



PM_{2.5} SIP

Appendix F

Modeling Protocols

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Appendix F.1

WRF Modeling Protocol

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Date

March 2016 (Rev. 1/18)

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Project Number:

06-35892A

ALLEGHENY COUNTY HEALTH DEPARTMENT

PM_{2.5} STATE IMPLEMENTATION PLAN

FOR THE 2012 NAAQS

WRF MODELING PROTOCOL

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Acronyms and Abbreviations

ACHD	Allegheny County Health Department
ASTER	Advanced Space-borne Thermal Emission and Reflection Radiometer
CFL	Courant-Friedrichs-Lewy
ERA	European Center for Medium-Range Weather Forecasting Re-Analysis
ESRL	Earth Systems Research Laboratory
FDDA	Four Dimensional Data Assimilation
ISHO	Integrated Surface Hourly Observations
KPIT	Surface and upper-air identifier for Pittsburgh Airport
LCC	Lambert Conformal Conic map projection
LSM	Land-Surface Model
LST	Local Standard Time
MADIS	Meteorological Assimilation Data Ingest System observation archive
MARAMA	Mid-Atlantic Regional Air Management Association
METSTAT	Meteorological Statistical Program
NAAQS	National Ambient Air Quality Standards
NCAR	National Center for Atmospheric Research
NCEP	National Center for Environmental Prediction
NCDC	National Climatic Data Center
NOAA	National Oceanographic and Atmospheric Administration
NOHRSC	National Operational Hydrologic Remote Sensing Center
NWS	National Weather Service
PBL	Planetary Boundary Layer
PRISM	Parameter-elevation Regressions on Independent Slopes Model
RMSE	Root Mean Square Error
RTG	Real-Time Global
SCAS-OSU	Spatial Climate Analysis Service at Oregon State University
SIP	State Implementation Plan
SNODAS	Snow Data Assimilation System
SST	Sea Surface Temperature
RPO	Regional Planning Organization
UTC	Coordinated Universal Time
WPS	WRF Pre-processing System
WRAP	Western Regional Air Partnership
WRF	Weather Research and Forecasting model

1. INTRODUCTION

Ramboll Environ US Corporation (Ramboll Environ) is performing the air quality modeling necessary to demonstrate attainment of the 2012 fine particulate matter (PM_{2.5}) National Ambient Air Quality Standards (NAAQS) within the Allegheny County, PA nonattainment area. It has been demonstrated that the PM_{2.5} air quality problem at the South Allegheny Middle/High School (Liberty) monitoring site is due to a combination of regional and local emission sources. The air quality modeling approach will account for the influences of long-range transport of PM_{2.5} (and precursors) into the region, as well as resolve local source impacts at the Liberty monitoring site.

Air quality modeling requires various input datasets, including emissions sources, meteorology, and pre-existing pollutant concentrations. The accuracy of the modeling predictions depends on several factors, including the accuracy of emissions and the representativeness of the meteorological dataset. The air quality impact analysis is only as comprehensive as the emission inventory on which the analysis is based, and only as accurate as the meteorological dataset applied to disperse and transport the pollutants. Ramboll Environ will be conducting the meteorological modeling to provide meteorological fields for use in air dispersion modeling within the PM_{2.5} nonattainment area of Allegheny County, PA. This meteorological modeling protocol details the methodology and application of the Weather Research and Forecasting (WRF) meteorological model for this Study.

1.1 Background

In 1997, the Environmental Protection Agency (EPA) promulgated annual and 24-hour PM_{2.5} NAAQS with thresholds of 15 and 65 µg/m³, respectively. The form of the annual PM_{2.5} NAAQS is the 3-year average of the annual PM_{2.5} concentrations. The form of the 24-hour PM_{2.5} NAAQS is the three year average of the 98th percentile 24-hour PM_{2.5} concentration in a year.

In December 2006, EPA lowered the 24-hour PM_{2.5} NAAQS from 65 to 35 µg/m³ and kept the annual PM_{2.5} NAAQS at 15 µg/m³. On December 14, 2012, EPA further lowered the annual PM_{2.5} NAAQS to 12 µg/m³.

The PM_{2.5} attainment demonstration SIPs for the 2012 annual PM_{2.5} NAAQS are due by October 2016, this includes a demonstration of attainment of the PM_{2.5} NAAQS at the Liberty Borough monitoring site.

1.2 Overview of PM_{2.5} Air Quality in Allegheny County

Allegheny County was designated nonattainment for 2006 24-hour PM_{2.5} as part of the multi-county Pittsburgh-Beaver Valley Area based on 2001-2003 monitored data.

The entirety of Allegheny County was designated nonattainment for 2012 annual PM_{2.5} based on 2011-2013 monitored data.

Table 1 displays the annual and 24-hour PM_{2.5} Design Values for monitoring sites in Allegheny County for the three most recent three-year periods (2011-2013, 2012-2014, 2013-2015). Figure 1 displays the locations of the monitoring sites in Allegheny County. PM_{2.5} concentrations have been on a downward trend at all monitoring sites in Allegheny County. The annual PM_{2.5} Design Values at 4 of the 9 monitoring sites violated the NAAQS based on 2003-2005 observations, however using the latest three years of monitoring data, only the Liberty monitor still exceeds the annual PM_{2.5} NAAQS (12.0 µg/m³) with a 2013-2015 Design Value that is 0.6 µg/m³ above the NAAQS. Similar downward trends are seen in 24-hour PM_{2.5} Design Values so that by 2013-2015, the Liberty monitor attains the 24-hour PM_{2.5} NAAQS (35 µg/m³) with a 24-hour PM_{2.5} Design Value of 33 µg/m³.

Annual CAMx photochemical grid model simulations will be conducted using grid resolutions of 36/12/4/1.333/0.444 km for the base year of 2011. As was done in the Allegheny County 24-hour PM_{2.5} modeling, the subgrid-scale PiG puffs will be sampled at and near key locations (e.g., Liberty) and added to the CAMx grid model predictions. Should the performance of the PiG approach prove to be inadequate, a hybrid approach may be used with CAMx supplying the background concentrations and AERMOD supplying the contribution of the closest sources to the Liberty Monitor.

Table 1. Latest annual and 24-hour PM_{2.5} Design Values for monitoring sites in Allegheny County

Monitoring Site	Annual PM _{2.5} Design Values			24-Hour PM _{2.5} Design Values		
	2011-2013	2012-2014	2013-2015	2011-2013	2012-2014	2013-2015
Avalon	11.4	10.6	10.6	25	22	23
Lawrenceville	10.3	10.0	9.8	23	21	21
Liberty	13.4	13.0	12.6	37	35	33
South Fayette	9.6	9.0	8.8	24	20	21
North Park	8.8	8.5	8.5	19	17	18
Harrison	10.6	10.0	9.8	25	22	22
North Braddock	11.7	11.4	11.2	29	26	25
Clairton	9.8	9.5	9.9	22	23	25

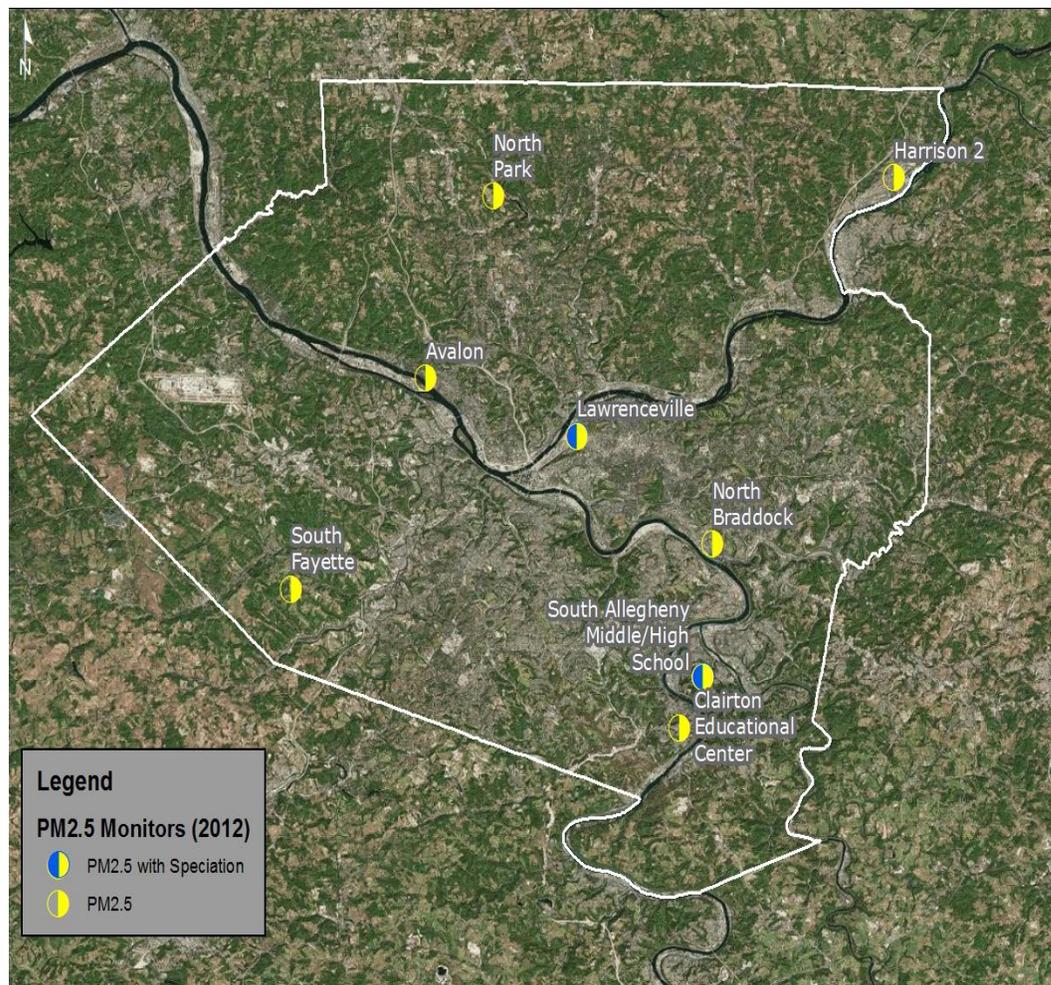


Figure 1. Locations of PM_{2.5} monitoring sites within Allegheny County.

1.3 Objectives of Meteorological Modeling in Allegheny County

Meteorological information is needed for air quality dispersion modeling. Parameters such as wind speed, wind direction, air temperature, and humidity are required by models to determine the rate that pollutants disperse and react in the atmosphere. Meteorological measurements are gathered at various locations within Allegheny County, however the spatial coverage of the measurements is insufficient to describe the three-dimensional structure of the atmosphere away from measurement locations. Using measurement data as inputs, gridded meteorological models are able to estimate meteorological conditions in regions far from measurement sites. The results of these models are often used to establish conditions near remote pollutant sources or remote locations downwind of pollutant sources. As discussed in the following section, within the domain of Allegheny County, the WRF meteorological model has been determined to produce appropriate representative meteorological conditions and will be used to provide meteorological inputs for the air quality modeling.

The existing 1.333 km WRF domain from the ongoing SO₂ SIP modeling does not fully cover the Allegheny County PM_{2.5} nonattainment area. It was determined that a new meteorological dataset with an updated domain would be needed to more accurately represent the meteorological conditions within the nonattainment area.

2. MODEL SELECTION

The development of a WRF dataset to accurately represent meteorological conditions over the PM_{2.5} SIP study area in a high resolution domain is necessary for air quality modeling. Optimizing WRF performance for the study area will be based on various WRF modeling techniques. Some aspects of the model configuration can be recommended based on recognition of the state-of-the-art procedures of WRF modeling. This includes aspects concerning the numerical solver settings and selected physical models. The Rapid Radiative Transfer Model - Global (RRTMG) radiation models, Thompson microphysics model, and Noah Land Surface Model (LSM) represent the state-of-the-art models for general WRF modeling in the mid-latitudes. The Advanced Research WRF (ARW) core, currently version WRF 3.7.1, is supported by the National Center for Atmospheric Research (NCAR) Mesoscale and Microscale Meteorology Division (NCAR, 2015) and will be used to develop the meteorological dataset.

This section discusses the methodologies to be used to select the WRF meteorological model for Allegheny County. The WRF model is the current preferred model for atmospheric research and operational forecasting needs at mesoscale resolution (approximately 5 to several hundred km). The model is the state-of-the-art atmospheric simulation system commonly used to drive air quality dispersion models on the regional level.

2.1 Overview of Selected Meteorological Model

Over the past decade, emergent requirements for numerical simulation of urban and regional scale air quality have led to intensified efforts to construct high-resolution emissions, meteorological, and air quality data sets. It is now possible, for example, to exercise sophisticated mesoscale prognostic meteorological models and Eulerian and Lagrangian photochemical/aerosol models, for multi-seasonal periods over near-continental scale domains, in a matter of weeks with the application tailored to a specific air quality modeling project.

The WRF model contains separate modules to compute different physical processes, such as surface energy budgets and soil interactions, turbulence, cloud microphysics, and atmospheric radiation. Within WRF, the user has many options for selecting the different schemes for each type of physical process. The WRF Pre-processing System (WPS)

generates the initial and boundary conditions used by WRF, based on topographic datasets, land use information, and larger-scale atmospheric and oceanic models.

2.2 Description of WRF

WRF was selected for high resolution meteorological modeling of the region for the period of January 1st through December 31st, 2011. WRF's research and operational application ensures state-of-the-science physics and adaptability to a wide range of environments, through a broad selection of physics options, allowing us to develop the best-performing configuration for simulating meteorology in the region.

The non-hydrostatic version of the Advanced Research version of the Weather Research and Forecast (WRF-ARW) model (Skamarock et al., 2008) is a three-dimensional, limited-area, primitive equation, prognostic model that has been used widely in regional air quality model applications. The basic model has been under continuous development, improvement, testing and open peer review for more than 10 years. It has been used worldwide by hundreds of scientists for a variety of mesoscale studies, including cyclogenesis, polar lows, cold-air damming, coastal fronts, severe thunderstorms, tropical storms, subtropical easterly jets, mesoscale convective complexes, desert mixed layers, urban-scale modeling, air quality studies, frontal weather, lake-effect snows, sea breezes, orographically induced flows, and operational mesoscale forecasting. WRF is a next-generation mesoscale prognostic meteorological model routinely used in urban- and regional-scale photochemical, fine particulate and regional haze regulatory modeling studies. Developed jointly by the National Center for Atmospheric Research (NCAR) and NCEP, WRF is maintained and supported as a community model by researchers and practitioners around the globe. The code supports two modes: the Advanced Research WRF (ARW) version and the Non-hydrostatic Mesoscale Model (NMM) version. WRF-ARW has become the new standard model used in place of the older Mesoscale Meteorological Model (MM5) for regulatory air quality applications in the U.S. It is suitable for use in a broad spectrum of applications across scales ranging from hundreds of meters to thousands of kilometers.

3. METEOROLOGICAL MODELING

This section describes the methodology which will be used for conducting the WRF simulation for the January to December 2011 modeling period, and describes the model configuration used in the WRF meteorological dataset for the ACHD PM_{2.5} air dispersion modeling.

3.1 Model Domain Configuration

The WRF Domain configuration will be comprised of a system of simultaneous nested grids. Figure 2 shows the WRF modeling grids at 36/12/4/1.333/0.444 km. All WRF grids will be defined on a Lambert Conformal Conic (LCC) projection centered at 40°N, 97°W with true latitudes at 33°N and 45°N (the so-called standard Regional Planning Organization (RPO) projection). The outermost domain with 36 km resolution will include the entire continental United States and parts of Canada and Mexico. The inner 12 km regional grid will cover nearly all of the eastern United States and portions of Quebec and Ontario Canadian Provinces, and is identical to the Mid-Atlantic Regional Air Management Association (MARAMA) grid. The 4 km domain will cover all of Pennsylvania and portions of surrounding states. Figure 3 shows the 1.333 km domain with grid cells, covering Allegheny County. Figure 4 shows the 444 m domain, the region close to the Liberty and North Braddock monitors. The blue lines in Figure 3 and Figure 4 represent the usable area of the WRF domain, or where the anomalous edge effects resulting from the boundary conditions of the parent domain no longer influence the inner domain (approximately 5 grid cells). Table 2 provides the domain specifications used in the modeling study.

Table 2. WRF Domain Specifications

Grid Spacing (km)	Number of Points (West-East)	Number of Points (South-North)	Starting Point (West-East)	Starting Point (South-North)
36	165	129	-	-
12	187	187	88	38
4	217	160	76	72
1.333	70	70	74	66
0.444	31	46	43	19

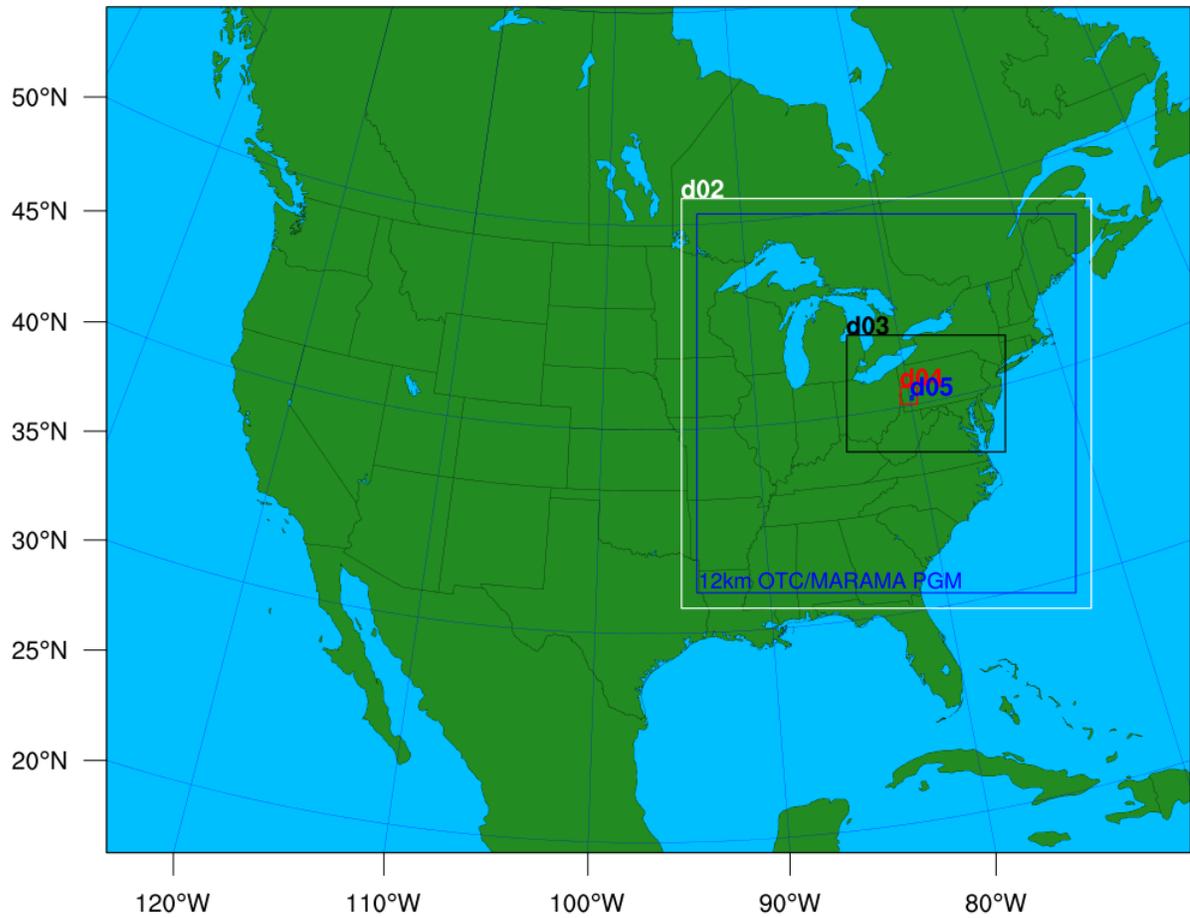


Figure 2. ACHD WRF (36/12/4/1.333/0.444 km) Modeling Domains.

