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 ambient air concentrations and total depositions rates for use in determining chronic exposures were calculated as a COPC average air concentration or deposition rate over the 6 years of on-site meteorological data used in the model. The 1-hour COPC concentrations for use in determining acute exposures were calculated as the highest 1-hour air concentration from the entire 6-year meteorological data set. (Exposure to air concentrations via inhalation is the only pathway that is evaluated in the acute risk assessment.)

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 deposition 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 (or source group), and the resulting concentration and deposition rates calculated by the model (referred to as a unit response) can be adjusted using COPC-specific emission rates to obtain COPC-specific concentrations and deposition rates. This precluded the need to run the model for each individual COPC (i.e., each of the 79 COPCs with emission rates) in this MPHRA.

All source groups, except for the BTS system and EDS units, included a single stack. The BTS system is comprised of four identical units, each with a single stack, and each of the two EDS units is comprised of two stacks. The BTS design condition is that all four units will operate with the same air flows and emission rates. Therefore, the unit emission rate used in the MPHRA represents the combined BTS system with the four BTS stacks included in a single source group in AERMOD. To establish some spatial definition (albeit very small), four discrete BTS stack locations were input, and each BTS emission rate was set equal to 0.25 g/s to account for each stack's contribution to the combined BTS unit emission rate. Similarly, emissions from each EDS unit are conveyed through the EDS ventilation system which discharges through two identical OTSs, each with its own dedicated stack. Therefore, the EDS emission rate was set equal to 0.5 g/s to account for each stack's contribution to the total EDS emission rate.

When modeling with unit emission rates, the unit response must be adjusted to perform chemical-specific exposure and risk assessments. This adjustment was 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 [µg/m^3])
Q	=	estimated chemical-specific stack emission rate (g/s)
Cy	=	maximum ground-level unit response concentration (µg/m^3 per g/s).

Similarly, the chemical-specific wet and dry deposition rate adjustments were 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 group. The long-term and short-term COPC-specific emission rates presented in Table 2-2 and Table 2-3, respectively, were used to adjust the AERMOD unit response. The resulting COPC-specific air concentrations and deposition rates were then used to estimate media concentrations.

3.1.3 Partitioning of Emissions

To effectively model the emissions from PCAPP and EDS, each emitted chemical must be characterized as occurring either in the vapor or particulate phase. Organic chemicals occur as either vapor or as vapor condensed onto the surface of particulates (i.e., particle-bound). In general, most chemicals with very low volatility are modeled in the particle phase. Particle-bound modeling is used to approximate situations where a portion of a semivolatile organic compound is volatilized in a high temperature environment and condensed to the surface of a particle entrained in the exhaust gas after the gas cools in the stack. Neither PCAPP nor EDS employ high temperature environments followed by stack gas cooling. Therefore, particle-bound phase modeling was not conducted for this assessment. Based on their vapor pressures (i.e., fraction of COPC in vapor phase [F_v]), COPCs emitted from PCAPP and EDS were expected to be found either in the vapor phase or particle phase as follows:

- COPCs with very low volatility (F_v less than 0.05) occur only in the particle phase; and
- volatile COPCs (F_v of 1.0) occur only in the vapor phase.

Except for the five EDS metal COPCs with F_v less than 0.05, the COPCs expected to be emitted from PCAPP and EDS are volatile with F_v of 1.0.

3.1.4 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 uses two types of meteorological data files, both of which are produced by the AERMOD Meteorological Data Preprocessor Program (AERMET). One file contains surface scalar parameters, and the other contains vertical profiles of meteorological data. For applications involving elevated terrain effects, the AERMOD terrain preprocessor program (AERMAP) produces 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.

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 dry gas deposition inputs. Table 3-1 lists the Control Option specifications used in this MPHRA.

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.

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 requirement
Dry deposition	Calculate and output	MPHRA calculation input requirement
Wet deposition	Calculate and output	MPHRA calculation input requirement
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	Rangeland for all 36 wind sectors (Category No. 3).	Surrounding land use (Section 2.2.2 of USEPA, 2014a)
seasonal categories		
midsummer (Category 1)	June through August	Temperature and growing season (Section 2.2.1 of USEPA, 2014a)
autumn (Category 2)	September, October	
late autumn (Category 3)	January, February, November, December	
winter with snow (Category 4)	not applicable, no continuous snow cover	
transitional spring (Category 5)	March through May	

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 stack design parameters as inputs to the AERMOD model. This design includes a total of eight emission sources associated with hazardous waste operations at PCAPP and two sources (stacks) associated with each EDS unit. Table 3-2 summarizes the source locations and stack design parameters for these 12 emission sources.

As noted in Table 3-2, two identical EDS units, each with two stacks, were included in the AERMOD runs. While two EDS units will be constructed at PCD, only one unit will operate at a time. The other unit only will be used as a backup if the primary unit is not operational. As a conservative measure, both EDS units were included in the model runs and the MPHRA

included the air concentration and deposition rates from the EDS unit producing the maximum results.

Because the EDS units will only operate during daylight hours, the AERMOD input file included variable emission rates for the two EDS source groups. This was accomplished by selecting only the hours of the day the EDS units would operate. As such, the AERMOD input file specified an emission factor of 1 for the hours of 8:00 am to 8:00 pm and an emission factor of 0 for the remaining hours of the day. Specifying emissions over a 12-hour period is consistent with the derivation of the long-term emission rates as discussed in Section 2 and in more detail in Appendix B-2 (i.e., based on 12 hours per day and not 24 hours per day).

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. If a stack is short enough, relative to adjacent structures, plume dispersion can be influenced by turbulence from the structures. This phenomenon, known as structure-induced downwash, generally results in a higher ground-level concentration in the vicinity of a stack and influencing structure(s).

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, 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. All PCAPP and EDS structures were analyzed to determine their potential to influence the dispersion of stack emissions. Structures other than buildings included in this analysis were the above-ground storage tanks, the AFA filter banks and associated duct work, pipe racks, and the bioreactor modules. All of these structures are solid or practically solid structures that have the potential for inducing wake effects as air flows across the structure and are appropriately considered in the BPIPPRM analysis. Figure 3-1 graphically shows the PCAPP structures and emission points included in the BPIPPRM analysis. Figure 3-2 provides a three-dimensional illustration of the EDS structures and emission points included in the BPIPPRM analysis

3.2.2.3 Land Use Type

The rural or urban dispersion 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 site location, the entire area within 3 km (1.9 miles) of the site location is rural. Therefore, the rural land use dispersion coefficient was selected for use in the model input control pathway. Figure 3-3 presents an aerial photograph of the land use within 3 km of the PCAPP AFA stack, which is the center of the receptor grid.

Table 3-2. Summary of Source Parameters for PCAPP and EDS Emission Sources

Source ID	Source Description	Location, UTM		Base Elevation		Stack Height		Stack Temperature		Stack Velocity[a]		Stack Diameter	
		East	North										
		(m)	(m)	(m)	(ft)	(m)	(ft)	(K)	(^{o} F)	(m/s)	(ft/s)	(m)	(ft)
AFA	AFA stack	560,539	4,244,449	1448	4750	26.2	86	305.4	90	18.1	59.2	2.0	6.7
30-Day	Tanks vent	560,711	4,244,408	1446	4746	12.2	40	324.7	125	6.1	20.0	0.10	0.25
BTS1	Four BTS OTS stacks	560,776	4,244,331	1446	4746	4.6	15	325.2	126	27.5	90.3	0.46	1.5
BTS2		560,776	4,244,362	1446	4746	4.6	15	325.2	126	27.5	90.3	0.46	1.5
BTS3		560,776	4,244,414	1446	4746	4.6	15	325.2	126	27.5	90.3	0.46	1.5
BTS4		560,776	4,244,445	1446	4746	4.6	15	325.2	126	27.5	90.3	0.46	1.5
WRS	BC feed tank OTS stack	560,845	4,244,453	1446	4746	16.8	55	319.3	115	18.2	60.0	0.20	0.67
BRS	BRS OTS stack	560,795	4,244,460	1447	4746	7.6	25	355.3	180	14.6	47.8	0.20	0.67
EDS1A	Two EDS Unit 1 stacks	559,057	4,243,724	1451	4760	4.6	15	294.1	70	16.2	53.1	0.46	1.5
EDS1B		559,058	4,243,725	1451	4760	4.6	15	294.1	70	15.8	51.9	0.46	1.5
EDS2A	Two EDS Unit 2 stacks	559,118	4,243,724	1451	4760	4.6	15	294.1	70	16.2	53.1	0.46	1.5
EDS2B		559,119	4,243,725	1451	4760	4.6	15	294.1	70	15.8	51.9	0.46	1.5

a. All stacks are vertical and unobstructed.