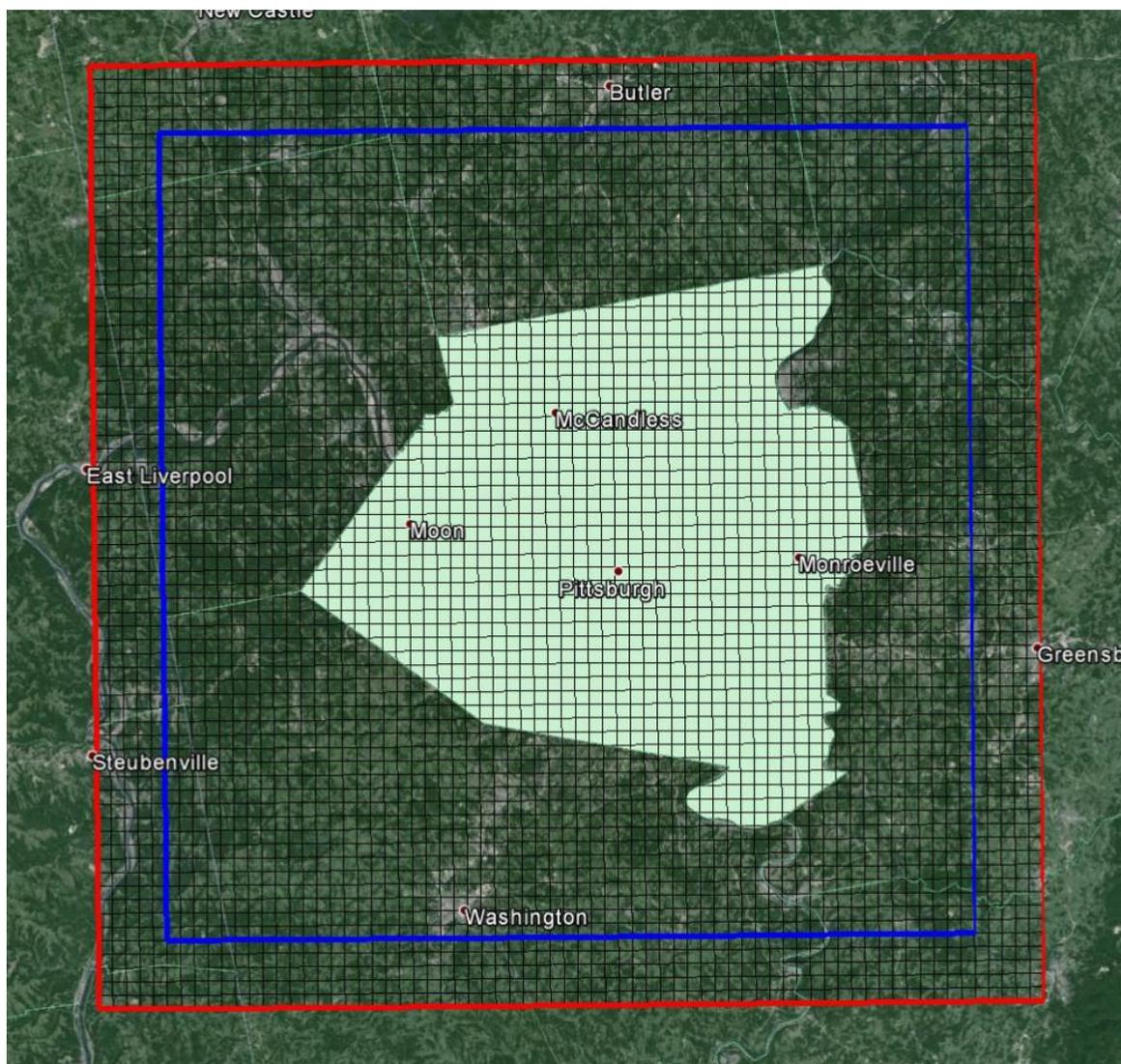


Figure 3. WRF grid d04 (1.333 km, outer red rectangle) covering Allegheny County nonattainment area. Blue rectangle show usable area of 1.333 km domain.

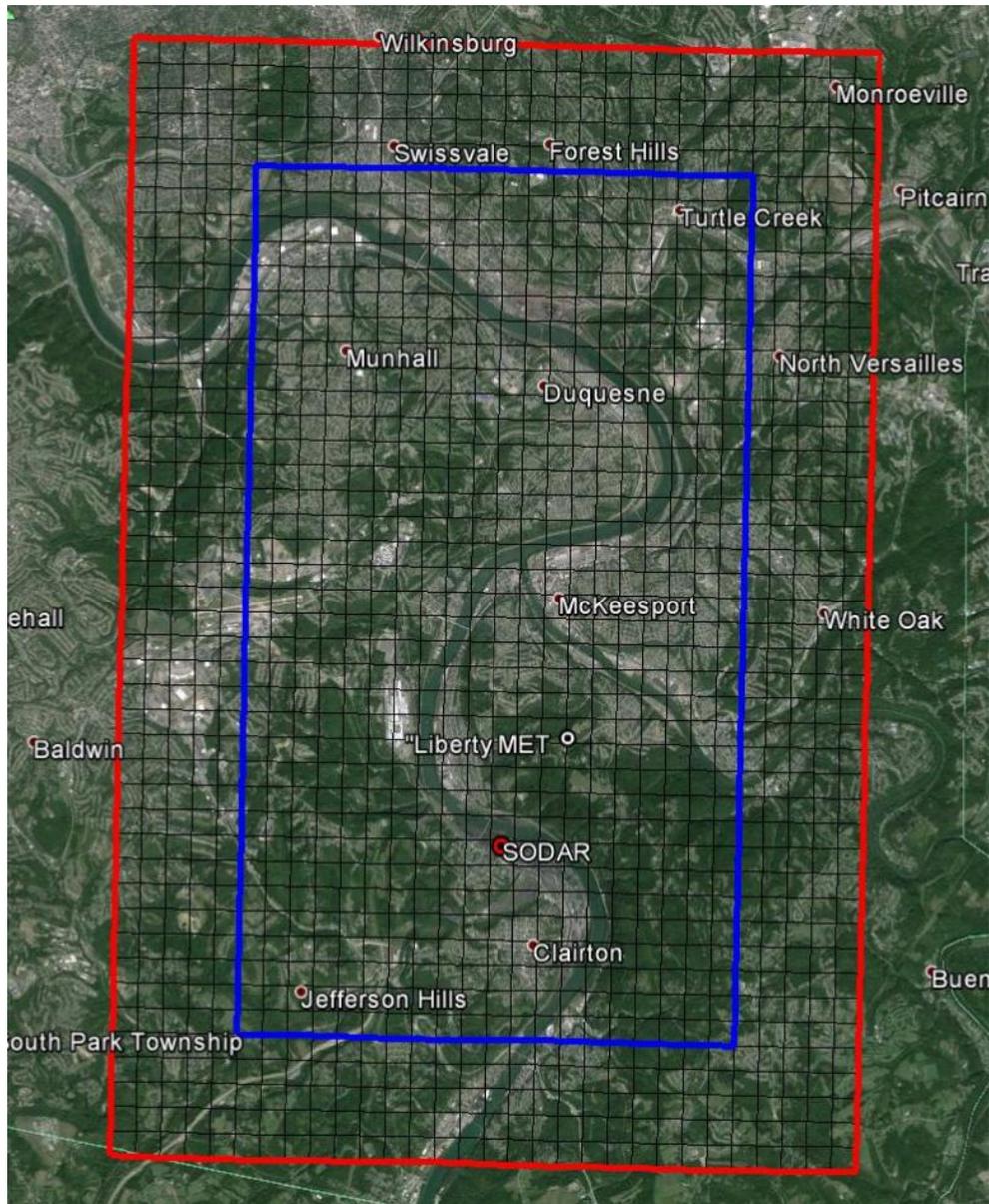


Figure 4. WRF grid d05 (0.444 km, outer red rectangle) covering the southeast portion of the Allegheny County nonattainment area. Blue rectangles show usable area of 0.444 km domain.

3.2 Model Application

A brief summary of the WRF configuration and input data Ramboll Environ will be using for this meteorological modeling is provided below. The WRF model configuration will be based on the most recent ACHD SO₂ SIP WRF modeling dataset with updated options. The updated configuration will account for the latest model version and lessons learned in more recent WRF datasets, in order to improve performance of temperature, moisture, and precipitation fields in this demonstration.

3.2.1 Model Vertical Resolution

The WRF modeling will employ high vertical resolutions from the surface to the 100 mb pressure level. High vertical resolution enables the model to more accurately capture the convective updraft velocities in summer and low level temperature inversions frequently present during winter. The ACHD WRF modeling will use 37 vertical layers with an approximately 11 meter thick lowest layer. Table 3 gives the vertical layer structure to be used in this modeling project.

Table 3. ACHD WRF Dataset Model Levels

Level	Eta	Pressure (mb)	Height (m)	ΔZ (m)
1	1.0000	1013	0.0	
2	0.9985	1012	11.2	11.2
3	0.9970	1010	22.4	11.2
4	0.9955	1009	33.7	11.2
5	0.9940	1008	44.9	11.2
6	0.9925	1006	56.1	11.3
7	0.9910	1005	67.4	11.3
8	0.9895	1003	78.7	11.3
9	0.9870	1001	97.5	18.8
10	0.9845	999	116.4	18.9
11	0.9820	997	135.3	18.9
12	0.9795	994	154.2	18.9
13	0.9770	992	173.2	19.0
14	0.9745	990	192.2	19.0
15	0.9720	987	211.2	19.0
16	0.9690	985	234.1	22.9
17	0.9660	982	257.1	22.9
18	0.9610	977	295.4	38.4
19	0.9510	968	372.6	77.1
20	0.9360	955	489.4	116.8
21	0.9210	941	607.6	118.2
22	0.9010	923	767.4	159.8
23	0.8810	904	929.7	162.4
24	0.8600	885	1103.1	173.4
25	0.8200	849	1441.9	338.8
26	0.7600	794	1973.0	531.1
27	0.7000	739	2534.6	561.6
28	0.6000	648	3550.4	1015.8
29	0.5000	557	4689.7	1139.3
30	0.4000	465	5991.9	1302.2
31	0.3000	374	7520.7	1528.8
32	0.2200	301	8979.7	1459.0
33	0.1500	237	10514.7	1535.0
34	0.1000	191	11832.4	1317.6
35	0.0600	155	13084.9	1252.5
36	0.0270	125	14313.8	1228.9
37	0.0000	100	15513.7	1199.9

3.2.2 Topographic Inputs

Topographic information for the WRF will be developed using a combination of the standard WRF terrain databases and high-resolution terrain. The 36 km domain will be based on the 10 minute global data; the 12 km domain will be based on the 2 minute data; the 4 and 1.333 km domain will be based on the 30 second data, and the 0.444 km will be based on the high-resolution Advanced Space-borne Thermal Emission and Reflection Radiometer (ASTER) Global Digital Elevation Model (DEM) 1 arc second ~ 90 meter data.

3.2.3 Vegetation Type and Land Use Inputs

Vegetation type and land use information will be developed using the United States Geological Survey (USGS) land use databases from the most recently released WRF databases provided with the WRF distribution. Standard WRF surface characteristics corresponding to each land use category will be employed.

3.2.4 Atmospheric Data Inputs

WRF relies on other model or re-analysis output to provide initial and boundary conditions (IC/BC). The first guess fields will be taken from the ~70 km European Center for Medium-Range Weather Forecasting Re-Analysis (ERA)-Interim dataset. These will be objectively re-analyzed using traditional observational data (meteorological towers) to the higher resolution of each WRF grid, using the OBSGRID program. These fields are used both to initialize the model, and used with analysis nudging (on selected domains) to guide the model to best match the observations.

3.2.5 Time Integration

Third-order Runge-Kutta integration will be used (`rk_ord = 3`). The maximum time step, defined for the outer-most domain (36 km) only, should be set by evaluating the following equation:

$$dt = \frac{6dx}{F_{map}}$$

Where dx is the grid cell size in km, F_{map} is the maximum map factor (which can be found in the output from REAL.EXE), and dt is the resulting time-step in seconds. For the case of the 36 km RPO domain, $dx = 36$ and $F_{map} = 1.08$, so dt should be taken to be less than 200 seconds. Longer time steps risk Courant-Friedrichs-Lewy (CFL) condition errors, associated with large values of vertical velocity, which tend to occur in areas of steep terrain (especially during stable conditions typical of winter).

3.2.6 Diffusion Options

Horizontal Smagorinsky first-order closure (`km_opt=4`) with sixth-order numerical diffusion and suppressed up-gradient diffusion (`diff_6th_opt=2`) will be used.

3.2.7 Lateral Boundary Conditions

Lateral boundary conditions will be specified from the initialization dataset on the 36 km CONUS domain with continuous updates nested from each "parent" domain to its "child" domain, using one-way nesting (`feedback=0`).

3.2.8 Top and Bottom Boundary Conditions

The top boundary condition will be selected as an implicit Rayleigh dampening for the vertical velocity. Consistent with the model application for non-idealized cases, the bottom boundary condition will be selected as physical, not free-slip.

3.2.9 Water Temperature Inputs

The water temperature data will be taken from the NCEP RTG daily global one-twelfth degree analysis, and will be updated every 24 hours (as opposed to fixed for each WRF initialization).

3.2.10 Snow Cover

The model runs will use the 1 km resolution snow data from the SNOW Data Assimilation System (SNODAS). SNODAS is a modeling and data assimilation system developed by the NOAA National Weather Service's National Operational Hydrologic Remote Sensing Center (NOHRSC) to provide the best possible estimates of snow cover and associated variables to support hydrologic modeling and analysis. SNODAS includes procedures to ingest and

downscale output from Numerical Weather Prediction (NWP) models and to simulate snow cover using a physically based, spatially-distributed energy and mass-balance snow model (NOHRSC, 2004). This is the finest-resolution dataset that Ramboll Environ is aware of, even though it is roughly twice the resolution of the 444 m finest grid.

3.2.11 FDDA Data Assimilation

WRF was created as a forecast tool, but can also be applied in “hindcast” mode. In forecast mode, the initial conditions for a run might be the most recent analysis (a gridded version of the current state of the atmosphere). In hindcast mode, we know the state of the atmosphere both at the beginning *and end* of (and during) the WRF run. Using these 6-hourly analyses, an extra error term is introduced into the WRF equations, nudging the WRF atmosphere toward the real atmosphere. This is known as Four Dimensional Data Assimilation (FDDA) or analysis nudging, and is applied to every grid cell in the domain. It works best at larger grid spacing scales and for larger domains.

Observational nudging is the process of nudging just the single grid cell toward a single-point observation. The observation could be taken at a traditional meteorological tower, or by a weather balloon, or other non-traditional sources. OBS nudging works best at finer grid spacing scales.

The WRF model will be run with a combination of analysis and observation nudging. Analysis nudging will be used for winds, temperature, and humidity on the 36 km and 12 km domains. The nudging will use both surface and aloft nudging, but nudging for temperature and mixing ratio will not be performed in the lower atmosphere (i.e., within the boundary layer) due in part because nudging temperature and moisture at the surface may have detrimental effects on finer scale structures. The WRF simulation will use observation nudging within the 4 km and 1.333 km domains for winds, temperature, and humidity. Observation nudging will be performed using the Meteorological Assimilation Data Ingest System (MADIS, 2015) observation archive. The observations taken at South Allegheny Middle/High School, along with the county airport, will be used to nudge the 444m domain.

3.2.12 Physics Options

The WRF model contains many different physics options. Table 4 lists the recommended WRF physics options chosen for the WRF configuration. Sensitivity tests for the months of January 2011 and July 2011 will be performed to test additional cumulus parameterizations, observational nudging coefficients, planetary boundary layer schemes, and land surface models to see whether improved WRF performance can be achieved.

Table 4. Physics Options used in the ACHD WRF Dataset

Physics	Parameterization Scheme	Description
Longwave/Shortwave Radiation	Rapid Radiative Transfer Model for GCM (RRTMG)	Scheme with the MCICA method of random cloud overlap
Microphysics	Thompson	Scheme with ice, snow, and graupel processes suitable for high resolution simulations
Cumulus	Multi-scale Kain-Fritsch	Uses scale-dependent dynamic adjustment timescale, LCC-based entrainment. Also uses new trigger function based on Bechtold
Planetary Boundary Layer (PBL)	YSU	Non-local-K scheme with explicit entrainment layer and parabolic K profile in unstable mixed layer

Land Surface Model (LSM)	Noah	Scheme with soil temperature and moisture in four layers, fractional snow cover and frozen soil physics
Surface Layer	Monin-Obukhov	Based on Monin-Obukhov with Zilitinkevich thermal roughness length and standard similarity functions

3.2.13 Application Methodology

The WRF model will be executed in 5.5-day blocks initialized at 12Z every five days. Model results will be output every 60 minutes and output files will be split at twelve (12) hour intervals. Twelve (12) hours of spin-up will be included in each 5-day block before the data will be used in the subsequent evaluation. The model will be run at the 36, 12, 4, 1.333, and 0.444 km resolution from January 2011 through December 2011.

4. METEOROLOGICAL MODEL PERFORMANCE EVALUATION

Both a quantitative and qualitative evaluation of the ACHD WRF simulation will be conducted. The quantitative evaluation will compare both integrated surface hourly and on-site meteorological observations with WRF predictions matched by time and location. The qualitative evaluation will compare twice daily vertical profiles with upper-air data with WRF predictions also matched by time and location. Additionally, monthly total spatial precipitation fields based on observations (PRISM data) will be compared with the WRF gridded monthly total precipitation fields. Below we summarize the main features of the WRF simulation model performance evaluation.

4.1 Quantitative Evaluation Using METSTAT

A quantitative model performance evaluation of the ACHD WRF simulation will be performed using the publicly-available METSTAT software (Ramboll Environ, 2015) evaluation tool. Output from meteorological models will be compared against meteorological observations from the various networks operating in the study area. This is carried out both graphically and statistically to evaluate model performance for winds, temperatures, humidity, and the placement, intensity, and evolution of key weather phenomena. The purpose of these evaluations is to establish a first-order acceptance/rejection of the simulation in adequately replicating the gross weather phenomena in the study area. Thus, this approach screens for obvious model flaws and errors.

4.1.1 Quantitative Statistics

The quantitative analysis will be conducted using METSTAT. Statistical measures calculated by METSTAT include observation and prediction means, prediction bias, and prediction error that are given as follows.

Mean observation (M_o) is calculated using values from all sites for a given time period by

Eq. (1):

$$M_o = \frac{1}{IJ} \sum_{j=1}^J \sum_{i=1}^I O_j^i \quad (1)$$

where O_j^i is the individual observed quantity at site i and time j , and the summations are over all sites (I) and over time periods (J).

Mean Prediction (M_p) is calculated from simulation results that are interpolated to each observation used to calculate the mean observation for a given time period by Eq. (2):

$$M_p = \frac{1}{IJ} \sum_{j=1}^J \sum_{i=1}^I P_j^i \quad (2)$$

where P_j^i is the individual predicted quantity at site i and time j . Note the predicted mean wind speed and mean resultant direction are derived from the vector-average (for east-west component u and north-south component v), from which the

Bias (B) is calculated as the mean difference in prediction-observation pairings with valid data within a given analysis region and for a given time period by Eq. (3):

$$B = \frac{1}{IJ} \sum_{j=1}^J \sum_{i=1}^I (P_j^i - O_j^i) \quad (3)$$

Gross Error (E) is calculated as the mean *absolute* difference in prediction-observation pairings with valid data within a given analysis region and for a given time period by Eq. (4):

$$E = \frac{1}{IJ} \sum_{j=1}^J \sum_{i=1}^I |P_j^i - O_j^i| \quad (4)$$

Note that the bias and gross error for winds are calculated from the predicted-observed residuals in speed and direction (not from vector components u and v). The direction error for a given prediction-observation pairing is limited to range from 0 to $\pm 180^\circ$.