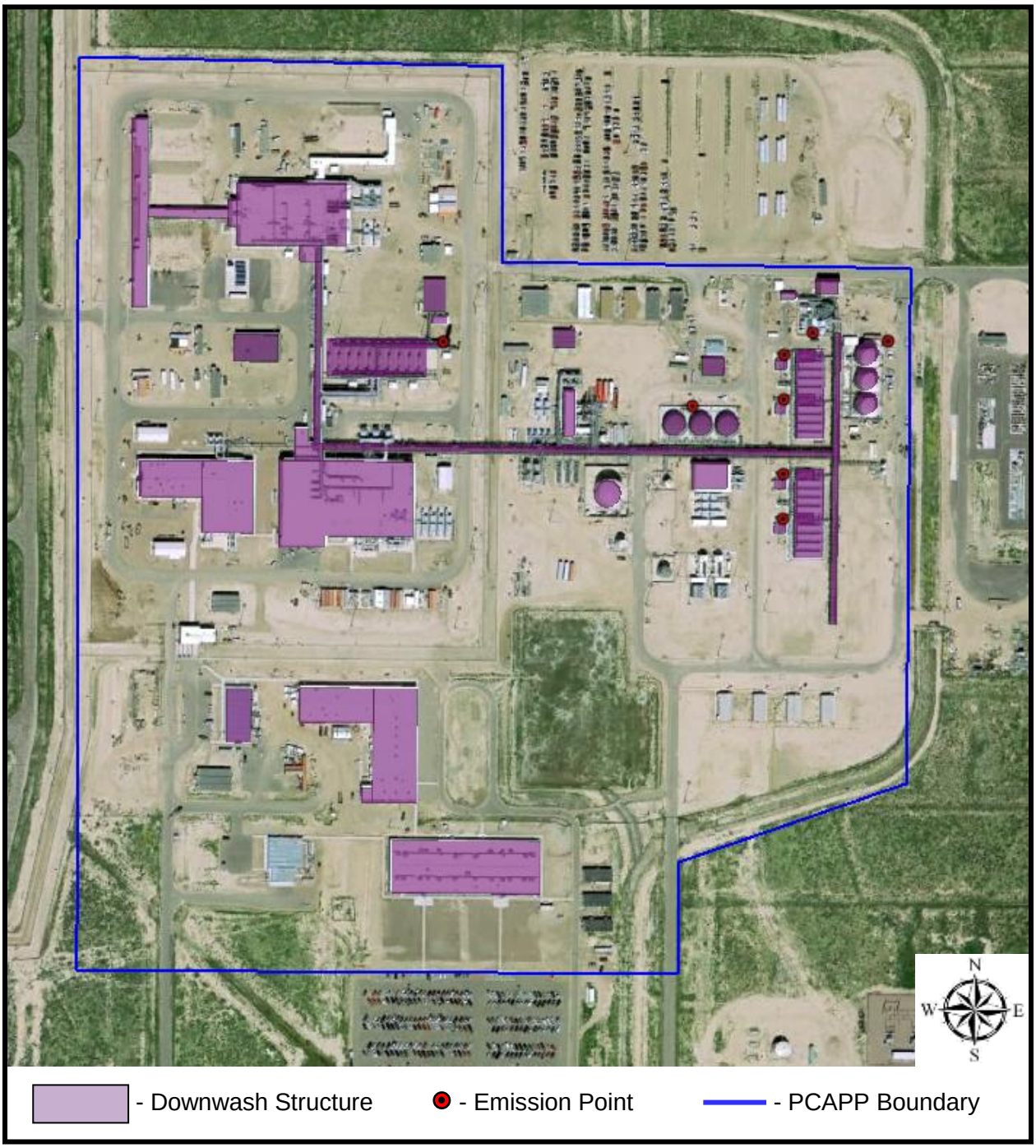

Figure 3-1. Location of the PCAPP downwash analysis structures and emission points.

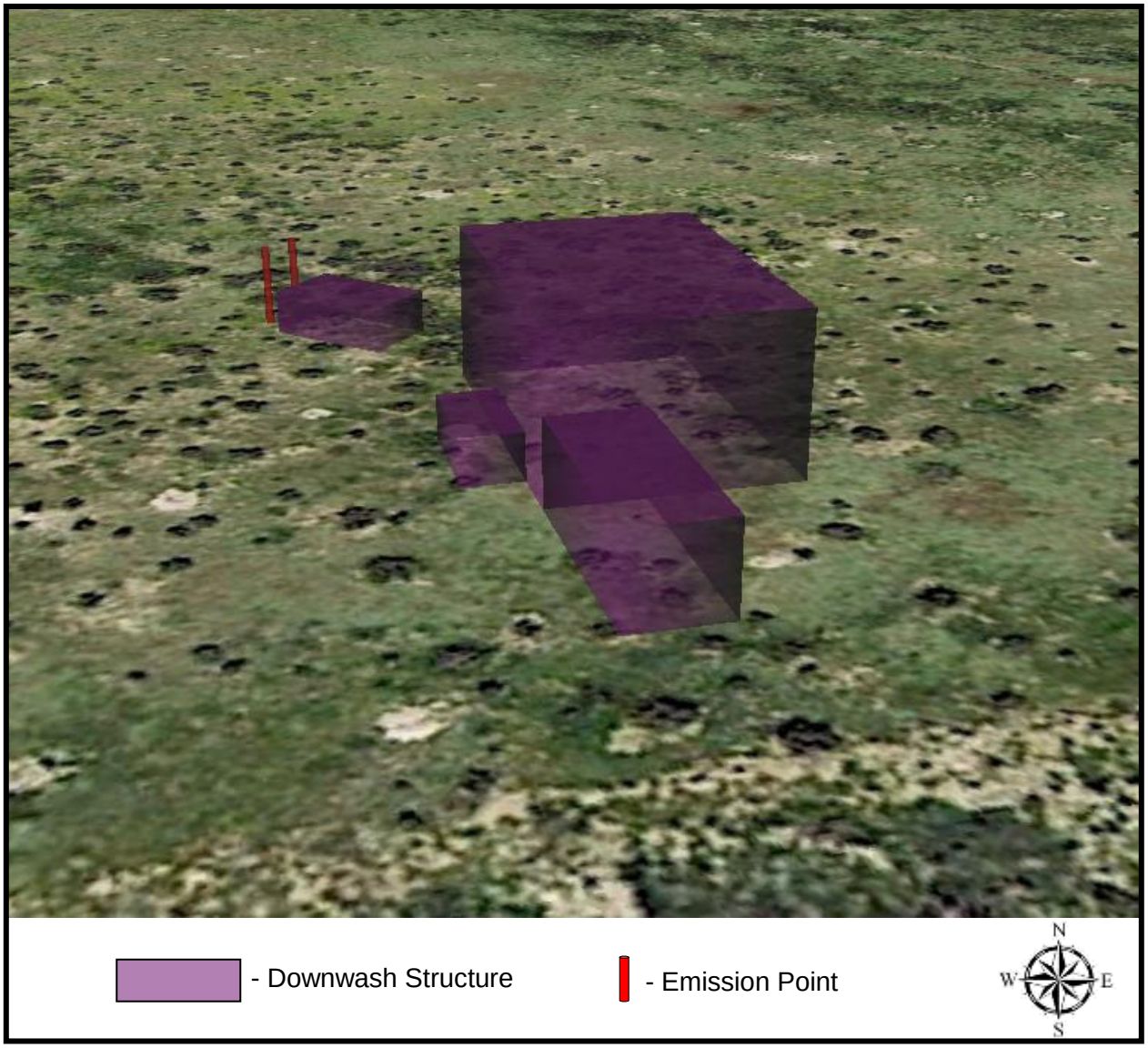

Figure 3-2. Three-dimensional illustration of EDS downwash analysis structures and emission points.

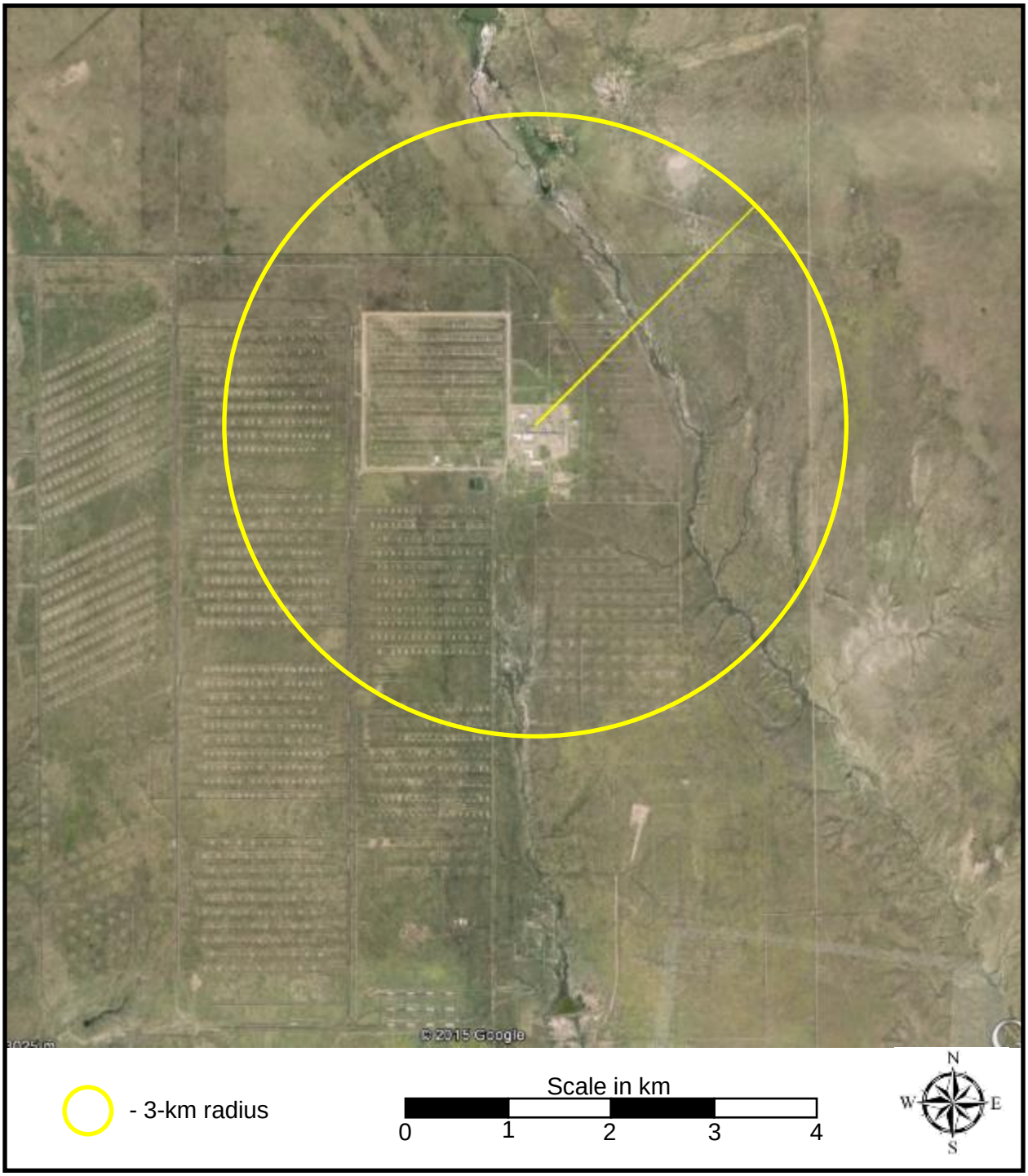

Figure 3-3. Aerial photograph depicting land use within a 3-km radius of the AFA stack.

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 vapor-phase COPCs potentially released by PCAPP or EDS sources. Because these gas deposition parameters are not needed for particle-phase COPCs, the metal COPCs associated with EDS are not included in Table 3-3. These gas deposition parameters are the only chemical-specific inputs required by AERMOD deposition calculations. To increase the efficiency of the AERMOD calculations and provide a reasonably conservative set of chemical-specific inputs, surrogate COPCs were developed for each gas phase model run (i.e., ambient air concentration, dry deposition, and wet deposition).

The gas deposition parameter values listed in Table 3-3 were sorted to identify the COPCs that have the 5 largest and 5 smallest values for each gas deposition parameter. Table 3-4 presents a list of the COPCs with the largest and smallest gas deposition parameter values. Thirty (30) different COPCs are listed. The gas deposition parameters for each of these 30 COPCs were used as input values to calculate COPC-specific ambient air concentrations, dry deposition rates, and wet deposition rates in AERMOD based on a unit emission rate and AFA stack parameters over the entire receptor grid.

Table 3-5 presents the highest COPC-specific unit response ambient air concentrations and dry and wet deposition rates at any receptor for these 30 COPCs for the AFA stack. Only the gas deposition parameter values were varied in these AERMOD runs. Table 3-5 shows that deposition parameter values for dichlorodifluoromethane produce the highest air concentration, those for thiodiglycol produce the highest dry deposition rate, and those for 2,4-dinitrotoluene produce the highest wet deposition rate. (These three values are highlighted in Table 3-5.) Therefore, the parameter values for these three chemicals were used as surrogates for all other COPCs included in the MPHRA, thus yielding the highest possible inhalation exposures and media concentrations relative to the known COPCs.

3.2.2.5 Particle-Phase Dry Deposition Parameters

AERMOD provides two methods for calculating dry deposition rates based on particle size. Method 1 is used when 10 percent or more of the total particulate mass is particles with a diameter of 10 micrometers (microns [µm]) or larger. In order to use Method 1, the particle size distribution of the emissions must be reasonably known. Method 2 is used when less than 10 percent of the total particulate mass is particles with a diameter of 10 µm or larger. The deposition velocity for Method 2 is given as the weighted average of the deposition velocity for particles in the fine mode (i.e., less than 2.5 µm in diameter) and the deposition velocity for the coarse mode (i.e., greater than 2.5 µm but less than 10 µm in diameter).