Root Mean Square Error (RMSE) is calculated as the square root of the mean squared difference in prediction-observation pairings with valid data within a given analysis region and for a given time period by Eq (5):

$$RMSE = \left[\frac{1}{IJ} \sum_{j=1}^J \sum_{i=1}^I (P_j^i - O_j^i)^2 \right]^{\frac{1}{2}} \quad (5)$$

The RMSE, as with the gross error, is a good overall measure of model performance. However, since large errors are weighted heavily (due to squaring), large errors in a small sub-region may produce a large RMSE even though the errors may be small and quite acceptable elsewhere.

4.1.2 METSTAT Processing

METSTAT was developed to calculate and graphically present statistics associated with temporally paired meteorological model predictions and observations. The METSTAT program includes a micro-meteorological module that can scale model mid-layer predicted winds to 10 m heights, and mid-layer predicted temperatures to 2 m heights, using a common stability-dependent non-iterative surface-layer similarity theory algorithm (Louis, 1979). WRF always outputs 10 m winds and 2 m temperatures and absolute humidity, and these are read by METSTAT and used directly without surface-layer scaling.

The horizontal analysis range can be given for an entire output grid, by a coordinate box, or as a list of specific site identifiers (such as WBAN or AIRS numbers), as labeled on the observational file. This allows for an evaluation at a single site, a subset of specific sites or

over an entire regional domain. The program then proceeds to calculate statistics for each hour and for each day of the time window.

The process will involve statistical comparisons of model data from the WRF grid cells to observational measurements located with each grid cell, using METSTAT. METSTAT evaluates wind speed and direction, air temperature, and air humidity using both bias-like and error-like statistics. METSTAT has been widely applied to WRF runs for many years, across many modeling domains. Using a consistent definition of the statistical quantities to be calculated and a consistent methodology for pairing observations in time, METSTAT allows for more straightforward comparisons between model applications in widely different regions and time periods.

4.1.3 Statistical Benchmarks

METSTAT calculates statistical performance metrics for bias, error and correlation for surface winds, temperature, and mixing ratio (i.e., water vapor or humidity). To evaluate the performance of a meteorological model simulation for air quality model applications, a number of performance benchmarks for comparison are typically used. Table 5 lists the meteorological model performance benchmarks for simple (Emery et al., 2001) and complex (Kemball-Cook et al., 2005) situations. The simple benchmarks were developed by analyzing well-performing meteorological model evaluation results for simple, mostly flat terrain conditions and simple meteorological conditions (e.g., stationary high pressure) that were mostly conducted to support air quality modeling studies (e.g., ozone SIP modeling). The complex benchmarks were developed during the Western Regional Air Partnership (WRAP) regional haze modeling and are performance benchmarks for more complex conditions, such as the complex terrain of the Rocky Mountains and Alaska (Kemball-Cook et al., 2005). McNally (2009) analyzed multiple annual runs that included complex terrain conditions and suggested an alternative set of benchmarks for temperature under more complex conditions. The purpose of the benchmarks is to understand how good or poor the results are relative to other model applications run for the United States.

In this section, Ramboll Environ will compare the initial WRF meteorological variables to the benchmarks as an indication of WRF model performance. These benchmarks include bias and error in temperature, wind direction and mixing ratio as well as the wind speed bias and Root Mean Squared Error (RMSE) between the models and databases.

Table 5. Meteorological Model Performance Benchmarks for Simple and Complex Conditions

Parameter	Emery et al. (2001)	Kemball-Cook et al. (2005)	McNally (2009)	Resulting Criteria
Conditions	Simple	Complex	Complex	Complex
Temperature Bias	$\leq \pm 0.5$ K	$\leq \pm 2.0$ K	$\leq \pm 1.0$ K	$\leq \pm 1.0$ K
Temperature Error	≤ 2.0 K	≤ 3.5 K	≤ 3.0 K	≤ 3.0 K
Temperature IOA	≥ 0.8	(not addressed)	(not addressed)	≥ 0.8
Humidity Bias	$\leq \pm 1.0$ g/kg	$\leq \pm 0.8$ g/kg	$\leq \pm 1.0$ g/kg	$\leq \pm 1.0$ g/kg
Humidity Error	≤ 2.0 g/kg	≤ 2.0 g/kg	≤ 2.0 g/kg	≤ 2.0 g/kg
Humidity IOA	≥ 0.6	(not addressed)	(not addressed)	≥ 0.6
Wind Speed Bias	$\leq \pm 0.5$ m/s	$\leq \pm 1.5$ m/s	(not addressed)	$\leq \pm 1.5$ m/s
Wind Speed RMSE	≤ 2.0 m/s	≤ 2.5 m/s	(not addressed)	≤ 2.5 m/s
Wind Speed IOA	≥ 0.6	(not addressed)	(not addressed)	≥ 0.6
Wind Dir. Bias	$\leq \pm 10$ degrees	(not addressed)	(not addressed)	$\leq \pm 10$ degrees
Wind Dir. Error	≤ 30 degrees	≤ 55 degrees	(not addressed)	≤ 55 degrees

The output from the ACHD WRF simulation will be compared against on-site meteorological data obtained from the Liberty monitoring station operated by Allegheny County and the National Climate Data Center's (NCDC) global-scale, quality-controlled DS3505 integrated surface hourly observational (ISHO) data as verification data (NOAA-NCDC, 2015). Global hourly and synoptic observations are compiled from numerous sources into a single common ASCII format and common data model. The DS3505 database contains records of most official surface meteorological stations from airports, military bases, reservoirs/dams, agricultural sites, and other sources dating from 1901 to the present.

A standard set of statistical metrics from the METSTAT package will be used. These metrics will be calculated on hourly, daily and monthly time frames for wind speed, wind direction, temperature, and humidity at the surface, using all available observational weather data. The WRF surface meteorological model performance metrics will be compared against the simple and complex model performance goals using "soccer plots." Soccer plots use two WRF performance metrics as X-axis and Y-axis values (e.g., temperature bias as X, and temperature error as Y) along with the performance benchmarks. The closer the symbols are to the zero origin, the better the model performance. It is also easy to see when the two WRF performance metrics fall within the benchmark lines. We will present monthly surface meteorological model performance across the 36/12/4/1.333/0.444 km domains.

4.2 Qualitative Evaluation Using Upper-Air Data

Upper-air data from the Pittsburgh National Weather Service office radiosonde (KPIT, WBAN 94823) dataset will be used to evaluate WRF vertical profiles of predicted temperature and moisture above that location. This upper-air observation location was selected as the closest sounding site to the Allegheny County PM_{2.5} study area. The KPIT radiosonde dataset is collected and maintained by the National Weather Service (NWS). Radiosondes are launched from KPIT twice per day, at approximately 0 and 12 UTC (7 AM and 7 PM LST). Radiosondes provide high-resolution vertical profiles of temperature, humidity, wind speed, and wind direction throughout the troposphere. The data are made publicly available by NOAA on the Earth System Research Laboratory (ESRL) Radiosonde Observation website (www.esrl.noaa.gov/raobs). Ramboll Environ downloaded and stored the radiosonde data from 2011 in FSL format for use in WRF model dataset comparisons.

The advantages of traditional radiosonde datasets are the length of the dataset and that they are direct measurements, as opposed to remote sensing. Disadvantages include the low frequency at only twice per day, and that the lowest reported level comes from a different sensor than the rest of the profile and may lead to unrealistic profiles. For the performance evaluation, vertical profile plots will show WRF modeled data from the 1.333 km domain and observed upper-air soundings in order to evaluate the performance of the vertical atmospheric structure.

4.3 Qualitative Evaluation of Precipitation

Precipitation removes chemicals and particulates from the air via wet deposition, and so is an important parameter for high-quality dispersion modeling. A qualitative comparison of WRF-simulation estimated monthly precipitation with monthly analysis fields based on observations will be shown to evaluate the amount and spatial extent of rainfall throughout the 36/12/4/1.333/0.444 km domains.

High-resolution (4 km) Parameter-elevation Regressions on Independent Slopes Model (PRISM) datasets cover the contiguous US in both monthly and daily output versions (Daly et al., 2008). The PRISM datasets are spatial maps of climate elements across the United States built by the Spatial Climate Analysis Service at Oregon State University (SCAS-OSU). Gridded maps of mean monthly and annual precipitation and temperature were built using meteorological station measurements and a set of statistical weighting procedures and corrections based on distance, elevation, topographic orientations and influences, and land-surface type (SCAS-OSU, 2001). The process and results have been extensively peer-

reviewed and generally accepted by the climatological community as state-of-the-art representations.

5. RECOMMENDATIONS

The meteorological modeling protocol will result in a recommended configuration for a WRF model simulation for January 2011 through December 2011 for the annual PM_{2.5} nonattainment portion of Allegheny County.

Along with the protocol documentation, the recommended meteorological model will be produced in formats usable by air dispersion and chemical transport models.

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Appendix F.2

CAMx Modeling Protocol

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July, 2017 (Rev. 1/18)

Project Number:
06-35842A

ALLEGHENY COUNTY HEALTH DEPARTMENT PM_{2.5} STATE IMPLEMENTATION PLAN FOR THE 2012 NAAQS CAM_x MODELING PROTOCOL

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1. OVERVIEW

Modeling is a tool used to simulate real-world conditions. For air-quality studies, “air-dispersion modeling,” as described by the U.S. Environmental Protection Agency (EPA), “uses mathematical formulations to characterize the atmospheric processes that disperse a pollutant emitted by a source. Based on emissions and meteorological inputs, a dispersion model can be used to predict concentrations at selected downwind receptor locations.”¹ Thus, an atmospheric model incorporates the three components of the air-pollution system, namely, the sources, dispersion, and receptors of atmospheric contaminants.

An air quality modeling *protocol* is a plan prepared to help assure that the modeling is conducted using the most scientifically grounded approaches that are agreed to in advance of the modeling that is used to estimate future air-quality levels from atmospheric models. Such a plan is used as a road map for conducting the modeling to demonstrate attainment of air-quality goals. A particular condition of concern addressed in this CAMx Modeling Protocol for the Allegheny County, PA nonattainment area (NAA) is the southeastern portion of the county in the Monongahela River Valley (“Mon Valley”).

As discussed in more detail herein, the following are the primary models used in the attainment demonstration modeling: the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system², the Motor Vehicle Emissions Simulator (MOVES) model³, the Weather Research and Forecasting (WRF) meteorological model⁴, and the Comprehensive Air Quality Model with extensions (CAMx)⁵, which includes a Plume-in-Grid (PiG) option for local source impacts and a Particulate Source Apportionment Technology (PSAT) that will be important for obtaining the separate contributions of local sources. Together, these models, along with additional models and techniques, are used to show that the emission control strategy proposed by Allegheny County along with regional emission controls will lead to

(1) <https://www.epa.gov/scram/air-quality-dispersion-modeling>

(2) <https://www.cmascenter.org/smoke>

(3) <https://www.epa.gov/moves>

(4) <https://www.mmm.ucar.edu/weather-research-and-forecasting-model>

(5) <http://www.camx.com>

attainment of the 2012 National Ambient Air Quality Standards (NAAQS) for PM_{2.5} by December, 2021.

This section explains the official designations for particulate matter that is 2.5 microns or less in diameter (PM_{2.5}) and the need to carry out an attainment demonstration for the Allegheny County, PA PM_{2.5} nonattainment area according to this protocol. Stakeholders, including contractors, of the PM_{2.5} protocol are also discussed.

1.1 PM_{2.5} Designations

In 1997, EPA promulgated annual and 24-hour PM_{2.5} NAAQS with thresholds of 15 and 65 µg/m³, respectively. The form of the annual PM_{2.5} NAAQS is the 3-year average of the annual PM_{2.5} concentrations. The form of the 24-hour PM_{2.5} NAAQS is the three year average of the 98th percentile 24-hour PM_{2.5} concentration in a year. In December 2006, EPA lowered the 24-hour PM_{2.5} NAAQS from 65 to 35 µg/m³ and kept the annual PM_{2.5} NAAQS at 15 µg/m³. On December 14, 2012, EPA lowered the primary annual PM_{2.5} NAAQS from 15 to 12 µg/m³, but kept the secondary annual PM_{2.5} NAAQS at 15 µg/m³. The primary NAAQS is designed to protect public health, whereas the secondary NAAQS is design to protect public welfare, such as visibility impairment, crop and materials damage and soiling.

The PM_{2.5} attainment demonstration State Implementation Plans (SIPs) for the 2012 annual PM_{2.5} NAAQS were due by October 2016. This includes a demonstration of attainment of the PM_{2.5} NAAQS at the South Allegheny High School (Liberty) monitoring site, the only PM_{2.5} monitor within the nonattainment area that currently violates the PM_{2.5} NAAQS.

1.2 Overview of PM_{2.5} Air Quality in Allegheny County

The Liberty-Clairton area in Allegheny County was designated as nonattainment with respect to the 1997 PM_{2.5} NAAQS based on 2001-2003 monitored data and the 2006 24-hour PM_{2.5} NAAQS based on 2006-2008 monitoring data. The entirety of Allegheny County was designated nonattainment for 2012 annual PM_{2.5} based on 2011-2013 monitored data.

[Table 1-1](#) displays the annual and 24-hour PM_{2.5} Design Values (DVs) for monitoring sites in Allegheny County for several recent three-year periods (2011-2013, 2012-2014, 2013-2015, and 2014-2016). [Figure 1-1](#) displays the locations of the PM_{2.5} monitoring sites in Allegheny County. PM_{2.5} concentrations have

generally been on a downward trend at all monitoring sites in Allegheny County, as shown in [Figure 1-2](#) and [Figure 1-3](#).

While more than one site in Allegheny County violated the annual PM_{2.5} NAAQS prior to the 2011-2013 timeframe, only the Liberty monitor violated the annual PM_{2.5} NAAQS based on 2011-2013 and with more recent monitored data. Liberty 24-hour data has shown DVs just below or above the 24-hour NAAQS with recent data, with the most recent data for 2014-2016 just above the standard.

Table 1-1. Latest annual and 24-hour PM_{2.5} Design Values for monitoring sites in Allegheny County

Monitoring Site	Annual PM _{2.5} Design Values				24-Hour PM _{2.5} Design Values			
	2011-2013	2012-2014	2013-2015	2014-2016 ¹	2011-2013	2012-2014	2013-2015	2014-2016 ¹
Avalon	11.4	10.6	10.6	10.4	25	22	23	22
Lawrenceville	10.3	10.0	9.7	9.5	23	21	21	20
Liberty	13.4	13.0	12.6	12.8	37	35	33	36
South Fayette	9.6	9.0	8.8	8.5	24	20	21	19
North Park	8.8	8.5	8.5	8.2	19	17	18	18
Harrison	10.6	10.0	9.8	9.8	25	22	22	21
North Braddock	11.7	11.4	11.2	11.0	29	26	25	25
Clairton	9.8	9.5	9.9	9.8	22	23	25	26

¹2014-2016 design values for Avalon, South Fayette, North Park, and Clairton are considered to be invalid by EPA due to low data recovery.



Figure 1-1. Locations of PM_{2.5} monitoring sites within Allegheny County.

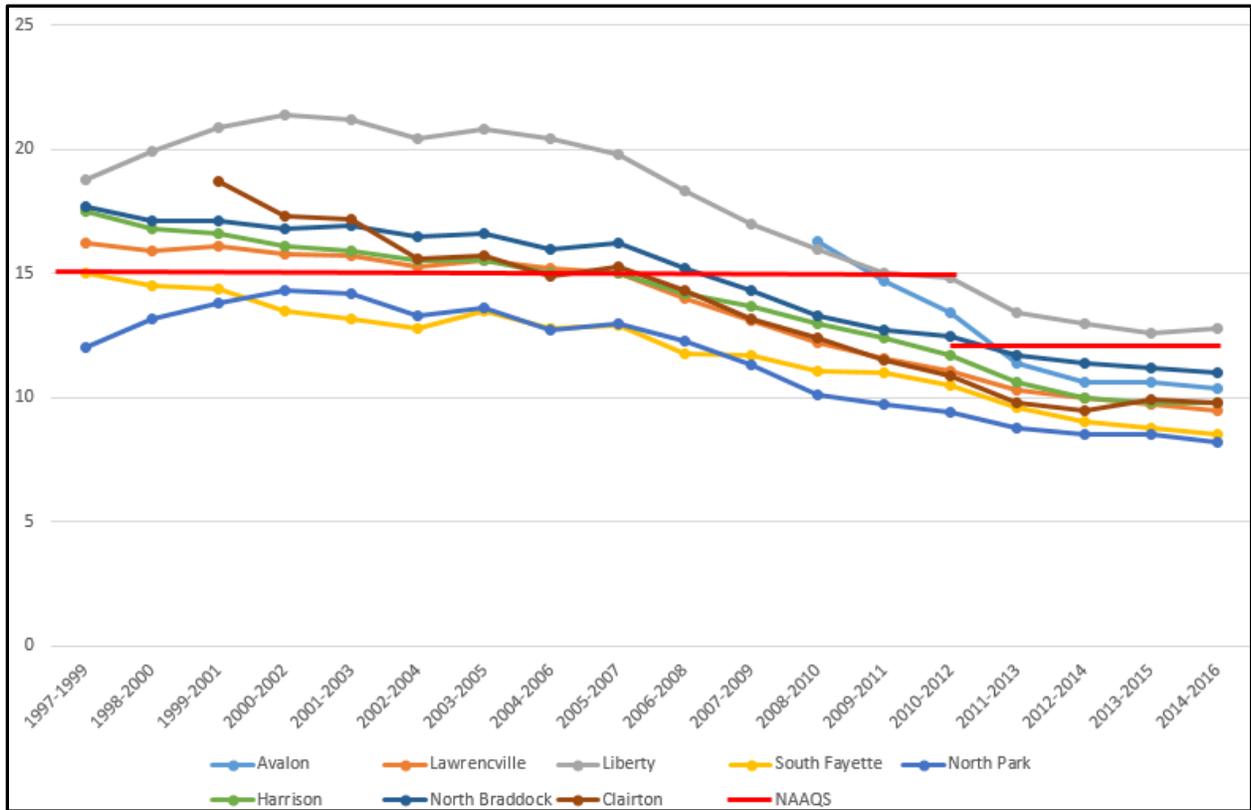


Figure 1-2. Trends in annual PM_{2.5} Design Values for Monitoring Sites in Allegheny County.