Table 3-3. Summary of COPC Gas Deposition Parameter Values

Chemical	CAS Number	Diffusivity in Air	Diffusivity in Water	Cuticular Resistance	Henry's Law Constant
		(cm^2/s)	(cm^2/s)	(s/cm)	(Pa-m^3/mol)
		D_a	D_w	*rcl*	*H*
1,1,2,2-tetrachloroethane	79-34-5	0.071	7.90E-06	4.95E+04	3.45E+01
1,1-dichloroethane	75-34-3	0.074	1.05E-05	1.16E+05	5.67E+02
1,1-dichloroethene	75-35-4	0.090	1.04E-05	5.78E+04	2.63E+03
1,2,3-trichlorobenzene	87-61-6	0.001	1.00E-05	2.60E+02	1.27E+02
1,2,4-trichlorobenzene	120-82-1	0.030	8.23E-06	4.82E+02	1.42E+02
1,2,4-trimethyl benzene	95-63-6	0.078	9.03E-06	1.30E+04	6.24E+02
1,2-dichlorobenzene	95-50-1	0.069	7.90E-06	1.28E+03	1.93E+02
1,2-dichlorobutane	616-21-7	0.075	8.71E-06	1.51E+04	2.17E+03
1,2-dichloroethane	107-06-2	0.104	9.90E-06	1.31E+05	9.93E+01
1,2-dichloropropane	78-87-5	0.078	8.73E-06	6.18E+04	2.84E+02
1,3-dichlorobenzene	541-73-1	0.069	7.86E-06	4.57E+02	3.14E+02
1,4-dichlorobenzene	106-46-7	0.069	7.90E-06	5.04E+02	2.43E+02
1,4-dithiane	505-29-3	0.078	9.03E-06	9.81E+04	4.98E-01
1,4-oxathiane	15980-15-1	0.086	9.94E-06	5.94E+05	5.45E-01
1-chlorobutane	109-69-3	0.093	1.08E-05	3.61E+04	1.69E+03
1-hexene	592-41-6	0.099	1.15E-05	3.00E+04	4.17E+04
2,4-dichlorophenol	120-83-2	0.001	1.00E-05	3.48E+01	3.24E-01
2,4-dinitrotoluene[a]	121-14-2	0.203	7.06E-06	2.62E+01	9.38E-03
2-butanone	78-93-3	0.081	9.80E-06	3.88E+07	5.67E+00
2-chlorobutane	78-86-4	0.093	1.08E-05	5.49E+04	2.44E+03
2-chloroethoxyethane	112-26-5	0.058	6.73E-06	5.27E+02	7.91E-02
2-ethyl 1,3-butadiene	3404-63-5	0.101	1.16E-05	1.01E+04	2.48E+04
2-hexanone	591-78-6	0.088	1.02E-05	3.37E+05	9.44E+00
2-methyl phenol	95-48-7	0.074	8.30E-06	5.58E+01	1.22E-01
2-methylnaphthalene	91-57-6	0.070	8.08E-06	4.71E+02	5.25E+01
3-methyl phenol	108-39-4	0.074	1.00E-05	3.27E+01	8.76E-02
4-methyl phenol	106-44-5	0.074	1.00E-05	2.54E+01	8.00E-02
4-methyl-2-pentanone	108-10-1	0.075	7.80E-06	8.24E+05	1.42E+01
acenaphthylene	208-96-8	0.044	7.50E-06	3.59E+01	1.16E+01
acetone	67-64-1	0.124	1.14E-05	3.36E+08	3.95E+00
acetylene	74-86-2	0.216	2.50E-05	1.34E+08	2.20E+03
acrolein	107-02-8	0.105	1.22E-05	5.80E+05	1.22E+01
alpha-methylstyrene	98-83-9	0.079	9.14E-06	7.08E+03	2.58E+02
ammonia	7664-41-7	0.287	3.33E-05	6.97E+11	1.63E+00
benzene	71-43-2	0.088	1.02E-05	2.51E+04	5.67E+02
bis(2-chloroisopropyl) ether	108-60-1	0.001	1.00E-05	1.07E+05	9.33E+01
carbon disulfide	75-15-0	0.104	1.00E-05	7.45E+02	3.04E+03
chlorine	7782-50-5	0.001	1.00E-05	8.00E+05	1.19E+03
chlorobenzene	108-90-7	0.073	8.70E-06	6.02E+03	3.75E+02
chloroethane	75-00-3	0.271	1.15E-05	2.11E+04	8.92E+02
chloroform	67-66-3	0.104	1.00E-05	1.62E+05	3.75E+02
chloromethane	74-87-3	0.126	6.50E-06	1.89E+06	8.94E+02
chloromethoxyethane	3188-13-4	0.092	1.06E-05	3.17E+05	4.08E+01

Table 3-3. Summary of COPC Gas Deposition Parameter Values (continued)

Chemical	CAS Number	Diffusivity in Air	Diffusivity in Water	Cuticular Resistance	Henry's Law Constant
		(cm^2/s)	(cm^2/s)	(s/cm)	(Pa-m^3/mol)
		D_a	D_w	*rcl*	*H*
cis-1,2-dichloroethene	156-59-2	0.001	1.00E-05	3.83E+04	4.15E+02
dichlorodifluoromethane	75-71-8	0.001	1.00E-05	1.43E+06	3.48E+04
diethyl ether	60-29-7	0.078	8.60E-06	5.41E+07	2.69E+01
ethane	74-84-0	0.196	2.28E-05	1.65E+03	5.07E+04
ethanol	64-17-5	0.123	1.30E-05	3.29E+09	5.07E-01
ethylbenzene	100-41-4	0.075	7.80E-06	1.65E+04	8.00E+02
HD	505-60-2	0.065	7.49E-06	2.18E+03	3.34E+00
hexane	110-54-3	0.097	1.13E-05	2.73E+04	1.82E+05
hydrogen chloride	7647-01-0	0.001	1.00E-05	3.62E+10	7.83E+02
hydrogen cyanide	74-90-8	0.210	2.44E-05	9.01E+12	1.35E+01
methane	74-82-8	0.299	3.46E-05	8.64E+04	6.67E+04
methyl tert-butyl ether	1634-04-4	0.096	1.11E-05	1.11E+07	5.95E+01
methylene chloride	75-09-2	0.101	1.17E-05	9.07E+04	2.23E+02
monoethanolamine	141-43-5	0.123	1.42E-05	6.23E+07	3.29E-03
naphthalene	91-20-3	0.059	7.50E-06	3.65E+02	4.86E+01
nitrobenzene	98-95-3	0.076	8.60E-06	7.51E+02	2.43E+00
octane	111-65-9	0.081	9.35E-06	5.53E+04	3.25E+05
pentane	109-66-0	0.110	1.27E-05	9.67E+03	1.27E+05
phenanthrene	85-01-8	0.001	1.00E-05	2.33E+01	2.33E+00
phenol	108-95-2	0.082	9.10E-06	3.33E+01	4.05E-02
propene	115-07-1	0.157	1.82E-05	1.62E+04	1.99E+04
styrene	100-42-5	0.071	8.00E-06	1.13E+04	2.74E+02
tert-butyl alcohol	75-65-0	0.108	1.25E-05	2.18E+07	9.17E-01
tetrachloroethene	127-18-4	0.072	8.20E-06	6.04E+03	1.82E+03
thiirane	420-12-2	0.124	1.43E-05	2.84E+06	3.51E+01
thiodiglycol	111-48-8	0.077	8.93E-06	3.57E+03	1.87E-04
toluene	108-88-3	0.087	8.60E-06	1.74E+04	6.69E+02
trans-1,2-dichloroethene	156-60-5	0.070	1.19E-05	3.05E+04	9.52E+02
trichloroethene	79-01-6	0.079	9.10E-06	1.88E+04	1.01E+03
vinyl chloride	75-01-4	0.106	1.23E-05	7.35E+03	2.74E+03
xylenes	1330-20-7	0.085	9.81E-06	2.00E+04	6.72E+02

a. 2,4-dinitrotoluene is not a COPC potentially released by PCAPP or EDS sources. However, it was included in the gas deposition sensitivity analysis and is therefore included in this table.

Table 3-4. Summary of Five Largest and Five Smallest Gas Deposition Parameter Values for COPCs

Rank	Henry's Law Constant		Diffusivity of Chemical in Air[a]		Diffusivity of Chemical in Water[b]		Cuticular Resistance	
	COPC	Value	COPC	Value	COPC	Value	COPC	Value
Smallest	thiodiglycol	1.87E-04	1,2,3-trichlorobenzene	0.001	chloromethane	6.50E-06	phenanthrene	2.33E+01
2nd Smallest	monoethanolamine	3.29E-03	2,4-dichlorophenol	0.001	2-chloroethoxyethane	6.73E-06	4-methyl phenol	2.54E+01
3rd Smallest	2,4-dinitrotoluene	9.38E-03	bis(2-chloroisopropyl) ether	0.001	2,4-dinitrotoluene	7.06E-06	2,4-dinitrotoluene	2.62E+01
4th Smallest	phenol	4.05E-02	chlorine	0.001	HD	7.49E-06	3-methyl phenol	3.27E+01
5th Smallest	2-chloroethoxyethane	7.91E-02	cis-1,2-dichloroethene	0.001	acenaphthylene	7.50E-06	phenol	3.33E+01
5th Largest	ethane	5.07E+04	hydrogen cyanide	0.21	ethane	2.28E-05	acetone	3.36E+08
4th Largest	methane	6.67E+04	acetylene	0.216	hydrogen cyanide	2.44E-05	ethanol	3.29E+09
3rd Largest	pentane	1.27E+05	chloroethane	0.271	acetylene	2.50E-05	hydrogen chloride	3.62E+10
2nd Largest	hexane	1.82E+05	ammonia	0.287	ammonia	3.33E-05	ammonia	6.97E+11
Largest	octane	3.25E+05	methane	0.299	methane	3.46E-05	hydrogen cyanide	9.01E+12

a. Dichlorodifluoromethane also has a diffusivity in air value of 0.001 cm^2/s and was therefore included in the sensitivity analysis.
b. Naphthalene also has a diffusivity in water of 7.50E-06 cm^2/s and was therefore included in the sensitivity analysis.

Table 3-5. Summary of the AERMOD Results Based on the Gas Deposition Parameters for the 30 COPCs listed in Table 3-4

Source No.	COPC	CAS Number	Chemical/Physical Properties				AFA Maximum Unit Response[a]		
			Henry's Law Constant	Diffusivity of Chemical in Air	Diffusivity of Chemical in Water	Cuticular Resistance	Annual Concentration	Annual Dry Deposition	Annual Wet Deposition
			(Pa-m^3/mol)	(cm^2/s)	(cm^2/s)	(s/cm)	(µg/m^3)	(g/m^2/yr)	(g/m^2/yr)
AFA1	1,2,3-trichlorobenzene	87-61-6	126.7	0.001	1.00E-05	260	0.05036	0.00019	0
AFA2	2,4-dichlorophenol	120-83-2	0.324	0.001	1.00E-05	34.8	0.05029	0.001	0
AFA3	2-chloroethoxyethane	112-26-5	0.0791	0.058	6.73E-06	527	0.05036	0.0002	0.0001
AFA4	3-methyl phenol	108-39-4	0.0876	0.074	1.00E-05	32.7	0.05024	0.00156	0.00009
AFA5	4-methyl phenol	106-44-5	0.0800	0.074	1.00E-05	25.4	0.05020	0.00195	0.0001
AFA6	acenaphthylene	208-96-8	11.6	0.044	7.50E-06	35.9	0.05026	0.00135	0
AFA7	acetone	67-64-1	3.95	0.124	1.14E-05	3.36E+08	0.05037	0.00001	0
AFA8	acetylene	74-86-2	2,199	0.216	2.50E-05	134,276,978	0.05038	0	0
AFA9	ammonia	7664-41-7	1.63	0.287	3.33E-05	6.97E+11	0.05037	0.00003	0.00001
AFA10	bis(2-chloroisopropyl) ether	108-60-1	93.3	0.001	1.00E-05	106,897	0.05038	0	0
AFA11	chlorine	7782-50-5	1,186	0.001	1.00E-05	799,553	0.05038	0	0
AFA12	chloroethane	75-00-3	892	0.271	1.15E-05	21,100	0.05038	0.00001	0
AFA13	chloromethane	74-87-3	894	0.126	6.50E-06	1.89E+06	0.05038	0.00001	0
AFA14	cis-1,2-dichloroethene	156-59-2	415	0.001	1.00E-05	38,310	0.05038	0	0
AFA15	ethane	74-84-0	50,663	0.196	2.28E-05	1,649	0.05037	0.00003	0
AFA16	ethanol	64-17-5	0.507	0.123	1.30E-05	3.29E+09	0.05037	0.00003	0.00002
AFA17	HD	505-60-2	3.34	0.065	7.49E-06	2,175	0.05037	0.00003	0
AFA18	hexane	110-54-3	182,385	0.097	1.13E-05	27,300	0.05038	0	0
AFA19	hydrogen chloride	7647-01-0	783	0.001	1.00E-05	3.62E+10	0.05038	0	0
AFA20	hydrogen cyanide	74-90-8	13.5	0.210	2.44E-05	9.01E+12	0.05037	0.00002	0
AFA21	methane	74-82-8	66,672	0.299	3.46E-05	86,370	0.05038	0	0
AFA22	monoethanolamine	141-43-5	0.00329	0.123	1.42E-05	6.23E+07	0.05022	0.00159	0.00042
AFA23	naphthalene	91-20-3	48.6	0.059	7.50E-06	365	0.05036	0.00015	0
AFA24	octane	111-65-9	325,253	0.081	9.35E-06	55,270	0.05038	0	0
AFA25	pentane	109-66-0	126,656	0.110	1.27E-05	9,668	0.05038	0.00001	0
AFA26	phenanthrene	85-01-8	2.33	0.001	1.00E-05	23.3	0.05027	0.00127	0
AFA27	phenol	108-95-2	0.0405	0.082	9.10E-06	33.3	0.05023	0.00161	0.00017
AFA28	thiodiglycol	111-48-8	0.000187	0.077	8.93E-06	3,570	0.04956	0.00963	0.00031
AFA29	dichlorodifluoromethane	75-71-8	34,800	0.001	0.00001	1.43E+06	0.05038	0	0
AFA30	2,4-dinitrotoluene	121-14-2	0.00938	0.203	7.06E-06	26.2	0.05014	0.00244	0.00048

a. Red font indicates the largest maximum unit response value. Yellow highlight indicates the COPCs selected as surrogate for vapor phase model runs.

Actual particle size information obtained from stack emission testing were not available for PCAPP or EDS sources. However, HEPA filters are installed on each PCAPP and EDS source prior to the stack. These filters were specified to remove particulates greater than 0.3 µm in size. Therefore, Method 2 was utilized to calculate the dry deposition of particulate emissions. The required input source parameters for each source for Method 2 include the fine mass fraction (i.e., the fraction of particle mass emitted in the fine mode, less than 2.5 µm) and mass mean particle diameter (µm). Based on the expected HEPA filter performance, 100 percent of the particle mass was assumed to be emitted in the fine mode with a mass mean particle diameter of 0.3 µm. A sensitivity analysis was conducted prior to the full AERMOD runs to verify that using a smaller mass mean particle diameter would not result in larger deposition rates. The results of the sensitivity model runs indicated that using mass mean particle diameters between 0.005 and 0.3 µm produced the same dry deposition rates for each of the emission sources.

3.2.2.6 Source Groups

AERMOD allows the user to add together contributions from particular sources by identifying source groups. Several source groups may be set up in a single model run, and the combined contributions for the emission sources within a source group are provided in the model output. The MPHRA included an assessment of potential emissions from the following seven source groups:

- AFA stack
- 30-day Storage Tanks vent
- Four BTS OTS stacks
- WRS BC feed tank OTS
- BRS OTS stack
- Two AFS stacks for EDS1
- Two AFS stacks for EDS2

Assigning these source groups was necessary for the MPHRA modeling because the potential emission rates of the COPCs vary for sources included in the seven source groups. The emission rates and stack parameters are identical for the four BTS process stacks; therefore, the AERMOD results for these four stacks were combined into a single source group. In addition, the two AFS stacks for each of the EDS units were combined into a single source group, as the emission rates are identical for the two stacks. All other identified source groups consist of a single stack.