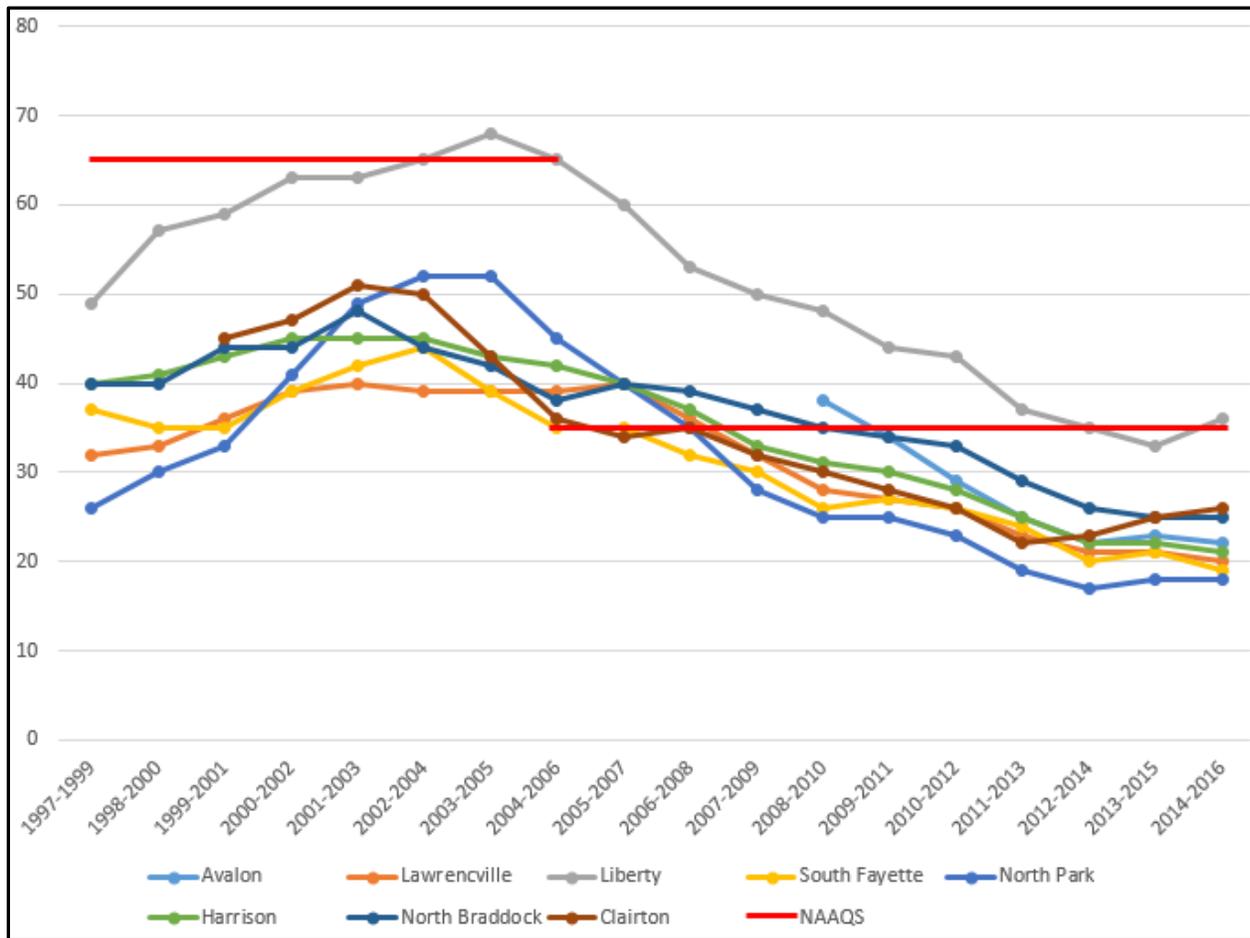


Figure 1-3. Trends in 24-hour PM_{2.5} Design Values for Monitoring Sites in Allegheny County.

1.3 Stakeholders

The Allegheny County Health Department (ACHD) is responsible for demonstrating attainment in the Allegheny County nonattainment area. A final attainment demonstration will be submitted to the Pennsylvania Department of Environmental Protection (DEP), on behalf of the ACHD, for submittal to the U.S. Environmental Protection Agency (EPA) Region 3 office as part of the Pennsylvania SIP.

ACHD has selected Ramboll Environ to assist them in the PM_{2.5} attainment demonstration modeling. ACHD staff, stakeholders, and Ramboll Environ have participated in the development of the PM_{2.5} modeling procedures that are documented in this Modeling Protocol. Stakeholders include persons from air quality agencies, local industry, environmental advocacy groups, environmental consulting companies, universities, and the general public.

2. PROBLEM STATEMENT

This section explains the nature of the PM_{2.5} problem and provides a conceptual model for high PM_{2.5} concentrations in the Allegheny County nonattainment area. Monitored data results are also given.

2.1 Geographic Situation

Allegheny County is located in western Pennsylvania and contains rural land, densely populated residential areas, and industrial facilities. Allegheny County has many regions with complex terrain, such as the area immediately surrounding the Liberty monitor in the Mon Valley.

The base of the river valley lies at 718 feet in elevation above mean sea level (MSL), while adjacent hilltops can be greater than 1,250 feet MSL. Large temperature differences can be seen between hilltop and valley floor observations (e.g., 2 to 7°F) during clear, low-wind, nighttime conditions. Strong nighttime drainage flows can cause differences of up to 180° in wind direction with 3-4 mph downward flows. Also, strong nighttime inversions can lead to poor dispersion scenarios on several days of the year (Sullivan, 1996).

2.2 PM_{2.5} Contributions in Allegheny County

Data analysis has shown that Allegheny County is impacted by both regional and localized PM_{2.5}. All monitor sites can be impacted by both long-range transport of pollutants and some degree of urban and/or local contributions.

ACHD performed speciation data analysis from monitored results as well as source apportionment modeling using Positive Matrix Factorization (PMF) for sites with speciation data (ACHD, 2012a, 2012b)⁶. Results have shown the largest PM_{2.5} contributions from long-range transport include secondary ammonium sulfate and nitrate. Urban anthropogenic contributions from vehicles and other sources can influence sites throughout the county. At sites like Liberty, localized PM_{2.5} contributions can include industrial carbon-rich sources and other components.

In defining the nonattainment area boundaries of the Allegheny County nonattainment area under the 2012 PM_{2.5} NAAQS, EPA performed a 5-factor

⁶ Updated analyses using more recent data are being prepared by ACHD for this SIP.

analysis (EPA, 2013). As part of this analysis EPA prepared pollution roses that analyzed the highest observed 24-hour PM_{2.5} concentrations at Liberty as a function of wind direction. Some of these results are shown in [Figure 2-1](#) that displays a PM_{2.5} concentration distribution by wind direction, and a map of the Liberty and Clairton monitors along with the nearby U. S. Steel Clairton Plant. The highest observed PM_{2.5} concentrations at the Liberty monitor tend to occur when winds are from the southwest quadrant that aligns the transport of emissions toward the Liberty monitor.

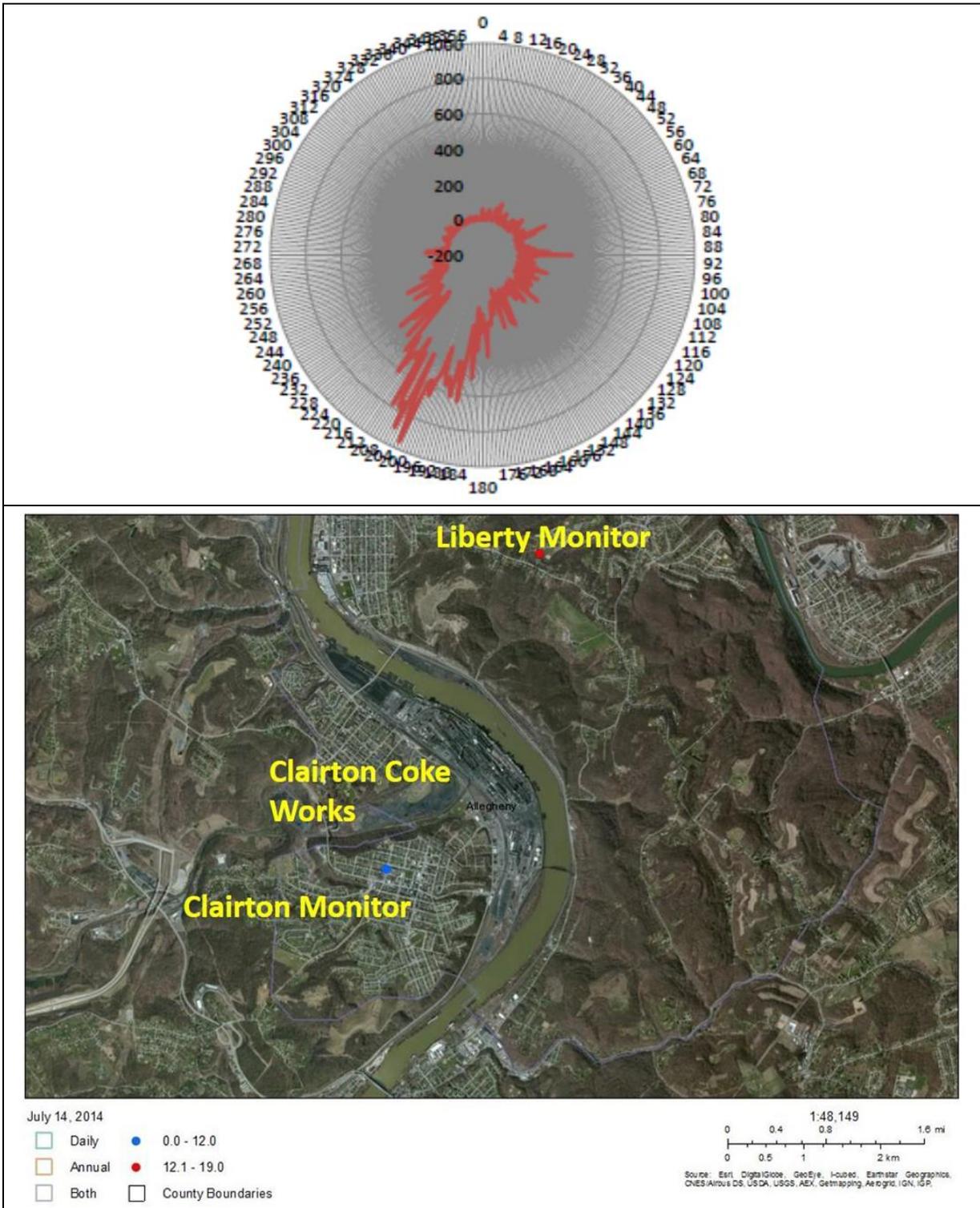


Figure 2-1. Concentration Distribution by Wind Direction on High PM_{2.5} Days at the Liberty monitor (top) and relationship between monitors and the Clairton Plant (bottom).

Analysis of chemical speciation data can reveal the amount of localized excess by individual species. The pie chart in [Figure 2-2](#) below shows the average “excess” PM_{2.5} species at Liberty for 2011. This excess was determined by first averaging Chemical Speciation Network (CSN) measurements from sites across the Pittsburgh metropolitan statistical area (MSA) to be used as regional background concentrations. The local excess PM_{2.5} contribution at Liberty was then calculated as the difference of Liberty and background concentrations by species. Note: other/unknown can include particle-bound water, unknown/unmeasured species, and/or differences between the analytical techniques used for measurements of the compounds. Also, organic carbon (OC) is shown here as measured by the CSN monitor. Organic aerosol (OA) is often estimated as 1.4*OC as a way to correct the measured organic carbon.

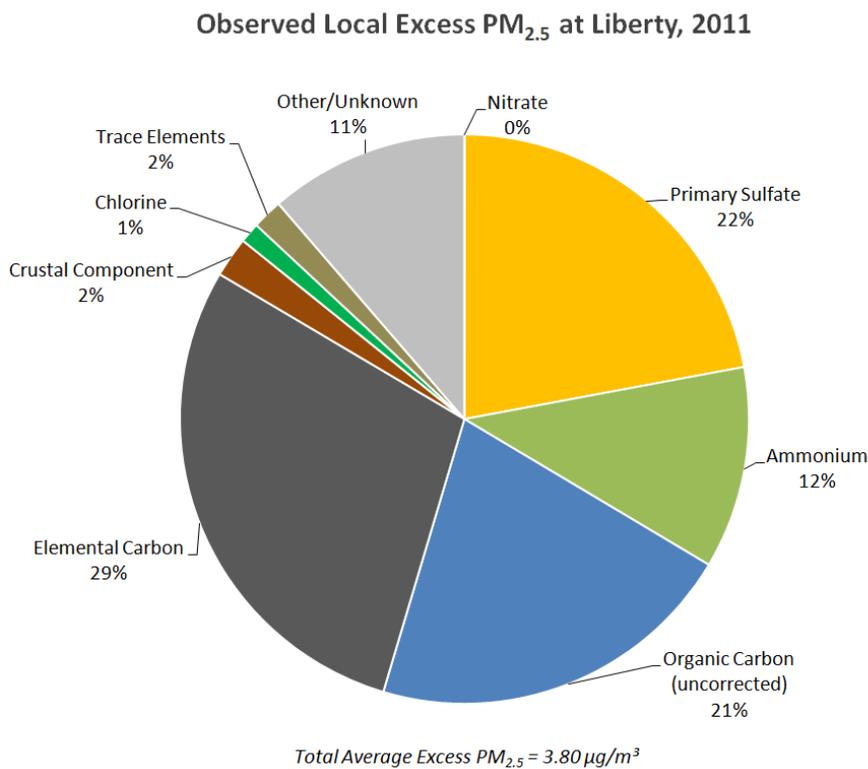


Figure 2-2. Excess PM_{2.5} concentrations at the Liberty monitoring site compared to surrounding MSA sites, 2011.

ACHD and EPA studies indicate that PM_{2.5} attainment demonstration modeling for the Liberty monitoring site must take into account both regional transport of PM_{2.5} from sources in the eastern U.S. and contributions from nearby local sources.⁷

⁽⁷⁾ http://www.heinz.org/UserFiles/Library/2011-air_quality-research.pdf

3. SELECTION OF MODELING ELEMENTS

This section outlines the models, modeling domains and modeling period used for the Allegheny County PM_{2.5} attainment demonstration modeling. The current EPA PM_{2.5} (Draft) Modeling Guidance for PM_{2.5} attainment demonstrations modeling was released in December 2014 (EPA, 2014). EPA has also developed the Modeled Attainment Test Software (MATS⁸) tool that implements the recommended annual and 24-hour PM_{2.5} DV projection approach from their guidance (EPA, 2014).

3.1 Model Selection

Three types of models will be used in the Allegheny County PM_{2.5} attainment demonstration modeling to simulate emissions, meteorology and air quality.

3.1.1 Meteorological Model Selection

The Weather Research and Forecasting (WRF) model⁹ will be used to represent meteorological conditions in this study area. The Advanced Research WRF (ARW) version of WRF was selected for the Allegheny County PM_{2.5} attainment demonstration modeling and is further described in a separate WRF Modeling Protocol (Ramboll Environ, 2016).

3.1.2 Emissions Model Selection

A suite of emission models will be used to generate air quality model-ready emissions for various source categories. The air quality model requires hourly, gridded, and speciated emissions inputs. The Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system¹⁰ is an emissions processing system that generates hourly gridded speciated emission inputs (Coats, 1995; Houyoux et al., 2000). SMOKE is principally an emission processing system and not a true emissions modeling system in which emissions estimates are simulated from “first principles”. This means that, with the exception of mobile and biogenic sources, its purpose is to provide an efficient tool for converting emissions inventory data into the formatted emission files required by an air quality simulation model. For mobile sources, SMOKE actually simulates emission rates based on input mobile-source activity data, meteorological data, and emission factors.

⁽⁸⁾ <https://www.epa.gov/scram/photochemical-modeling-tools>

⁽⁹⁾ <https://www.mmm.ucar.edu/weather-research-and-forecasting-model>

⁽¹⁰⁾ <http://www.smoke-model.org/index.cfm>

SMOKE was originally designed to allow emissions data processing methods to utilize emergent high-performance-computing (HPC) as applied to sparse-matrix algorithms. Indeed, SMOKE is the fastest emissions processing tool currently available to the air quality modeling community. The sparse matrix approach utilized throughout SMOKE permits both rapid and flexible processing of emissions data. The processing is rapid because SMOKE utilizes a series of matrix calculations instead of less efficient algorithms used in previous systems such as EPS and EMS. The processing is flexible because the steps of temporal projection, controls, chemical speciation, temporal allocation, and spatial allocation are separated into independent operations wherever possible. The results from these steps are merged together at a final stage of processing. SMOKE has been available since 1996, and it has been used for emissions processing in a number of regional air quality modeling applications. Continuing model development activities with SMOKE now occur at the University of North Carolina (UNC) Institute for the Environment.

Notable features of SMOKE from an applications standpoint include: (a) control strategies can include changes in the reactivity of emitted pollutants, a useful capability, for example, when a solvent is changed in an industrial process; (b) no third party software is required to run SMOKE, although some input file preparation may require other software; (c) support of various air quality model emissions input formats (for different photochemical models); and (d) enhanced quality assurance pre- and post-processing.

SMOKE supports area, mobile, fire and point source emission processing and also includes biogenic emissions modeling through a rewrite of the Biogenic Emission Inventory System, Version 3 (BEIS3). SMOKE (and SMOKE-BEIS3) will be used to process emissions for the Allegheny County PM_{2.5} modeling.

3.1.3 Air Quality Model Selection

Two photochemical grid models (PGMs) have been used in recent PM_{2.5} attainment demonstration SIP modeling: (1) the Community Multiscale Air Quality (CMAQ) modeling system¹¹ (Byun and Ching, 1999); and (2) the Comprehensive Air Quality

⁽¹¹⁾ <http://www.cmaq-model.org>

Model with extensions (CAMx¹²; ENVIRON, 2016). Both models are publicly available and have been used in numerous ozone and PM_{2.5} SIPs that have been approved by EPA.

CAMx was developed with all new code during the late 1990s using modern and modular coding practices. This has made the model an ideal platform for the extension to treat a variety of air quality issues including ozone, particulate matter (PM), visibility, acid deposition, and air toxics. The flexible CAMx framework has also made it a convenient and robust host model for the implementation of a variety of mass balance and sensitivity analysis techniques including Process Analysis (PA), Decoupled Direct Method (DDM), and the Ozone/Particulate Source Apportionment Technology (OSAT/PSAT).

Ramboll Environ will utilize CAMx Version 6.30 (released in April 2016) for modeling of the Allegheny Country nonattainment area utilizing WRF meteorological model output for modeling domains with 36, 12, 4, and 1.33 km horizontal resolution. This will include regional and localized PM_{2.5} impacts, formed by both primary and secondary mechanisms. Model performance will be examined for comparison to monitored results. CAMx was selected over CMAQ because it includes several features not included in the current version of CMAQ that are important for PM_{2.5} modeling of the Allegheny County area:

- CAMx supports two-way grid nesting that will allow the modeling of regional- as well as local-scale impacts within the same simulation.
- CAMx includes a subgrid-scale Plume-in-Grid (PiG) module that simulates near-source plume dispersion and chemistry and includes an ability for subgrid-scale sampling of the puffs that can better represent the contributions of local sources. The plume-in-grid treatment (APT) that was found in previous versions of CMAQ is not included in the current version.
- CAMx includes the CB6 chemical mechanism that represents the latest understanding of photochemistry.
- CAMx includes Particulate Source Apportionment Technology (PSAT) that will be important for obtaining the separate contributions of local sources.

If CAMx model performance exhibits performance issues such as a tendency toward underestimation for total PM_{2.5} (sum of all fine particulate species) in the baseline

⁽¹²⁾ <http://www.camx.com>

year 2011, local modeling for near-field primary PM_{2.5} may be performed using EPA's AMS/EPA Regulatory Model (AERMOD)¹³ model version 16216r. This AERMOD modeling may use meteorological inputs based on a nested 444 m horizontal resolution WRF grid, and the Mesoscale Model Interface tool (MMIF). If needed, the AERMOD local modeling will be performed for both baseline and future year cases.

3.2 PM_{2.5} Components

Analysis of speciated PM_{2.5} data indicates that excess near the Liberty monitor is composed of both primary and secondary components of PM_{2.5} (ACHD, 2012a, 2012b). Therefore, emission inputs for CAMx will include all PM_{2.5} precursor pollutants (sulfur dioxide, nitrogen oxides, volatile organic compounds, ammonia) along with primary filterable and condensable PM_{2.5}.

If additional local plume modeling is necessary, AERMOD modeling will be performed for primary filterable and condensable PM_{2.5} for selected near-field sources. The AERMOD results would be combined in post-processing with CAMx results with the contribution of primary emissions from local sources eliminated. This would be done by using the PSAT source apportionment modeling of local sources so their contributions can be eliminated in the current and future year CAMx modeling so that local sources are not double counted when the AERMOD local source results are added to the CAMx regional results.