3.2.3 Receptor Information

The MPHRA is based on two distinct areas of concern: (1) off-site impact locations, and (2) on-site impact locations. The off-site impact locations were used to determine the RME individual location, while the on-site impact locations were used to evaluate the acute on-site worker exposure scenario.

3.2.3.1 Off-site Receptor Locations

Off-site receptor locations were established at appropriate distances to ensure sufficient density and areal extent to adequately characterize the pattern of impacts in the area. A nested rectangular grid was used that extended a sufficient distance from the PCD boundary. This tiered receptor grid was oriented with the AFA stack at its center and included the following array of receptors:

- 100 m (328 ft) spacing out to a distance of 5 km (3.1 miles), which encompasses the local water body
- 500 m (1,640 ft) spacing out to a distance of 10 km (6.2 miles)
- 1 km (0.6 mile) spacing out to a distance of 25 km (15.6 miles)
- 100 m (328 ft) spacing along the PCD fence line

Figure 3-4 presents the layout of the tiered off-site receptor grid. Figure 3-5 illustrates the receptor locations that encompass the local water body.

3.2.3.2 On-site Receptor Locations

The on-site receptor grid was oriented with the AFA stack at its center and included the following array of receptors out to the PCD fence line:

- 100 m (328 ft) spacing out to a distance of 3 km (1.9 miles)
- 500 m (1,640 ft) spacing out to the remainder of the PCD fence line
- 100 m (328 ft) spacing along the PCD fence line

In addition, receptors were included at 50 m (164 ft) spacing within and along the PCAPP and EDS boundaries. Figure 3-6 presents the layout of the on-site receptor grid.

3.2.3.3 Terrain Data

Accuracy of receptor location elevation data is critical in evaluating the dispersion of a plume. If the terrain data are not accurate, the model may underestimate or overestimate the maximum concentrations and deposition rates. Terrain data used to determine receptor elevations consisted of 1/3 arc-second National Elevation Dataset (NED) data (approximately 10 meters) obtained from the USGS. The AERMOD terrain preprocessor, AERMAP, was used to calculate terrain elevations for each receptor location using the 1/3 arc-second NED data. Grade elevations were obtained from facility design drawings for the PCAPP and EDS emission units and downwash structures and manually entered into the AERMOD input file.

3.2.4 Meteorological Information

AERMOD utilizes two meteorological data files: (1) a file of surface boundary layer parameters, and (2) a file of profile variables including wind speed, wind direction, and turbulence parameters. These two meteorological input files are generated by AERMET. Both of these meteorological input files are sequential ASCII files, and AERMOD automatically recognizes the format generated by AERMET as the default format. AERMOD processes all available meteorological data in the specified input file by default.

A surface meteorological monitoring station (PCD02) has been in operation at the PCD, near the PCAPP location, since December 1997. The station is located in the northern portion of the PCD, approximately 2 km (1.2 miles) west-northwest of the PCAPP and approximately 1.8 km (1.1 miles) north-northwest of the EDS. Figure 1-3, presented previously, shows the relative locations of the PCD02 station, PCAPP and EDS sites. The PCD02 site coordinates are:

- latitude: 38° 21’ 21.6” N
- longitude: 104° 19’ 50.9” W
- elevation: 1,440 m above mean sea level

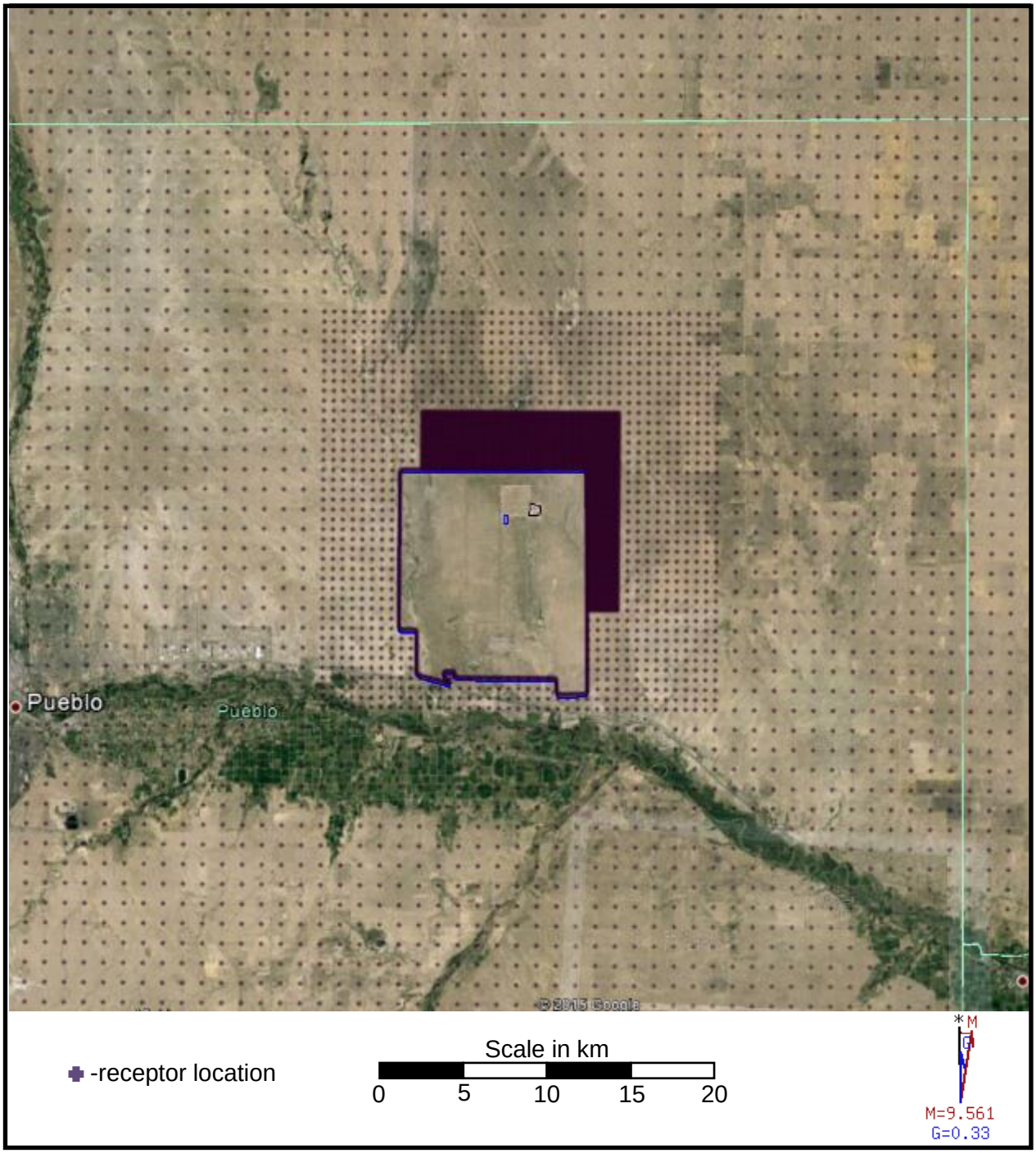

Figure 3-4. Tiered off-site receptor grid layout.