3.3 Modeling Years

The 2011 calendar year was selected for the baseline modeling and model performance evaluation. The 2011 modeling year was selected because it was part of the 2011-2013 monitoring timeframe used for designations and is representative of PM levels in the region. Additionally, there are comprehensive 2011 modeling databases that includes the 2011 National Emissions Inventory (NEI2011v2). Emissions for the 2021 future year will be used for the projected case and attainment demonstration modeling using the 2011 base year meteorological inputs. The EPA 2011NEIv2 platform (2011v6.2) currently includes future years of 2017 and 2025, and ACHD will provide future year emission estimates for their local sources.

¹³ <https://www.epa.gov/scram/air-quality-dispersion-modeling-preferred-and-recommended-models>

We will assume that that the 2021 future year Boundary Conditions (BCs) for the 36 km CONUS domain (i.e., international transport) will remain unchanged from the current (2011) year. CAMx will be applied on the 36/12 km domains using two-way grid nesting and the results post-processed to generate BC inputs for the 4 km western Pennsylvania domain (i.e., one-way grid nesting between the 12 and 4 km domains). CAMx will then be applied on the 4/1.33 km domains using two-way grid nesting.

The CAMx 4/1.33 km output for the 2011 base case and 2021 future year emission scenarios would be processed using MATS to project future year annual PM_{2.5} DVs to assess compliance with the 2012 annual PM_{2.5} NAAQS. Note that EPA is in the process of updating MATS to a new software tool called the Software for the Modeled Attainment Test – Community Edition (SMAT-CE¹⁴), which may be used for this study. MATS and SMAT-CE use EPA’s recommended procedures in their modeling guidance (EPA, 2014) that uses the relative modeling results for the base and future year emission scenarios to scale the observed current year PM_{2.5} Design Values (DVC) to project future year PM_{2.5} Design Values (DVF). The modeled derived scaling factors are referred to as Relative Response Factors (RRF) that are calculated as the ratio of the future year to current year modeling results:

$$DVF = DVC \times RRF$$

⁽¹⁴⁾ <https://www.epa.gov/scram/photochemical-modeling-tools>

4. MODELING PROCEDURE

This section delineates the procedures for the model simulations and post-processing required for the Allegheny County attainment demonstration modeling.

4.1 Horizontal Modeling Domains

WRF and CAMx will be run for a 36/12/4/1.33km domain structure as depicted in [Figure 4-1](#) and [Figure 4-2](#) (also provided in [Table 4-1](#)). The four domains will use a Lambert Conic Conformal (LCC) projection. The LCC grid projection will have a pole of projection of 40 degrees North, -97 degrees East and standard parallels of 33 and 45 degrees, the so-called standard Regional Planning Organization (RPO) projection. The four domains are defined as follows:

- A 36 km continental U.S. (CONUS) domain is defined to be the standard RPO CONUS domain.
- A 12 km northeastern U.S. (NEUS) domain identical to the NEUS domain used by the Ozone Transport Commission (OTC) 12 km domain that is also used by MARAMA.
- A 4 km domain that covers all of Pennsylvania (PA) and adjacent areas in West Virginia and Ohio.
- A nested grid of 1.33 km for the Allegheny County nonattainment area and portions of adjacent counties.

A fifth modeling domain centered over the Liberty and Clairton monitor with 0.444 km spatial resolution was also developed. This domain will not be used for CAMx modeling but may be used for potential AERMOD modeling associated with this project.

The proposed modeling domains were carefully devised to include all the major area and point sources of NO_x, SO₂, NH₃ and PM_{2.5} emissions in the corresponding regions. The WRF domains are defined to be slightly larger than the CAMx domains to eliminate any boundary artifacts in the WRF simulations from influencing the CAMx meteorological inputs. WRF produces modeling artifacts near its boundaries as the meteorological variables from the boundary conditions come into dynamic balance with WRF's numerical algorithms. By specifying a few grid cell buffers between the WRF and CAMx boundaries we can be sure that no artifacts are in the CAMx meteorological inputs. WRF domains are defined with at least a 5-grid cell buffer in all directions from the CAMx domains.

The CAMx run strategy is to use two-way grid nesting between the 36 km CONUS and 12 km NEUS domains, and then use one-way grid nesting to provide boundary conditions to a two-way grid nesting run of the 4 km PA and 1.33 km Allegheny County domains.

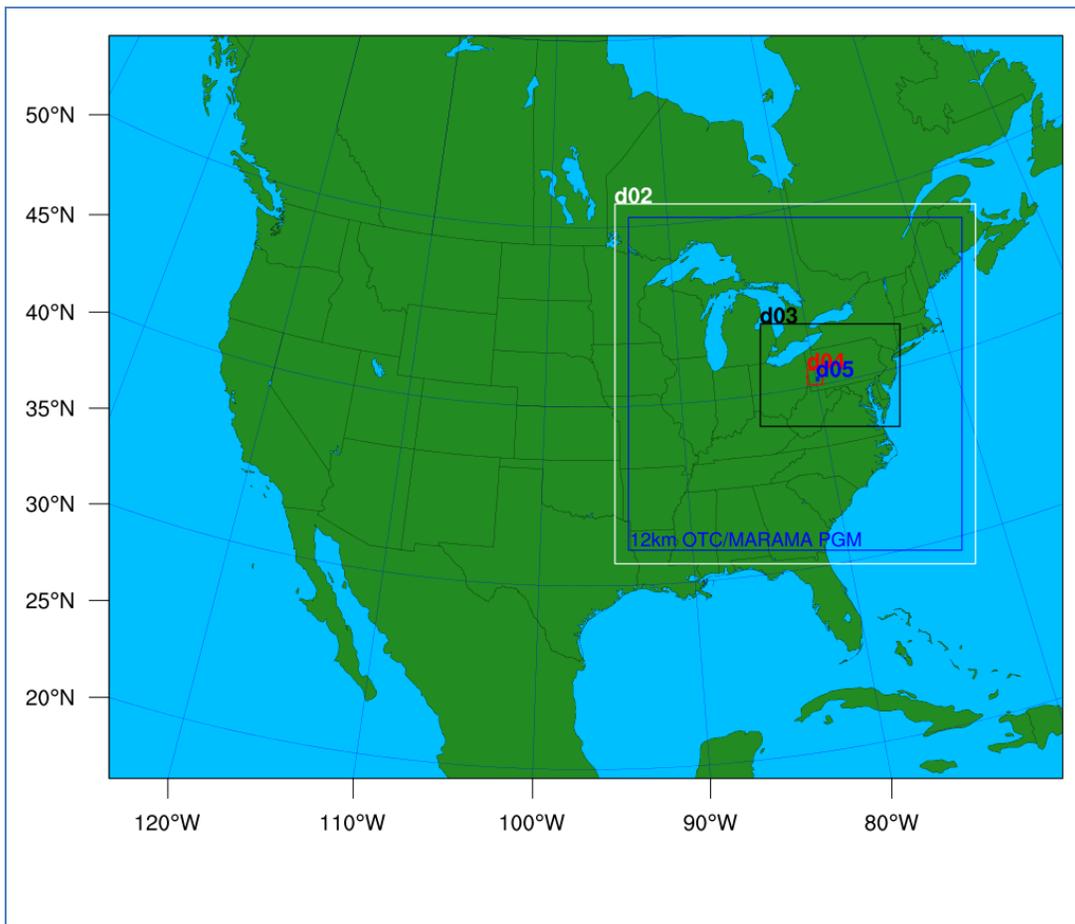


Figure 4-1. Large Scale WRF and CAMx Horizontal Modeling Domains at 36 km (CONUS; d01); 12 km (NEUS; d02); 4 km (PA; d03); 1.33 km (Allegheny County; d04); and 0.444 km (Southeastern Allegheny County; d05) Resolution.

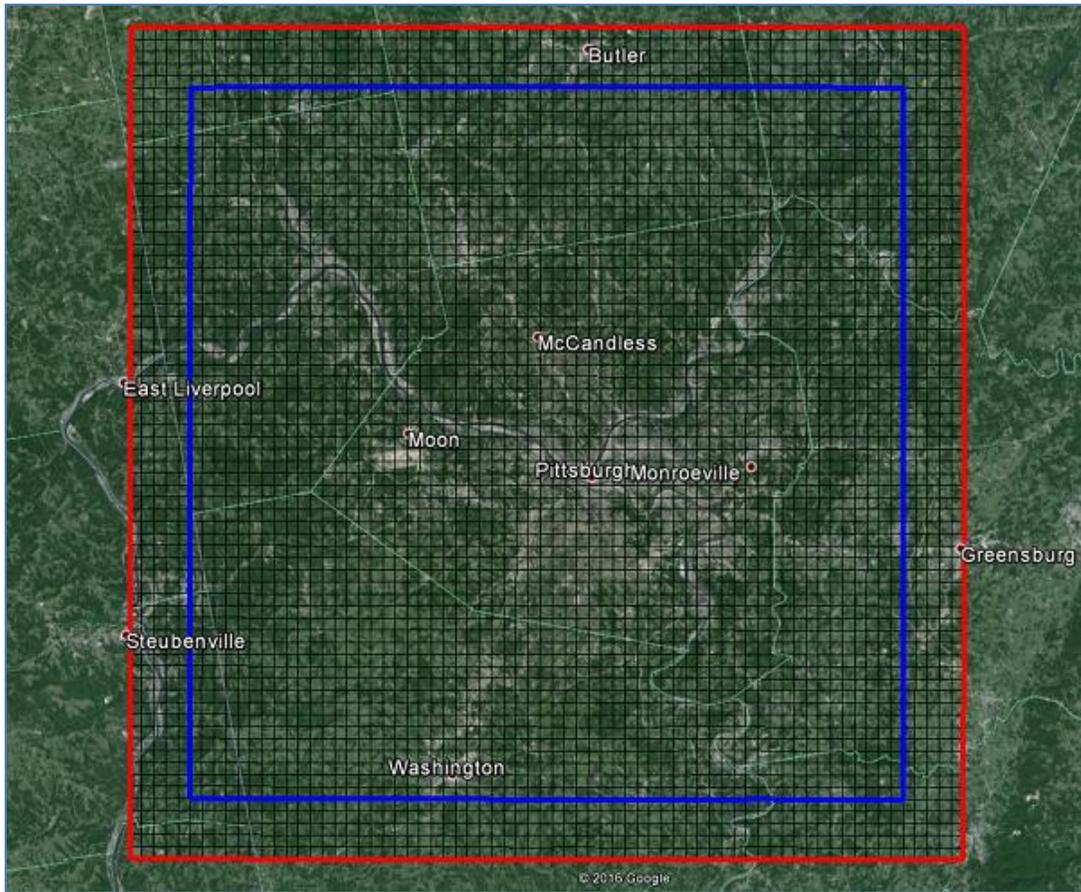


Figure 4-2. Allegheny County 1.33 km (d04) WRF (red) and CAMx (blue) Horizontal Modeling Domains.

Table 4-1. WRF and CAMx Horizontal Modeling Domains

Grid Spacing (km)	Domain Origin (km) (x,y)	Number of Cells (West-East)	Number of Cells (South-North)
WRF			
36	-2952, -2304	165	129
12	180, -972	187	187
4	1080, -120	217	160
1.33	1372, 140	70	70
0.444	1428, 164	31	46
CAMx¹			
36	-2412, -1620	132	82
12	240, -912	167	176
4	1100, -100	206	149
1.33	1378.67, 146.67	59	59

¹CAMx modeling domains include boundary or buffer cells.

4.2 Vertical Layer Structure

The WRF output will be processed using the WRFCAMx processor to generate CAMx meteorological inputs. WRFCAMx can perform layer collapsing to reduce the vertical layers in WRF to fewer vertical layers for the CAMx modeling to reduce the CAMx computational requirements.

Table 4-2 displays the approach to be used for collapsing the WRF 37 vertical levels (36 layers) to 25 vertical layers for the CAMx modeling.

Table 4-2. WRF 37 level (36 layer) and CAMx 25 layer structure.

WRF Meteorological Model					CAMx Air Quality Model		
WRF Level	Sigma	Pressure (mb)	Height (m)	Thickness (m)	CAMx Layer	Height (m)	Thickness (m)
36	0.0000	50.00	19260	2055	25	19260.0	3904.9
35	0.0270	75.65	17205	1850			
34	0.0600	107.00	15355	1725	24	15355.1	3425.4
33	0.1000	145.00	13630	1701			
32	0.1500	192.50	11930	1389	23	11929.7	2569.6
31	0.2000	240.00	10541	1181			
30	0.2500	287.50	9360	1032	22	9360.1	1952.2
29	0.3000	335.00	8328	920			
28	0.3500	382.50	7408	832	21	7407.9	1591.8
27	0.4000	430.00	6576	760			
26	0.4500	477.50	5816	701	20	5816.1	1352.9
25	0.5000	525.00	5115	652			
24	0.5500	572.50	4463	609	19	4463.3	609.2
23	0.6000	620.00	3854	461	18	3854.1	460.7
22	0.6400	658.00	3393	440	17	3393.4	439.6
21	0.6800	696.00	2954	421	16	2953.7	420.6
20	0.7200	734.00	2533	403	15	2533.1	403.3
19	0.7600	772.00	2130	388	14	2129.7	387.6
18	0.8000	810.00	1742	373	13	1742.2	373.1
17	0.8400	848.00	1369	271	12	1369.1	271.1
16	0.8700	876.50	1098	177	11	1098.0	176.8
15	0.8900	895.50	921	174	10	921.2	173.8
14	0.9100	914.50	747	171	9	747.5	170.9
13	0.9300	933.50	577	84	8	576.6	168.1
12	0.9400	943.00	492	84			
11	0.9500	952.50	409	83	7	408.6	83.0

- table continued on next page -

WRF Meteorological Model					CAMx Air Quality Model		
WRF Level	Sigma	Pressure (mb)	Height (m)	Thickness (m)	CAMx Layer	Height (m)	Thickness (m)
10	0.9600	962.00	326	82	6	325.6	82.4
9	0.9700	971.50	243	82	5	243.2	81.7
8	0.9800	981.00	162	41	4	161.5	64.9
7	0.9850	985.75	121	24			
6	0.9880	988.60	97	24	3	96.6	40.4
5	0.9910	991.45	72	16			
4	0.9930	993.35	56	16	2	56.2	32.2
3	0.9950	995.25	40	16			
2	0.9970	997.15	24	12	1	24.1	24.1
1	0.9985	998.58	12	12			
0	1.0000	1000	0		0	0	

4.3 Geophysical Data

Terrain and land use processing will include the most recent data available for use in CAMx and, if necessary, AERMOD. This includes:

- USGS NED terrain data, 0.3-1.0 arc-second resolution
- USGS NLCD land cover data, 1992 or 2001

CAMx also requires grid array of albedo and ozone column data. The albedo will be land use dependent. Ozone column data will come from the Total Ozone Mapping Spectrometer (TOMS) satellite data⁽¹⁵⁾. The TOMS data are used in the Tropospheric, Ultraviolet and Visible (TUV) radiation model¹⁶ to calculate photolysis rates. Frequently TOMS ozone column data are missing for extended periods so data needs to be filled. The CAMx TUV processor allows for the use of episode average data. If there are large periods of missing TOMS data during the modeling period, then we may use monthly or episode average TOMS data to work around the missing data.

⁽¹⁵⁾ <https://eosps0.gsfc.nasa.gov/missions/total-ozone-mapping-spectrometer-earth-probe>

⁽¹⁶⁾ <https://www2.acom.ucar.edu/modeling/tropospheric-ultraviolet-and-visible-tuv-radiation-model>

4.4 Meteorological Inputs

For CAMx, the WRF model will be used to generate three-dimensional grid meteorological inputs. If needed, AERMOD meteorological inputs will also be generated using the EPA's Mesoscale Model Interface tool (MMIF).

4.4.1 WRF Meteorological Modeling

The WRF meteorological modeling is discussed in a separate WRF Modeling Protocol (Ramboll Environ, 2016).

If AERMOD modeling is needed, the output from the 444 m resolution WRF domain will be processed with MMIF, following methodologies learned from the Liberty SO₂ SIP process.

4.5 Development of CAMx-Ready 2011 and 2021 Emissions

The emissions inventories and other data discussed in this section will be used to prepare CAMx-ready emission files using the SMOKE system and other methods as described below.

4.5.1 2011 Base Year Emissions

The 2011 MARAMA ALPHA2 emissions inventory will form the framework of base case emissions for 15 states in the Northeastern U.S. (CT, DC, DE, MA, MD, ME, NC, NH, NJ, NY, PA, RI, VA, VT, WV). The additional U.S states, Mexico and Canadian provinces, and offshore sources emissions will be based on inventories in EPA's 2011 NEI-based 2011v6.2 modeling platform (MP). The MARAMA and NEI inventories include sources of PM₁₀, PM_{2.5}, NO_x, CO, SO₂, NH₃, and VOC emissions on an annual basis.

The Northeastern regional emission inventory includes all air pollution sources categorized into eight sectors. A list of these sectors along with key processing features is provided below:

EGU Point Sources This sector includes emission units located primarily at electric power plants that are included in the EPA 2011 v6.2 MP inventory with SO₂/NO_x hourly data for temporal profiles. These sources are required to report Continuous Emission Monitoring Systems (CEMS) data to EPA's Clean Air Market Division (CAMD) under 40 CFR Part 75. Generally, these units burn fossil fuel and serve a generator of more than 25 MW. They are required to report NO_x and SO₂ emissions and activity data at an hourly resolution as required by Part 75. Air quality

modeling uses the hourly emissions data for these units to accurately reflect the temporal variation in emissions. For primary PM emissions, the annual values can be processed to hourly values using the CEMS hourly heat input observations.

Small EGU Point Sources This sector includes smaller EGUs that are not included in the EGU Point Source inventories. These point source emissions will be processed through SMOKE using speciation and temporal allocation data available in the EPA's modeling platform.

Non-EGU Point Sources This sector includes facilities and sources located at a fixed, stationary location. Other point sources include larger industrial, commercial and institutional facilities. The non-EGU point source emissions will be processed through SMOKE using speciation and temporal allocation data available in the modeling platform.

Aircraft/GSE/APU Point Sources This sector includes emissions from aircraft engines, ground support equipment (GSE) and auxiliary power units (APUs) that are identified as point sources (e.g., emissions are located at specific airport locations). The aircraft emissions will be processed through SMOKE using speciation and temporal allocation data available in the modeling platform.

Nonpoint Sources This sector includes sources which individually are too small in magnitude or too numerous to inventory as individual point sources. Nonpoint sources include smaller industrial, commercial and institutional facilities, as well as residential sources. S/L/T agencies and EPA estimate nonpoint emissions at the county level. This sector does not include locomotive emissions outside of the rail yards and commercial marine vessel emissions, which are included in the nonroad sector described below. For emissions modeling purposes, these types of emissions are defined by state and county identifiers, and Source Classification Codes (SCCs). The nonpoint emissions will be processed through SMOKE as "area" source using spatial surrogates, speciation and temporal allocation data.

Nonroad Sources in the NONROAD Model This category contains mobile sources included in NONROAD model within the National Mobile Inventory Model (NMIM). Nonroad emissions result from the use of fuel in a diverse collection of vehicles and equipment such as construction equipment, recreational vehicles, and landscaping equipment. The non-road emissions are typically compiled as both annual total emissions, and average day emissions by month. In order to take the best

advantage of the monthly and seasonal variability of the non-road emissions sources, the monthly option will be used for SMOKE modeling inputs. Just like the nonpoint category, month-specific nonroad emissions will be processed as “area” source using spatial surrogates.

Rail/CMV Nonroad Sources This category includes internal combustion engines used to propel commercial marine vessels (CMV) and locomotives. These sources will be processed separately as their own source group in the emission modeling. The marine sources do not include large ocean going (Class 3) vessels which are processed under the off-shore shipping category.

Onroad Sources This category contains mobile sources included in the MOVES model. Onroad emissions result from the combustion and evaporation of fuel used by motorized vehicles that are normally operated on public roadways. This includes passenger cars, motorcycles, minivans, sport-utility vehicles, light-duty trucks, heavy-duty trucks, and buses. We will use the MARAMA county-level 2011 on-road mobile source emissions. The SMOKE emissions modeling system will: (1) distribute the county-level emissions to the grid cells using spatial surrogate distributions; (2) apply day-of-week and hour-of-day temporal allocation factors; and (3) perform chemical speciation for the Carbon Bond Version 6 Revision 2 (CB6r2) chemical mechanism.

The modeling inventories will be updated to include corrections for local sources in the Allegheny County NAA. The correction will include actual 2011 emissions, stacks and location.

Local sources in Allegheny County will be based on actual emissions data reported for 2011. Types of sources that will be included:

- Stacks: elevated point sources
- Quench Towers: elevated point sources
- Ambient-Temperature Fugitives: elevated point sources with ambient exit temperatures and minimal flow rates.
- Coke Oven Batteries: elevated point sources

The local major point sources in Allegheny County will be modeled using the Plume-in-Grid (PiG) option in CAMx. Local sources will also be flagged for treatment using the PSAT source apportionment technology. The facilities treated as major local

sources include U. S. Steel Mon Valley Works (Clairton, Irvin, Edgar Thomson Plants), Shenango, Allegheny Ludlum, and McConway and Torley.

4.5.2 Biogenic Emissions

Biogenic emissions will be developed using the Biogenic Emission Inventory System, version 3.61 (BEIS3.61) within SMOKE. The SMOKE-BEIS tool creates gridded, hourly, model-species emissions from vegetation and soils. It estimates CO, VOC (most notably isoprene, terpene, and sesquiterpene), and NO emissions using day-specific meteorology.

4.5.3 Fires Emissions

Forest fire emissions will be developed using 2011 BlueSky inventory from EPA. Fire emissions are highly episodic and very location specific. In the 2011v6.2 platform, wildfires are in the ptwildfire sector and prescribed burning emissions are contained in the ptprescfire sector. The BlueSky fires emissions will be processed through SMOKE using MCIP meteorological data and plume rise algorithm within SMOKE to generate 3D emissions. The 3D emissions will then be converted into CAMx format using the CMAQ2CAMx program.

4.5.4 Sea Salt and Lightning

Sea salt emissions and NO_x emissions from lightning will be generated using CAMx processors for these two source categories. The sea salt emissions processor uses an ocean file that includes a spray zone along with the 2011 WRF hourly surface wind speeds to generate day-specific hourly gridded sea salt emissions. Sea salt emissions are not expected to have a large influence on air quality in Allegheny County area. The lightning emissions processor uses estimates of North American continental annual lightning NO_x emissions along with the 2011 WRF estimated convective activity to spatially and temporally allocate the annual lightning NO_x emissions to generate the day-specific hourly lightning NO_x emissions at the appropriate vertical heights for PGM modeling.

[Table 4-3](#) summarizes inventory data sources by source category and region for the base year.

Table 4-3. Base Year Inventory Data Sources

Source Category	Allegheny County (1.33 km Domain)	Mid-Atlantic (4 km Domain)	Eastern U.S. (12 km Domain)	Continental U.S. (36 km Domain)
Area / Nonroad	MARAMA Alpha2 2011	MARAMA Alpha2 2011	EPA 2011 v6.2 MP	EPA 2011 v6.2 MP
Onroad (Mobile)	MARAMA Alpha2 2011	MARAMA Alpha2 2011	EPA 2011 v6.2 MP	EPA 2011 v6.2 MP
Point	ACHD Local + MARAMA Alpha2 2011	ACHD Local + MARAMA Alpha2 2011	EPA 2011 v6.2 MP	EPA 2011 v6.2 MP
EGU Point	EPA 2011 v6.2 MP 2011 w/CAMD CEMS	EPA 2011 v6.2 MP 2011 w/CAMD CEMS	EPA 2011 v6.2 MP 2011 w/CAMD CEMS	EPA 2011 v6.2 MP 2011 w/CAMD CEMS
Fires	EPA 2011 v6.2 FIRES	EPA 2011 v6.2 FIRES	EPA 2011 v6.2 FIRES	EPA 2011 v6.2 FIRES
Biogenics	EPA 2011 NEIv2 BEIS	EPA 2011 NEIv2 BEIS	EPA 2011 NEIv2 BEIS	EPA 2011 NEIv2 BEIS
Sea Salt and Lightning	CAMx processors	CAMx processors	CAMx processors	CAMx processors

Notes:

1. MARAMA Alpha2 and EPA v6.2 MP are developed from 2011 NEI V2
2. Point sources include non-EGUs and small EGU.
3. EGU emissions include SO₂/NO_x CAMD CEMS data for temporal profile; EPA 2011 (annualized) for other pollutants
4. ACHD Local is corrected MARAMA inventory for emissions, stack parameters, coordinates, etc. 36/12 km domains are used to develop boundary conditions for 4/1.33 km domains

4.5.5 2021 Future Year Emissions

2021 future year emissions will be generated for the Allegheny County PM_{2.5} attainment demonstration modeling. In the future year modeling, natural source categories (biogenic, fires, sea salt and lightning) will be held constant and same as the 2011 base case. The following section describes the emissions inventories used in the future year CAMx run.

EGU Sources MARAMA “ALPHA2” inventory for the Northeastern U.S. consists of three emissions cases: the 2011 base case, the 2018 projection and the 2028 projection. For future year inventories, MARAMA developed the ERTAC EGU Forecasting Tool to project electricity generation and emissions from EGUs. The tool calculates future emissions of NO_x and SO₂ based on projections of future generation, the 2011 base year emission rates, and known future year emission controls, fuel switches, retirements, and new units. The future year emissions for other pollutants (CO, NH₃, PM₁₀, PM_{2.5}, and VOC) are calculated using the

generation projections from the ERTAC tool and a file of emission factors for each unit. We will use 2021 EGU emissions from the ERTAC v2.4L2 Forecasting Tool in the modeling.

Local sources in Allegheny County. ACHD will provide future year emissions for local sources which will be harmonized with other regional inventory to avoid any potential double counting of emissions. [Table 4-4](#) below summarizes the future year inventory by region and major source category.

Table 4-4. Future Year Inventory Data Sources

Source Category	Allegheny County (1.33 km Domain)	Mid-Atlantic (4 km Domain)	Eastern U.S. (12 km Domain)	Continental U.S. (36 km Domain)
Area	MARAMA Alpha2 Interpolated 2018/2028	MARAMA Alpha2 Interpolated 2018/2028	EPA v6.2 MP Interpolated 2017/2025	EPA v6.2 MP Interpolated 2017/2025
Nonroad	EPA v6.2 MP Interpolated 2017/2025	EPA v6.2 MP Interpolated 2017/2025	EPA v6.2 MP Interpolated 2017/2025	EPA v6.2 MP Interpolated 2017/2025
Onroad (Mobile)	MARAMA Alpha2 2018	MARAMA Alpha2 2018	EPA v6.2 MP 2017	EPA v6.2 MP 2017
Point	ACHD Local + MARAMA Alpha2 Interpolated 2018/2028	ACHD Local + MARAMA Alpha2 Interpolated 2018/2028	EPA v6.2 MP Interpolated 2017/2025	EPA v6.2 MP Interpolated 2017/2025
EGU Point	ERTAC v2.4L2 2021	ERTAC v2.4L2 2021	ERTAC v2.4L2 2021	ERTAC v2.4L2 2021
Fires	EPA 2011 v6.2 FIRES	EPA 2011 v6.2 FIRES	EPA 2011 v6.2 FIRES	EPA 2011 v6.2 FIRES
Biogenics	EPA 2011 NEIv2 BEIS	EPA 2011 NEIv2 BEIS	EPA 2011 NEIv2 BEIS	EPA 2011 NEIv2 BEIS
Sea Salt and Lightning	CAMx processors	CAMx processors	CAMx processors	CAMx processors

Notes:

1. MARAMA Alpha2 and EPA v6.2 MP are developed from NEI V2 w/projections
2. Point sources include non-EGUs and small EGUs
3. For onroad (mobile), 2018/2017 are used as conservative estimates for future case
4. For nonroad in 1.33 and 4 km domains, EPA interpolations used due to issues with the MARAMA 2018/2028 files
5. ERTAC 2021 is based on projected EGU emissions for OTC, LADCO, SESARM, and CENSARA regions
6. Fires and biogenics are held constant for future case
7. ACHD Local is projected based on known modifications/shutdowns (other sources held constant)
8. 36/12 km domains are used to develop boundary conditions for 4/1.33 km domains

4.5.6 Spatial surrogates development

EPA has developed spatial allocation surrogates at 36, 12, and 4 km grid resolutions for the CONUS domain using the latest 2010 Census and other new data. These EPA surrogates will be used in 36/12/4 km emission modeling. The spatial surrogates define how county-level non-point emissions estimates are allocated to the modeling grid cells in a mass consistent fashion. If a grid cell contains two or more counties, then both counties can potentially contribute emissions in that grid cell depending on the spatial surrogates. We will develop additional surrogates at 1.33 km resolution for this modeling study.

The EPA's spatial allocate surrogate tool¹⁷ will be used to develop the 1.33 km surrogates. The surrogate tool combines GIS-based data in shapefile format and modeling domain definitions to generate the appropriate gridded surrogate data sets.

Table 4-5 summarizes the spatial surrogates that will be used for spatial allocation in the SMOKE emissions modeling.

¹⁷ https://www.cmascenter.org/sa-tools/documentation/4.2/html/srgtool/SurrogateToolUserGuide_4_2.pdf

Table 4-5. Spatial surrogate distributions used in the SMOKE emissions modeling spatial allocations.

Shapefile	Description	Type	Year	Source
cty_popshu2k_revised	U.S. County Boundaries	Polygon	2005	U.S. Census Bureau
popshu_bg2010	Population/Housing	Polygon	2010	U.S. Census Bureau
rd_ps_tiger2010	Roadways	Line	2010	U.S. Census Bureau
waterway_ntad2011	Waterways	Line	2010	U.S. Bureau of Transport Statistics
rail_tiger2010	Railways	Line	2010	U.S. Census Bureau
exits	Highway Exits	Point	2010	ESRI
mjrds	Major Roads	Line	2010	ESRI
transterm	Transportation Terminals	Point	2010	ESRI
fema_bsf_2002bnd	Building footprints	Polygon	2010	FEMA
heating_fuels_acs0510_c2010	Home heating fuels	Polygon	2010	U.S. Census Bureau

4.5.7 Emission Modeling

During emission processing, annual emission inventories will be speciated to model species, temporally allocated to hourly emissions, and spatially allocated to grid cells as follows.

Spatial Allocation: SMOKE uses spatial surrogates (described above) to spatially distribute emissions to modeling grid cells. Spatial surrogates are generated by overlaying the PGM modeling grid on maps of geospatial indicators appropriate to each source category (e.g., housing units). GIS software is used to calculate the fraction of geospatial indicator coverage in each model grid cell.

Temporal Allocation: SMOKE will be used to allocate oil and gas (O&G), mining and EGU annual emissions to months and across the diurnal cycle to account for seasonal, day-of-week and hour-of-day effects.

Chemical Speciation: The emissions inventories will include the following pollutants: CO, NO_x, VOC, NH₃, SO₂, PM₁₀, and PM_{2.5}. The CB6r2 photochemical mechanism with active local methane emissions will be used for the CAMx

modeling. We will use SMOKE to convert inventoried VOC emissions into the CB6r2 mechanism-specific model species used in CAMx. Chemical speciation profiles will be assigned to inventory sources using cross-referencing data that match the profiles and inventory sources using Federal Information Processing Standard (FIPS) state/county codes and Source Classification Codes (SCCs). Note that CB6r2 chemistry also models local excess methane (ECH4) above background concentrations that will also be specified in the emission inputs. SMOKE also will apply source-specific speciation profiles to convert inventoried NO_x emissions to NO, NO₂, and HONO components. PM emissions will also be speciated to model species, namely primary organic aerosol (POA), primary elemental carbon (PEC), primary nitrate (PNO₃), primary sulfate (PSO₄), primary others (FPRM), and coarse PM (CPRM or PM₁₀-PM_{2.5}).

Quality Assurance: The QA capabilities in SMOKE will be used to generate standard and custom reports for checking the emissions modeling process. SMOKE generates diagnostic files and summary reports which need to be carefully reviewed for error and warning messages.

All pre-merged emissions components will be merged together to generate the final CAMx-ready two-dimensional gridded low-level (layer 1) and point source emission inputs. The CAMx photochemical grid model requires two types of emissions files, as described below, for every episode day; both types are FORTRAN binary files.

Surface-level two-dimensional emissions: This file contains all sources other than elevated point sources that have no or little plume rise, so are emitted directly into the lowest (surface) layer of the model. SMOKE outputs gridded, speciated, hourly emissions files (one for each day) for each source category. The component emissions are then merged together into one surface layer emissions file.

Elevated point source emissions: This file typically consists of emissions from major stationary point sources and includes stack parameters for each source so that plume rise may be calculated within CAMx. SMOKE outputs speciated hourly point source emissions files with stack parameters in an ASCII format that are converted into FORTRAN binary format that is readable by CAMx. If multiple point source files are produced for one day they are merged together into one file.

The surface-level file is a gridded file that is matched to a specific modeling grid. Therefore, we will generate separate CAMx model-ready emission files for the 36,

12, 4 and 1.33 km domains. The elevated point source file is independent of the modeling grid, because it contains horizontal (x, y) coordinates for each point source, and so one file includes all point sources in the modeling grids.

If AERMOD is needed for local modeling, local major sources that contribute excess $PM_{2.5}$ at monitor sites will be identified (see Section 4.5.1 above). The primary $PM_{2.5}$ component for these sources will be tagged for treatment by PSAT or removed from the CAMx modeling input (or, “zeroed-out”) and modeled with AERMOD.

4.6 Receptor Grids

If AERMOD is used, EPA modeling guidance recommends modeling concentrations at “nearby receptors,” receptors close to the $PM_{2.5}$ monitors in the Liberty/Clairton area. The AERMOD receptor locations will mirror the placement of subgrid-scale sampling receptors in the CAMx PiG plume module. For impacts at the Liberty site, a number of techniques will be explored to combine AERMOD and CAMx impacts on an hourly basis. The average AERMOD impacts for the group of receptors can be added to the hourly results from the corresponding 1.33 km grid cells from the CAMx results. Alternatively, interpolation techniques can be used to combine AERMOD and CAMx impacts.

4.7 CAMx Configuration

[Table 4-6](#) summarizes the CAMx configuration to be used in the Allegheny County $PM_{2.5}$ attainment demonstration modeling. The latest version of CAMx (Version 6.30 released in April 2016) at the time of the 2011 base case modeling will be used in the modeling. The model will be configured to predict both ozone and PM species.

CAMx will be set up to perform two-way grid nesting between the 36/12 km domains, with one-way nesting to a separate run of the 4/1.33 km domains using two-way grid nesting. This will allow us to cost-effectively conduct sensitivity tests and evaluate the effects of emission control strategies that are limited to Pennsylvania or Allegheny County without having to carry the extra domains.

The PPM advection solver will be used for horizontal transport along with the spatially varying horizontal diffusion approach based on the method of Smagorinsky (1963). A simple eddy viscosity (or “K-theory”) first-order closure approach will be used for vertical diffusion. The CB6r2 gas-phase chemical mechanism (Hildebrandt

Ruiz and Yarwood, 2013) is selected because it includes the very latest chemical kinetic rates and represents improvements over the CB05 and SAPRC99 chemical mechanisms. Additional CAMx inputs will be as follows:

- Meteorological Inputs: The WRF-derived meteorological fields will be prepared for CAMx using the latest version of WRFCAMx. The CMAQ-Kv method along with the KVPATCH adjustment will be used to generate vertical diffusivity for CAMx. Several alternative vertical diffusivity options (TKE, ACM2, etc.) may be evaluated in sensitivity tests.
- Initial/Boundary Conditions: The boundary conditions for the 36 km CONUS domain simulation will be based on the latest available information at the time of the 2011 base case simulation. Boundary conditions will be extracted from a 2011 simulation of the GEOS-Chem global chemistry model. Existing programs will be used to interpolate from the GEOS-Chem horizontal and vertical coordinate system to the CAMx LCC coordinate system and vertical layer structure and to map the GEOS-Chem chemical species to the CB6r2 chemical mechanism.
- Photolysis Rates: The modeling team will prepare the photolysis inputs as well as albedo/haze/ozone/snow inputs for CAMx based on the TOMS data. The TUV processor will be used to generate clear-sky photolysis rates which will be adjusted for the presence of clouds and aerosols by CAMx. If there are periods of more than a couple of days where daily TOMS data are unavailable, monthly average TOMS data will be used.
- Landuse: The team will generate landuse fields based on USGS GIRAS data.
- Spin-Up Initialization: Ten days of model spin up will be used on the 36/12 km configuration. A shorter spin up (~5 days) will be used for the 4/1.33 km simulations.
- Plume-in-Grid: The Plume-in-Grid (PiG) subgrid-scale plume module would be turned on for all identified local major sources in Allegheny County. Sampling receptor grids with a 100 m grid resolution will be used to obtain concentrations due to the PiG puffs in the vicinity of the key PM monitoring sites in Allegheny County. See Section 4.8 for more details.
- Particulate Source Apportionment: The Particulate Source Apportionment Technology (PSAT) will be turned on for the identified local sources in Allegheny County. If AERMOD is used for local major source primary PM contributions, the effects on the local sources can be removed from the CAMx modeling by subtracting out the PSAT contributions for the local major sources primary PM emissions. See Section 4.9 for more details.

Table 4-6. Science options selected for the CAMx Allegheny County PM_{2.5} modeling.