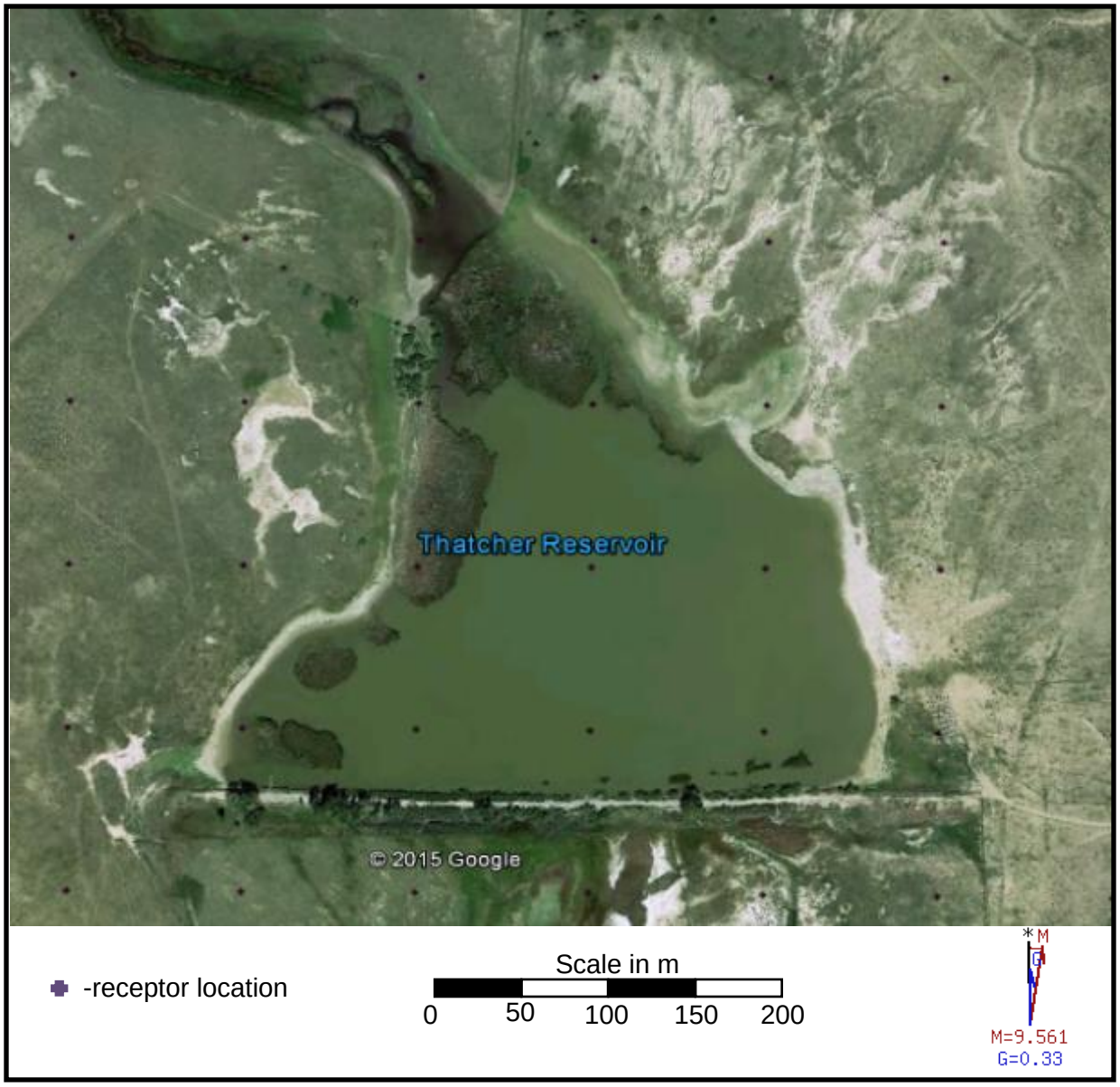

Figure 3-5. Water body receptor locations.

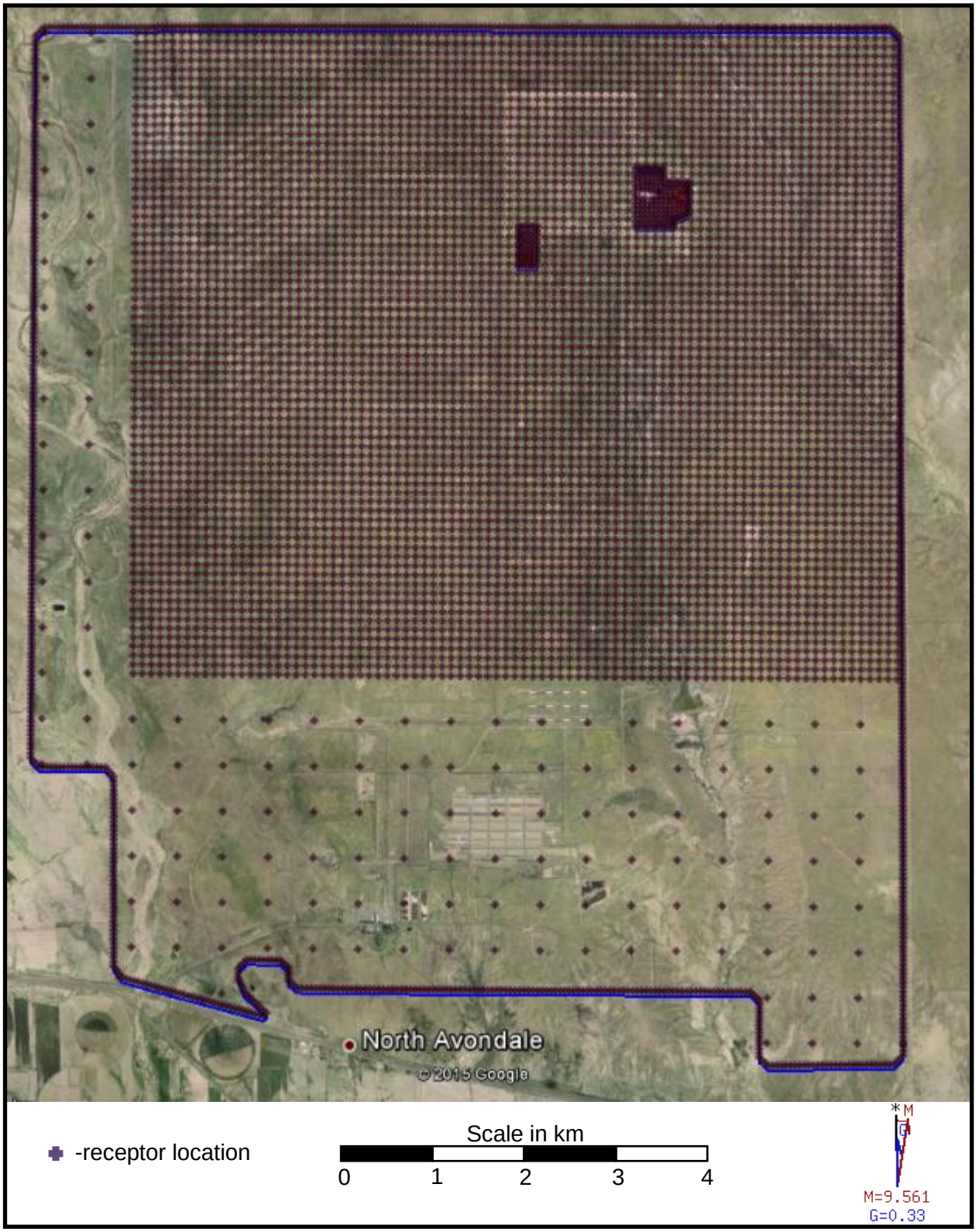

Figure 3-6. On-site receptor grid.

No significant terrain variations exist within 100 m (328 ft) of PCD02 or obstructions greater than 7 m (23 ft) within 500 m (1,640 ft) of PCD02. Multiple other meteorological towers are sited around PCD. The meteorological data from the PCD02 meteorological tower are most representative because it most accurately characterizes the transport and dispersion of pollutants from the PCAPP and EDS sources to the areas where the maximum concentrations are anticipated to occur.

Upper air data are needed to determine the mixing height for use in the air dispersion model. Upper air data are available from Fort Carson and Denver, Colorado, and from Dodge City, Kansas. Upper air data collected from the Denver station (Station 23062) are considered the most representative of the conditions around the PCD due to the impact of the mountains. Therefore, upper air data collected from the Denver station were used by CDPHE (see subsection 3.2.4.1) to generate the meteorological data input file.