Science Options	Configuration	Notes
Model Codes	CAMx Version 6.30	Released in April 2016
Horizontal Grid Mesh	36/12/4/1.33 km	
36 km grid	132 x 82 grid cells	36/12 km two-way grid nesting
12 km grid	167 x 176 grid cells	The 12 km model outputs provide BC's for the 4/1.3 km two-way grid nesting
4 km grid	206 x 149 grid cells	Two-way grid nesting between 4/1.33 km domains
1.33 km grid	59 x 59 grid cells	
Vertical Grid Mesh	25 vertical layers, defined by WRF	Layer collapse 36 WRF layers to 25 for CAMx
Grid Interaction	36/12 km two-way nesting 4/1.33 km two-way nesting	4/1.33 km and 1.33 km also set up as standalone configurations
Initial Conditions	10 day spin-up on 36/12 km grid	Clean initial conditions
Boundary Conditions	36 km BC's from global chemistry model	GEOS-Chem global chemistry model
Emissions		
Baseline Emissions Processing	SMOKE, MOVES, SMOKE-BEIS	2007 MANE-VU, LADCO and SEMAP and 2011 NEI
Sub-grid-scale Plumes	Plume-in-Grid for local major sources in Allegheny County	GREASD-PiG NO _x chemistry plume model
Chemistry		
Gas Phase Chemistry	CB6r2	Latest chemical reactions and kinetic rates (Hildebrandt Ruiz and Yarwood, 2013)
Aerosol Chemistry	Coarse-Fine (CF) aerosol scheme	Organic and inorganic aerosol/aqueous phase chemistry using 2 static size modes
Meteorological Processor	WRFCAMx Version 3.2	Compatible with CAMx v6.30
Horizontal Diffusion	Spatially varying	K-theory with Kh grid size dependence
- table continued on next page -		

Science Options	Configuration	Notes
Vertical Diffusion	CMAQ-Kv	Similar to CMAQ's integration methodology
Diffusivity Lower Limit	Kv-min = 0.1-2.0 m ² /s	KVPATCH to set landuse-dependent minimum Kv for layers below 200 m
Deposition Schemes		
Dry Deposition	Zhang dry deposition scheme	LAI-based algorithm using 26 landuse categories (Zhang et al., 2001)
Wet Deposition	Scavenging model for gases and aerosols	Deposition by rain/snow/graupel
Numerics		
Gas Phase Chemistry Solver	EBI Fast Solver	Based on Euler Backward Iterative scheme (Hertel et al., 1993)
Vertical Advection Scheme	Implicit scheme w/ vertical velocity update	
Horizontal Advection Scheme	Piecewise Parabolic Method (PPM) scheme	Piecewise Parabolic Method (PPM) scheme (Colella and Woodward,1984)
Integration Time Step	Wind speed dependent	~20-60 sec (1.3 km); ~0.5-1 min (4 km), 1-5 min (12 km), 5-15 min (36 km)

4.8 Plume-in-Grid Module

The subgrid-scale Plume-in-Grid (PiG) module will be used to track the near source chemistry and plume dynamics of the local major sources. The PiG module simulates plume chemistry and dispersion using a Gaussian puff module and releases its concentrations to the CAMx grid model when the plume size is commensurate with the size of the model grid cell (i.e., 1.33 km). As noted above, each local major source stack will be treated by two point source inputs for their primary PM and gaseous emissions, respectively, which will be tracked by different Source Groups/Regions in the CAMx PSAT source apportionment modeling. This is done so that, if needed, we can remove the contributions of the primary PM emissions from the local major sources and replace them with the AERMOD

simulation of the local major source primary PM emissions to avoid double counting (AERMOD does not treat secondary PM formation).

The PiG module will be run without rendering the PiG concentrations in the CAMx gridded averaging concentration output. Instead, we will obtain the live PiG concentrations on PiG sampling receptor grids. The PiG sampling receptor grid is defined following the same rules as used for defining a CAMx grid nest: the receptor spacing must be an integer multiple of the outer grid resolution (i.e., 4 km) and the sampling grid extent must exactly match the grid cell interfaces (i.e., the 4 km grid cell boundaries). For the PiG sampling grid, we propose to use a grid with 100 m receptor resolution in a 9x7 array of 4 km grid cells as shown in the bigger blue box in [Figure 4-3](#). This results in a 360x280 array of 100 m receptors where concentrations of the live puffs will be obtained. The 100 m PiG sampling grid will include 6 of the 8 PM_{2.5} monitoring sites in Allegheny County. Not included in the large PiG sampling receptor grid is the North Park background monitoring site in northwestern Allegheny County that has the lowest PM concentration in Allegheny County. The other site not included is the Harrison monitor in northeast Allegheny County that has the third highest PM concentrations of the 8 Allegheny County sites. As results at the Harrison monitoring site may be important, a smaller 40x40 100 m PiG receptor grid will be defined for the 4 km grid cell containing the Harrison monitoring site (see smaller blue box in [Figure 4-3](#)).

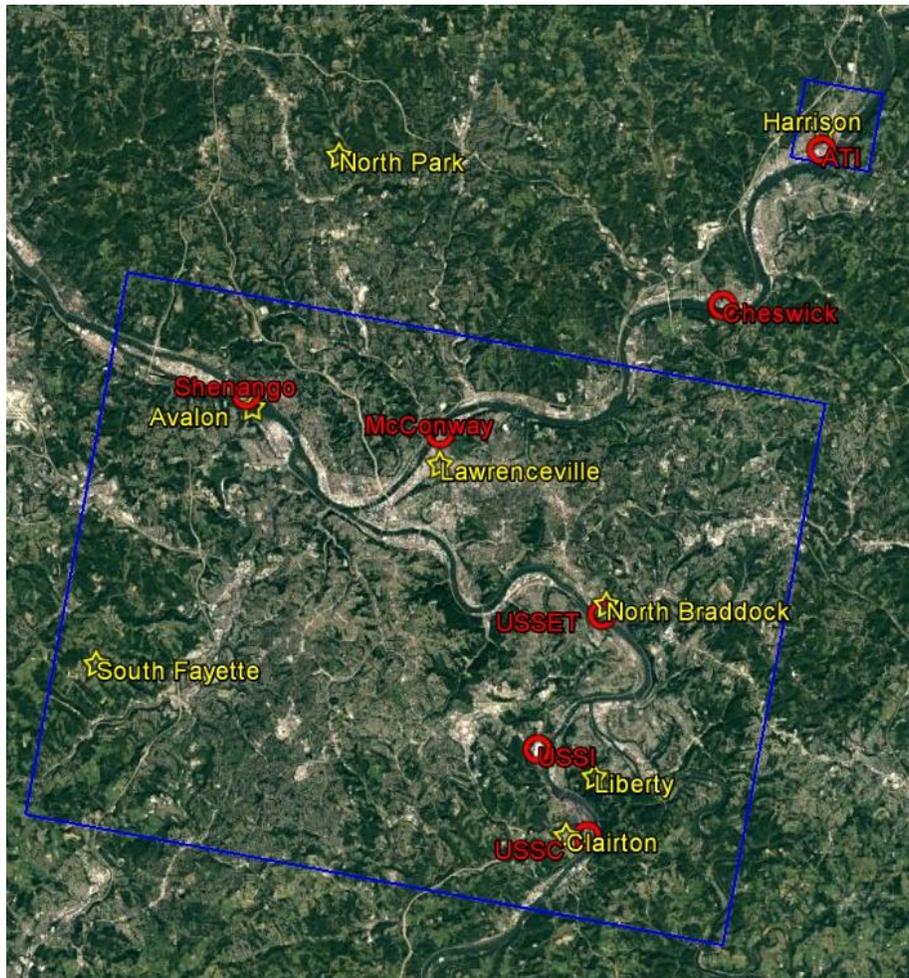


Figure 4-3. PiG live puffs sampling grids (blue boxes) that used a 100 m receptor network along with local major sources (red) and FRM PM_{2.5} monitoring sites (yellow) within Allegheny County

4.9 Source Apportionment Strategy

4.9.1 Overview

The CAMx PSAT source apportionment (SA) tool provides PM source contributions from user-defined Source Groups for up to five families of PM: (1) Sulfate (SO₄); (2) nitrate (NO₃) and ammonium (NH₄); (3) primary PM (EC, OA, FPM and CPM); (4) secondary organic aerosol (SOA); and (5) mercury. Source Groups are typically defined using a user-provided Source Region map of grid cell definitions of geographic regions (e.g., counties or states) and providing separate streams of inputs for different Source Categories (e.g., mobile, EGUs, biogenic, etc.).

Separate PM source apportionment is obtained for each Source Group that is defined as the intersection between Source Regions and Source Categories (e.g., on-road mobile sources from Allegheny County). The Source Region map will provide grid cell definitions of the geographic areas but is not able to exactly define specific geographic regions (e.g., a county) because some grid cells contain a boundary between two regions. In some cases, a large point source associated with one geographic region may lie in a Source Region map grid cell assigned to a different geographic region (e.g., several large EGUs are located along the Ohio river that are in separate states). In this case, the CAMx PSAT point source override feature will be used to link specific point source emissions to their correct Source Region.

4.9.2 PSAT Tracer Families

The SO₄, NO₃/NH₄, and primary PM families of PSAT tracers will be used. The SOA family of tracers will not be used since most SOA is from biogenic emission sources and the pathway for SOA formation is complicated requiring many reactive tracers that would double the run time of the CAMx SA simulation. The CAMx standard model output will allow us to estimate the amount of SOA from biogenic (SOAB) and anthropogenic (SOAA) sources that will provide insight on whether we should turn on the SOA source apportionment for the future year run. The mercury family of PSAT tracers will also not be used since it is not needed.

4.9.3 Definition of PSAT Source Groups for the 2011 Base Case

The CAMx 2011 4/1.33 km base case source apportionment will be configured with 5 Source Groups that will be defined using 5 Source Regions (i.e., one Source Category and 5 Source regions equals 5 Source Groups). The first two Source Regions will be defined by a Source Region map for the 4/1.33 km domains that will separate the domains into two geographic regions:

1. Allegheny County; and
2. Remainder of the 4 km PA domain.

The first two Source Groups/Regions will allow for an assessment of how much of the PM is coming from sources within and outside of Allegheny County. The next 3 Source Groups will be point source emissions from local sources that will use the point source override feature to define their Source Region numbers as follows:

3. Local Major Source Primary PM Emissions (AERMOD Sources);
4. Local Major Source Gaseous Emissions (i.e., PM precursors); and
5. Local Minor Sources Primary PM and Gaseous Emissions.

With IC/BC always included as Source Groups, the CAMx 2011 base case SA simulation would be run with 7 separate Source Groups.

4.9.4 Definition of PSAT Source Groups for the 2021 Future Case

The 2021 future year CAMx 4/1.33 km simulation will be performed using three Source Groups as follows:

1. Local Major Source Primary PM Emissions
2. Local Major Source Gaseous Emissions and Local Minor Source Primary PM and Gaseous Emissions
3. Remainder Anthropogenic and Natural Emissions

With IC/BC always included, there are 5 Source Groups for the initial future year CAMx SA simulation. Future year source groups will be consolidated to save computation time. The Source Groups 1 and 2 correspond to the same local sources as identified in Source Groups 3-5 in the 2011 base case run. Major Local Source PM and gaseous emissions would also be treated by the PiG module using the same 100 m sampling grids maps from the 2011 base case simulation.

5. EVALUATION OF RESULTS

This section delineates the procedures for post-processing modeled results and testing for attainment.

5.1 Meteorological Model Performance Evaluation

Meteorological inputs required by the CAMx model include hourly estimates of the three-dimensional distribution of winds, temperatures, mixing ratio, pressure, clouds, and precipitation, and other physical parameters or diagnosed quantities such as turbulent mixing rates (i.e., eddy diffusivities or K_v) that define planetary boundary layer heights. Accordingly, the objective of the WRF performance evaluation is to assess the adequacy of the surface and aloft meteorological fields for the Allegheny County $PM_{2.5}$ modeling episodes. The planned WRF Model Performance Evaluation is described in the separate WRF Modeling Protocol (Ramboll Environ, 2016).

5.2 Air Quality Model Performance Evaluation

This section describes a range of model testing methodologies potentially available to the modeling team in its efforts to adequately evaluate the performance of the air quality modeling system for the base year annual period. Model performance for CAMx (or combined CAMx/AERMOD) results will be based on the methodology given in the latest EPA Modeling Guidance (EPA, 2014), which recommends four types of model evaluation: Operational, Diagnostic, Dynamic and Probabilistic. The focus of our evaluation will be on the operational evaluation of the model, examining a specific set of gas phase and PM chemical species and a suite of statistical metrics for quantifying model response over the annual cycle. The emphasis is on assessing: (a) how accurately the model predicts observed concentrations; and (b) how accurately the model predicts responses of predicted air quality to changes in inputs.

5.2.1 Context for the Air Quality Model Performance Evaluation

When designing a model performance evaluation, it is important to understand how the modeling results will ultimately be used. EPA has published a draft final guidance document that encompasses ozone, fine particulate, and regional haze/visibility modeling (EPA, 2014). That document not only provides a framework for the Allegheny County model performance evaluation approach, but just as importantly describes the methodology by which to project base-year

pollutant levels to future years. A key concept in EPA's guidance is that the modeling projections are used in a relative sense to scale or roll back the observed individual PM species concentrations. The model-derived ratios of future-year to current-year concentrations are called Relative Response Factors (RRFs). Since the model is used to project future year PM_{2.5} species components rather than total PM_{2.5} mass, then the model performance for each of the PM components is actually more important than for total PM_{2.5} mass for which the standard was written.

These components are:

- Sulfate (SO₄);
- Nitrate (NO₃);
- Ammonium (NH₄);
- Organic Aerosol (OA);
- Elemental Carbon (EC); and
- Other Primary fine Particulate (OPP or Soil).

Therefore, the air quality model testing will concentrate on an operational evaluation of the model predictions for those PM components listed above as well as total PM_{2.5} mass. Where feasible and supported by sufficient measurement data, we will also evaluate the modeling system for its ability to accurately estimate coarse PM mass (CM) and other gas-phase precursors, product and indicator species. The correct simulation of gas-phase oxidant species is needed for PM since correct, unbiased simulation of gas-phase photochemistry is a necessary element of reliable secondary PM predictions. This evaluation will be carried out across the focus area for the entire year and also on a month-by-month to daily basis to help build confidence that the modeling system is operating correctly.

The PM_{2.5} modeling will be based on either CAMx alone or a hybrid modeling system using CAMx and AERMOD. If both CAMx and AERMOD are used, the model performance evaluation for the 2011 Base Year will include analyses of both CAMx and AERMOD predictions against available measurements at monitors throughout the 4 km and 1.33 km modeling domains. Performance will be assessed in two ways: (1) CAMx alone, simulating all sources; and (2) CAMx and AERMOD combined, where the CAMx PSAT source apportionment is used to remove the contributions of the local sources in the CAMx run, and the results will be added to AERMOD results at specific receptor locations to yield a sum of urban/regional and local source impacts.

5.2.2 Multi-Layered Model Testing Process

EPA's draft modeling guidance (EPA, 2014) affirms the recommendations of numerous modeling scientists over the past decade (see, for example, Dennis et al., 1990; Tesche et al., 1990, 1994; Seigneur et al., 2000; Russell and Dennis, 2000; Arnold et al., 2003; Boylan et al., 2003; Tonnesen et al., 2003) that a comprehensive, multi-layered approach to model performance testing should be performed, consisting of the four components: operational, diagnostic, mechanistic (or scientific) and probabilistic. As applied to PM_{2.5} modeling, this multi-layered framework may be viewed conceptually as follows:

- Operational Evaluation: Tests the ability of the model to estimate total and component PM concentrations. This evaluation examines whether the measurements are properly represented by the model predictions but does not necessarily ensure that the model is getting "the right answer for the right reason".
- Diagnostic Evaluation: For PM_{2.5}, this step tests the ability of the model to predict PM chemical composition including PM precursors (e.g., SO_x, NO_x, and NH₃) and associated oxidants (e.g., ozone and nitric acid), PM size distribution, temporal variation, spatial variation, and mass fluxes.
- Dynamic Evaluation: Tests the ability of the model to predict the response of PM to changes in variables such as emissions and meteorology.
- Probabilistic Evaluation: Takes into account the uncertainties associated with the model predictions and observations of PM.

Within the constraints of the SIP schedule and resources, the model evaluation effort will attempt to include elements of each of these components. The operational evaluation will obviously receive the greatest attention since this is the primary thrust of EPA's final modeling guidance. However, we will consider, where feasible and appropriate, diagnostic and mechanistic tests (e.g., use of probing tools, indicator species and ratios, aloft model evaluations, urban vs. rural performance analyses), traditional sensitivity simulations to explore uncertainty, and comparison of the model performance of this study with those from other groups.

5.2.3 Development of Consistent Evaluation Data Sets

The ground-level model evaluation database will be developed using several routine and research-grade databases. The first is the routine gas-phase concentration

measurements for ozone, NO, NO₂ and CO archived in EPA's Aerometric Information Retrieval System/Air Quality System (AIRS/AQS) database¹⁸. Other sources of information come from the various PM monitoring networks in the U.S. These include: IMPROVE¹⁹, CASTNet²⁰, SEARCH²¹, FRM²², CSN²³ and NADP²⁴ networks. Typically, these networks provide ozone, other gas phase precursors and product species, PM mass and species, deposition, and/or visibility measurements. Of key importance for the current modeling will be the AIRS/AQS, FRM, and CSN sites that measure ozone (and some precursors), total PM_{2.5} mass, and speciated PM_{2.5} components, respectively.

An important consideration in evaluating PM models is that each monitoring network employs a unique measurement approach that "measures" a different amount of a given species. For example, the IMPROVE network only speciates PM_{2.5}, so any sulfate or nitrate in the coarse mode (PM₁₀-PM_{2.5}) is included in the coarse mass (CM) "measurement". Thus, CAMx will be evaluated separately for each monitoring network. Additionally, there is often ambiguity in the mapping of modeled PM species to measurements. For example, PM monitors measure only the carbon component of OC, whereas in the model the entire mass of organics (OA or Organic Aerosol) is simulated, which includes carbon and the other elements attached to the carbon (e.g., hydrogen and oxygen). Thus, a factor is assumed to adjust the measured OC to OA. In the past an OA/OC factor of 1.4 has been used based on urban scale measurements of fresh OC emissions, and this has been the factor used in the original IMPROVE reconstructed mass equation (Malm et al., 2000). However, this OA/OC factor is likely too low, especially for aged OC compounds where ratios of 1.4 to 2.2 have been observed (Turpin and Lim, 2001). A recent study has shown that summertime OA/OC ratios are larger than wintertime values across the U.S. and that winter values are larger in the eastern U.S. than in the West (Simon et al., 2011). Currently an average OA/OC ratio value of 1.8 has been adopted for revised IMPROVE reconstructed mass equation.

(18) <https://www.epa.gov/outdoor-air-quality-data>

(19) <http://vista.cira.colostate.edu/Improve>

(20) <http://java.epa.gov/castnet/>

(21) <http://www.atmospheric-research.com>

(22) <http://www.epa.gov/ttnamti1/pmfrm.html>

(23) <https://www3.epa.gov/ttn/amtic/speciepg.html>

(24) <http://nadp.sws.uiuc.edu/>

However, in the urban Allegheny County region where we expect there to be fresh OA emissions an OA/OC ratio closer to 1.4 may be more appropriate. An alternative approach is to convert modeled OA to OC using species-specific OA/OC ratios (higher OA/OC ratios for more oxygenated organic compounds).

There are eight FRM PM_{2.5} monitoring sites within Allegheny County, including Avalon, Lawrenceville, Liberty, South Fayette, North Park, Harrison, North Braddock, and Clairton. Speciated PM_{2.5} CSN monitoring data is available from 2 sites, Liberty and Lawrenceville. Hourly AQS monitoring data for TEOM PM_{2.5} are available at Liberty and Lawrenceville.

5.2.4 Air Quality Model Evaluation Tools

The current modeling guidance document (EPA, 2014) focuses more on a holistic model evaluation approach compared to the original 1-hour ozone and draft PM guidance (EPA, 1991; 2001). Not only should we assess how well the model matches the observation, but we also need to determine whether the model is correctly simulating the processes that produce the elevated concentrations, which includes comparing against a conceptual model. [Table 5-1](#) lists a standard set of statistical performance measures that can be used to evaluate fine particulate models. The Atmospheric Model Evaluation Tool (AMET²⁵) will be the primary software tool used in the model evaluation. AMET can generate the whole suite of model performance metrics (Table 5-1) and graphical displays of model performance. These graphical displays include scatter plots, density plots, spatial bias and error plots, soccer plots and time series.

Ideally, the operational evaluation described above will confirm that the modeling system is performing consistently with its scientific formulation, technical implementation, and at a level that is at least as reliable as other current state-of-science methods. Should unforeseen model performance problems arise in the base case simulation, it may be necessary to draw into the evaluation supplemental diagnostic tools to aid in model testing. These diagnostic techniques are loosely referred to as “probing tools”. The actual need for their use, if any, can only be determined once the initial CAMx operational evaluation is completed. Should such diagnostic methods actually be needed, their usage would require additional

⁽²⁵⁾ https://www.cmascenter.org/amet/documentation/1.2/AMET_Users_Guide_v1.2.1.pdf

resources. Below, we identify the types of probing tools that could be brought to bear should their use become necessary.