Prior to about 2001, the meteorological data collected from the on-site station did not include the precipitation and relative humidity data required for the wet deposition algorithm in AERMOD. Therefore, the National Weather Service surface data collected at the Pueblo Memorial Airport station (Station 72464) were used to supplement the on-site station data for these impacts. The 2008 to 2010 on-site meteorological station, however, did provide the necessary precipitation and relative humidity data, and use of airport data was unnecessary. The Pueblo Memorial Airport is located within 16 km (10 miles) of PCD. Figure 1-2, presented previously, shows the location of the airport. Given the proximity of the airport to PCD, the airport precipitation and relative humidity data are representative of PCAPP and EDS site conditions and can be used to supplement the earlier data.

3.2.4.1 Meteorological Data Preprocessor

CDPHE operated AERMET to process the meteorological data into a format compatible with AERMOD. CDPHE used 6 years of meteorological data comprised of a composite of the 1998 to 2000 meteorological data set applied in the 2008 MPHRA and a more recent 2008 to 2010 meteorological data set produced by PCD02. As for the earlier data set, the 2008 to 2010 raw data from the PCD02 tower were provided to CDPHE, who performed QA on the data set and made adjustments, consistent with CDPHE practices. CDPHE then used AERMET to process the three types of data (i.e., the on-site PCD02 surface data, the Pueblo Airport precipitation data, and Denver upper air data) and produce the surface (.sfc) and profile (.pfl) files needed for input to AERMOD for 1998 to 2000 and 2008 to 2010 data sets.

Appendix C provides information pertaining to this process. Figure 3-7 presents a windrose of the 6 years of AERMET-processed surface meteorological data.

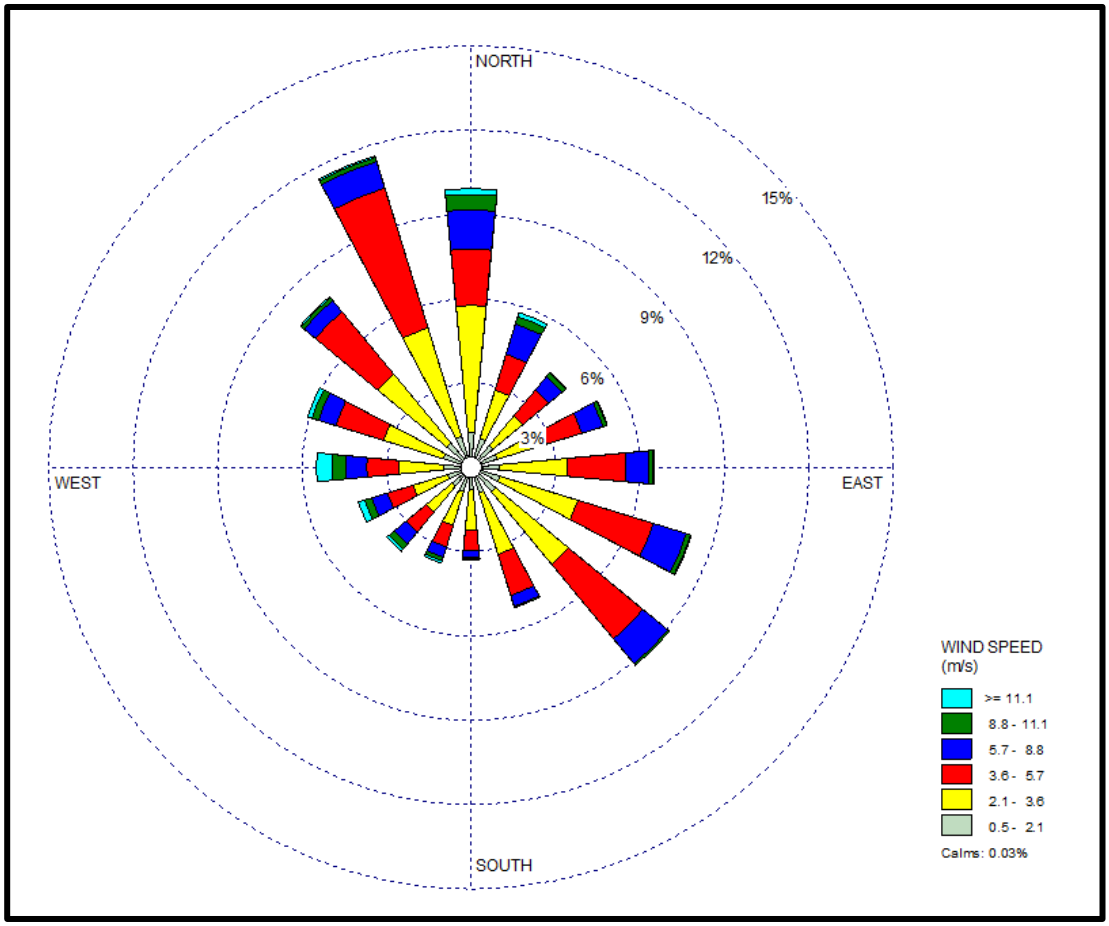

Figure 3-7. Windrose of 6 years of AERMET-processed surface meteorological data.

3.2.5 Output Options

AERMOD provides a number of optional output file formats. The “plot file” format is the most useful optional output for facilitating post-processing of the air parameter values in the model output. The plot file output option allows the user to select the source groups and averaging periods for which a plot file will be generated. The plot file format lists the x and y coordinates for each modeled receptor and the corresponding maximum unit response concentration and deposition values for each source group and averaging period selected. The plot file data are provided in a format that can easily be imported into a post-processing program (e.g., spreadsheet).

The output options selected for the MPHRA included plot files for annual and 1-hour averaging periods for each of the seven source groups. The annual plot files for each source group were used in a post-processing step to generate the maximum COPC-specific annual concentrations and deposition rates for the chronic risk assessment. The 1-hour plot files for each source group were used in a post-processing step to generate the maximum COPC-specific 1-hour air concentrations for the acute risk assessment.

3.3 POST-PROCESSING AERMOD RESULTS

AERMOD provides a plot file for each modeled source group that includes unit response concentrations and deposition rates from the 6-year meteorological period for each modeled receptor. The maximum unit response concentrations and wet and dry deposition rates for the various source groups occur at different receptor locations due, in part, to the following:

- Different effective plume heights, due to stack heights and stack gas flow rates and temperatures, for the various modeled sources and the subsequent downwind distance to plume centerline ground-level impacts.

- Differing receptor location elevations within the receptor grid in relation to the stack base elevations and the subsequent effect upon the distance between the plume centerline and each receptor location.

- The effect of precipitation on the source plumes. Precipitation tends to wash chemicals out of the plumes; therefore, the location of the maximum wet deposition rate will be closer to the source than the maximum dry deposition rate. The dry deposition rate is not affected by precipitation, but instead by plume interaction with terrain features.

The COPC-specific emission rates also vary for each emission source. Therefore, due to the combination of the varying unit response concentrations and deposition rates at each receptor for the various modeled source groups and the varying COPC emission rates for each emission source, a spreadsheet-based model output post-processor program was developed to determine the maximum total COPC-specific concentrations and deposition rates. The AERMOD output post-processor program combined the COPC-specific concentrations and deposition rates for all seven modeled source groups at each receptor location. Because only one EDS unit will operate at a time, the AERMOD output post-processor was programmed to select the EDS source group that resulted in largest COPC-specific concentration and deposition rates at each receptor and add those results to the concentration and deposition rates obtained for PCAPP source groups at those receptors. The combined results at each receptor location were then evaluated to determine the maximum cumulative COPC-specific concentrations and deposition rates from all modeled receptors (i.e., the RME location).
As a very conservative approach, the maximum total COPC-specific air concentrations and deposition rates were used to calculate exposure to the RME individual, even though the maximum air concentration, dry deposition rate, and wet deposition rate locations vary for each COPC. Thus, the different receptor locations positioned hundreds of meters away from each other were used to evaluate a single RME individual location.