Current “one-atmosphere” models such as CAMx have been outfitted with a number of “probing tools” that have proven to be very useful in testing and improving model performance and in evaluating emission control strategies. Among the probing tools available in CAMx are: (a) ozone and particulate source apportionment technology (OSAT and PSAT), (b) process analysis (PA), and (c) the decoupled direct method (DDM) of sensitivity analysis.

Because application of all these probing tools—source apportionment, DDM, and PA—are computational intensive and require a fair amount of analysis time to reap the benefits of using the methods, they do not lend themselves directly to the full simulation period. However, each method has potential for use in addressing key episodic periods or geographical locations in Allegheny County where performance in the base case simulation may present a problem or where particular attention needs to be focused on emissions controls (a specific PM_{2.5} violation monitor). In such focused applications, one or more of these probing tools may indeed serve a purpose and will be considered where appropriate.

Table 5-1. Core statistical measures to be used in the Allegheny County air quality model evaluation with ground-level data.

Statistical Measure	Mathematical Expression	Notes
Accuracy of paired peak (A_p)	$\frac{P - O_{peak}}{O_{peak}}$	P_{peak} = paired (in both time and space) peak prediction
Coefficient of determination (R²)	$\frac{\left[\sum_{i=1}^N (P_i - \bar{P})(O_i - \bar{O}) \right]^2}{\sum_{i=1}^N (P_i - \bar{P})^2 \sum_{i=1}^N (O_i - \bar{O})^2}$	P_i = prediction at time and location i ; O_i = observation at time and location i ; \bar{P} = arithmetic average of P_i , $i=1,2,\dots,N$; \bar{O} = arithmetic average of O_i , $i=1,2,\dots,N$
Normalized Mean Error (NME)	$\frac{\sum_{i=1}^N P_i - O_i }{\sum_{i=1}^N O_i}$	Reported as %
Root Mean Square Error (RMSE)	$\left[\frac{1}{N} \sum_{i=1}^N (P_i - O_i)^2 \right]^{1/2}$	Reported as %
Fractional Gross Error (FE)	$\frac{2}{N} \sum_{i=1}^N \frac{ P_i - O_i }{P_i + O_i}$	Reported as %
Mean Absolute Gross Error (MAGE)	$\frac{1}{N} \sum_{i=1}^N P_i - O_i $	Reported as concentration (e.g., $\mu\text{g}/\text{m}^3$)
Mean Normalized Gross Error (MNGE)	$\frac{1}{N} \sum_{i=1}^N \frac{ P_i - O_i }{O_i}$	Reported as %
Mean Bias (MB)	$\frac{1}{N} \sum_{i=1}^N (P_i - O_i)$	Reported as concentration (e.g., $\mu\text{g}/\text{m}^3$)
Mean Normalized Bias (MNB)	$\frac{1}{N} \sum_{i=1}^N \frac{(P_i - O_i)}{O_i}$	Reported as %
- table continued on next page -		

Statistical Measure	Mathematical Expression	Notes
Mean Fractionalized Bias (Fractional Bias, MFB)	$\frac{2}{N} \sum_{i=1}^N \left(\frac{P_i - O_i}{P_i + O_i} \right)$	Reported as %
Normalized Mean Bias (NMB)	$\frac{\sum_{i=1}^N (P_i - O_i)}{\sum_{i=1}^N O_i}$	Reported as %
Bias Factor (BF)	$\frac{1}{N} \sum_{i=1}^N \left(\frac{P_i}{O_i} \right)$	Reported as BF:1 or 1:BF or in fractional notation (BF/1 or 1/BF).

5.3 Attainment Tests

This section provides a summary of how the modeling results will be used to demonstrate attainment of the PM_{2.5} NAAQS in Allegheny County. It is expected that at least two types of CAMx simulations (and potentially hybrid CAMx/AERMOD simulations) will be performed:

- 2011 Base Case representing current emission conditions.
- 2021 “Base Case” where emission reflect growth, shut-downs, and “on-the-books” controls.
- Optional: 2021 “Control Case” that includes additional or revised controls

The procedures for demonstrating attainment of the PM_{2.5} NAAQS are given in EPA’s draft modeling guidance dated December 2014 (EPA, 2014). The EPA guidance (EPA, 2014) approach for making future year PM_{2.5} DV projections has been codified in the Modeled Attainment Test Software (MATS) and Software for Modeled Attainment Test – Community Edition (SMAT-CE).

These procedures use a modeled attainment test²⁶ that was first used to project future year PM_{2.5} DVs for the Clean Air Interstate Rule (CAIR)²⁷. The procedures use the modeling results in a relative sense to scale the observed PM_{2.5} DVs from the current- to future-year. The scaling factors are called Relative Response Factors

²⁶ <https://archive.epa.gov/airmarkets/programs/cair/web/pdf/revised-smat.pdf>

²⁷ <https://archive.epa.gov/airmarkets/programs/cair/web/html/index.html>

(RRFs) and are monitor- and PM species-specific and are based on the ratio of the future-year to current-year modeling results. The starting point for the PM_{2.5} DV projections is a site-specific baseline design value (DVB) that is calculated by averaging three DV periods centered on the base year under study, which is 2011 for the Allegheny County PM_{2.5} DV projections. Thus, the DVB will be based on three PM_{2.5} DVs (three year average of annual mean PM_{2.5} concentrations for the annual standard) of the 2009-2011, 2010-2012, and 2011-2013 periods. In this averaging scheme, PM_{2.5} concentrations from 2011 are “weighted” three times, 2010 and 2012 are weighted twice, and 2009 and 2013 are weighted once.

The Speciated Model Attainment Test procedures consists of two components: (1) the combination of total PM_{2.5} mass measurements from the Federal Reference Method (FRM) with speciated PM_{2.5} measurements such as those from the Chemical Speciation Network (CSN); and (2) the combination of the modeling results with the speciated FRM PM_{2.5} DVs to obtain future-year projected PM_{2.5} DVs.

One advantage to using the CAMx/PiG modeling system for making future year PM_{2.5} DV projections is that the CAMx modeling results can be used directly with the MATS tool. However, if the hybrid CAMx and AERMOD modeling approach is used, then special procedures must be utilized to account for the local source contributions and differences in the two modeling systems.

5.3.1 Speciation of FRM PM_{2.5} Mass Measurements

PM_{2.5} attainment/nonattainment can only be determined from the FRM (or FRM-equivalent) PM_{2.5} measurements, which measure just total PM_{2.5} mass. The FRM PM_{2.5} measurements are used to develop the PM_{2.5} DVs that determine an area’s attainment classification, and are used as the starting point for projecting future-year PM_{2.5} DVs to demonstrate attainment. Thus, representative speciated PM_{2.5} measurements need to be mapped to the FRM total mass measurements for the modeled attainment test. For most areas there is either a co-located speciated PM_{2.5} site, or such a site in the vicinity that can be used in the mapping. However, in some cases there is no nearby speciated PM_{2.5} site so speciation must be developed from all available data in the region and interpolated to the FRM monitoring site.

Speciated PM_{2.5} measurements are routinely collected on the same 1-in-3 day sampling schedule as used by the FRM network. Two routine speciated PM

monitoring networks are available across the U.S.: the Chemical Speciation Network (CSN) and the Interagency Monitoring of Protected Visual Environments (IMPROVE) networks. The FRM, CSN, and IMPROVE networks use different measurement technologies and each exhibits its own measurement artifacts. As the FRM is the de-facto regulatory definition of PM_{2.5}, EPA has developed procedures for adjusting the CSN and IMPROVE speciated PM_{2.5} measurements to account for the measurement artifacts of the different networks and to make the speciated PM measurements consistent with the FRM PM_{2.5} mass measurements. These adjustments include the following:

- Adjust nitrates downward to account for volatilization off of the FRM nylon filter;
- Add particle-bound water (PBW) that is assumed to be associated with nitrate and sulfate in the FRM measurements (hygroscopic species); and
- Estimate total carbonaceous mass accounting for the lack of blank-correction in the speciated PM_{2.5} measurements.

The resultant fine particle chemical speciation approach has been named the “sulfates, adjusted nitrates, derived water, inferred carbonaceous material balance approach” or SANDWICH. Details on the SANDWICH procedures are given in Frank (2006a,b).

As noted previously, for Allegheny County, CSN speciated PM_{2.5} measurements are available at the Liberty and Lawrenceville monitoring sites.

5.3.2 Special Considerations for Local-Scale Primary PM_{2.5} Impacts

There are several local industrial and other sources that contribute to PM_{2.5} concentrations at the Liberty FRM monitor. The contributions of these local sources will be evaluated either using the CAMx model with PiG and high resolution receptor grids, or with the AERMOD steady-state Gaussian plume model. If the CAMx PiG is used to simulate the local source contributions then the standard EPA Speciated Model Attainment Tests procedures in MATS and SMAT-CE can be used to make 2021 PM_{2.5} DV projections. However, if a hybrid CAMx/AERMOD modeling approach is used, then special considerations must be made. EPA’s modeling guidance (EPA, 2007; 2014) addresses an approach for dealing with the local-scale PM_{2.5} contributions including how to combine regional photochemical grid modeling results with local-scale Gaussian plume modeling results. In this approach, the current year observed PM_{2.5} DV is split into local and regional components. RRFs

that consist of the ratio of 2021 to 2011 modeling results are developed using AERMOD and CAMx and they are used to project the local and regional components of the current year DV to the future year (2021). The two components are then combined to obtain the projected 2021 PM_{2.5} DV. MATS and SMAT-CE do not treat this approach, but Ramboll Environ has developed tools for making the hybrid PM_{2.5} projection approach that have been used for both Birmingham and St. Louis modeling demonstrations.

5.4 Weight of Evidence Analyses

EPA's guidance recommends several options for supplemental analyses when making a "weight of evidence" (WOE) determination. These options are based on the results of the modeled attainment test, specifically how far above the standard the modeled future year concentrations are projected to be. Furthermore, there are three general types of WOE analyses in support of the attainment demonstration: (a) use of air quality model output; (b) examination of air quality and emissions trends; and (c) the use of corroborative modeling. We will consider the use of these methods in conducting the CAMx modeling because it could significantly strengthen the credibility and reliability of the modeling available to the states for their subsequent use. The exact details of the WOE analyses must wait until the Allegheny County modeling study evolves further. It is premature to prescribe which, if any, of the WOE analyses would be performed since the model's level of performance with the base case modeling is obviously not known at this time. It is a good idea to perform WOE analysis to corroborate the modeled attainment demonstration. Many of the WOE analyses are independent of the photochemical modeling being conducted by the study team and can potentially be performed by the project sponsors or interested stakeholders. Below are thoughts regarding what would likely be considered as part of the WOE analyses.

- Use of Emissions and Air Quality Trends: Emissions and air quality trend analysis is always an important component of a WOE analysis. When combined with meteorological analysis of the yearly ozone formation potential, it can be used to determine whether actual trends can corroborate the model projected determination of whether future-year air quality goals are achieved. Traditionally, these types of analyses are performed by the lead agency's own staff as part of their SIP development.
- Use of Corroborative Observational Modeling: While regulatory modeling studies for ozone attainment demonstrations have traditionally relied upon photochemical models to evaluate ozone control strategies, there has recently been growing emphasis on the use of data-driven models to

corroborate the findings of air quality models. As noted, EPA's guidance (EPA, 2014) now encourages the use of such observation-based (OBM) or observation-driven (OBD) models. These include receptor models such as Chemical Mass Balance (CMB) model and the Positive Matrix Factorization (PMF) model. We will consider the merits of using these techniques as supportive WOE. While the OBD/OBM models cannot predict future year air quality levels, they do provide useful corroborative information on the extent to which ozone formation in specific sub-regions may be VOC-limited or NO_x-limited, for example, or where controls on ammonia or SO₂ emissions might be most influential in reducing PM_{2.5}. Information of this type, together with results of DDM, PA, OSAT and PSAT as well as traditional "brute-force" sensitivity simulations, can be helpful in postulating emissions control scenarios since it helps focus on which pollutant(s) to control.

- Use of Corroborative Photochemical Modeling: Noteworthy in EPA's ozone, PM, and regional haze guidance documents is the encouragement of the use of alternative modeling methods to corroborate the performance findings and control strategy response of the primary air quality simulation model (EPA, 2014). This endorsement of the use of corroborative methodologies stems from the common understanding that no single photochemical modeling system can be expected to provide exact predictions of the observed ozone and PM species concentrations, especially over time scales spanning 1-hour to 1 year. Although the photochemical/PM models identified in EPA's modeling guidance document possess many up-to-date science and computational features, there still can be important differences in modeled gas-phase and aerosol predictions when alternative models are exercised with identical and/or similar inputs. Use of an alternative air quality modeling system (e.g., CMAQ) will permit the more explicit identification the expected range of model uncertainty and to corroborate the general effectiveness of the pollutant control strategies. Although such analysis will be limited by available resources.

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Appendix F.3

AERMOD Modeling Protocol

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AERMOD Modeling Protocol

**Allegheny County, PA PM_{2.5}
Nonattainment Area, 2012 NAAQS**

**Allegheny County Health Department
Air Quality Program**

July 2018 (Rev. 10/18)

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1 OVERVIEW

Based on review of the CAMx¹ modeling results for the Allegheny County, PA PM_{2.5} State Implementation Plan (SIP) for the 2012 National Ambient Air Quality Standards (NAAQS), the Allegheny County Health Department (ACHD) determined that additional local source modeling was needed for a refined analysis for the Liberty monitor site. The procedures outlined in this document constitute an air dispersion modeling protocol for a local area analysis (LAA) to demonstrate attainment for the Liberty site.

This protocol is a complement to the procedures outlined for the WRF² and CAMx modeling (Ramboll Environ, 2016b, 2017a) as well as the model evaluations (Ramboll Environ, 2016c, 2017b). The WRF/CAMx configuration was designed to allow for the separate tracking of large local source impacts in the case that a refined local modeling demonstration might be necessitated. The regional component of the CAMx results without the largest local source impacts will be combined with local source modeling for a more representative calculation of the projected PM_{2.5} species at Liberty. Projected design values from the CAMx modeling effort (Ramboll Environ, 2018) will be used as the final values for all sites except Liberty.

ACHD will utilize the U.S. Environmental Protection Agency (EPA) preferred AERMOD³ modeling system for this demonstration, with an alternative BLP⁴/AERMOD hybrid approach for buoyant line sources. AERMOD is recommended for near-field modeling (< 50 km) for primary pollutant simulations according to the Guideline on Air Quality Models⁵ (U.S. EPA, 2017). AERMOD has been demonstrated to perform adequately for many applications based on the results obtained from comprehensive field study results (Cimorelli et al., 2005; Perry et al., 2005).

The alternative BLP/AERMOD hybrid modeling approach uses plume rises calculated by the former preferred BLP model to derive release heights for elevated line volume sources in AERMOD. An alternative model demonstration for this technique was conducted and submitted to EPA Region 3 on July 27, 2018 (ACHD, 2018). This alternative technique was also used for the Allegheny, PA SO₂ SIP for the 2010 NAAQS (ACHD, 2017). Alternative modeling demonstrations require approval from the corresponding EPA regional office along with concurrence from the EPA Model Clearinghouse. The alternative technique was approved by EPA Region 3 on August 16, 2018, with concurrence from the Model Clearinghouse on August 10, 2018.⁶ (Documents regarding the alternative modeling demonstration will be included in Appendix H of the SIP.)

¹ Comprehensive Air Quality Model with Extensions (<http://www.camx.com/>)

² Weather Research and Forecasting Model (<https://www.mmm.ucar.edu/weather-research-and-forecasting-model>)

³ American Meteorological Society/Environmental Protection Agency Regulatory Model (<https://www.epa.gov/scram/air-quality-dispersion-modeling-preferred-and-recommended-models>)

⁴ Buoyant Line and Point Source dispersion model (<https://www3.epa.gov/ttn/scram/userg/regmod/blpug.pdf>)

⁵ Guideline on Air Quality Models, 40 CFR Part 51 Appendix W (https://www3.epa.gov/ttn/scram/guidance/guide/appw_17.pdf)

⁶ <https://cfpub.epa.gov/oarweb/MCHISRS/index.cfm?fuseaction=main.resultdetails&recnum=18-III-01>

2 PROBLEM STATEMENT

The CAMx protocol (Ramboll Environ, 2017a) provides a description of the nature of the localized PM_{2.5} problem at the Liberty monitor, along with monitored design values through 2016. Updated PM_{2.5} design values through 2017 are shown in Appendix A of this protocol.

Attainment tests based on the CAMx results using the EPA modeled attainment test software⁷ showed projected design values that were below the 2012 NAAQS⁸ for all sites except Liberty (Ramboll Environ, 2018). These attainment tests were based on modeled data that projects weighted monitored design values from 2009-2013 to a future case year of 2021.

The CAMx modeling – which included the use of Plume-in-Grid (PiG) for selected large sources of primary PM_{2.5} – showed good model performance at all sites in Allegheny County, including Liberty (Ramboll Environ, 2017b). However, the Liberty monitor failed to show attainment of the NAAQS likely due to the following factors:

- ERTAC⁹ 2.4L2 projections for electric generating unit (EGU) emissions used in the CAMx modeling were very conservative for 2021 EGU emissions. Compared to ERTAC 2.5 projection and recent actual CAMD¹⁰ emissions, future SO₂ and NO_x emissions may have been overestimated considerably in the Midwest and Mid-Atlantic region. (More information will be included in the Weight of Evidence section and Appendix K of the SIP.) Overestimates of SO₂ and NO_x would cause overprediction of future case modeled ammonium sulfates/nitrates as well as particle-bound water with the CAMx impacts.
- Some local primary PM_{2.5} emissions may have been overestimated with the inventory used for the CAMx modeling. More recent stack tests or emission factors for primary PM_{2.5} can be used for a refined modeling scenario with AERMOD.
- The spatial resolution of 1.33 km CAMx gridded cells, used for all locations in Allegheny County, may be too large to properly simulate localized impacts at Liberty. Impacts are averaged throughout a grid cell, potentially smoothing over concentration gradients (high or low) near the Liberty monitor. Additionally, the Liberty monitor lies near the edge of a 1.33 km grid cell, and the use of recommended 3 x 3 cell averages for MATS calculations may not have been adequate for the Liberty location.
- Source characterization with CAMx may not have been fully representative of some sources near Liberty, specifically at the U. S. Steel Clairton Plant. All local stationary sources were configured in CAMx as point sources, with constant emissions and fixed stack parameters. Refined modeling with AERMOD can more accurately account for many processes with the use

⁷ Modeled Attainment Test Software (MATS) version 2.6.1, and Software for the Modeled Attainment Test - Community Edition (SMAT-CE) version 1.2 (<https://www.epa.gov/scram/photochemical-modeling-tools>)

⁸ Annual standard = 12.0 µg/m³; 24-hour standard = 35 µg/m³ (<https://www.epa.gov/criteria-air-pollutants/naaqs-table>)

⁹ Eastern Regional Technical Advisory Committee (<https://www.epa.gov/air-emissions-inventories/eastern-regional-technical-advisory-committee-ertac-electricity-generating>)

¹⁰ EPA's Clean Air Markets Division (<https://www.epa.gov/airmarkets>)

of different source types (volumes, lines, etc.), building parameters (for downwash), and varying release heights (buoyant volumes).

- Based on analysis of the monitored CSN¹¹ speciation data compared to CAMx modeled species, species are not being properly apportioned by the modeled results and the EPA SANDWICH¹² reconstruction method used by the attainment test software. Modeled primary excess PM_{2.5} does not directly translate into monitored primary excess by species, and localized impacts in this case are likely better accounted for when modeling a local primary component separately from the regional components.

Based on the above factors, refined LAA modeling with AERMOD can better simulate localized impacts at Liberty. The methodology of combining local impacts from a dispersion model with regional impacts from a photochemical grid model is discussed in the 2014 draft modeling guidance (U.S. EPA, 2014). However, such combination of impacts is not available with the current versions of the EPA attainment test software, and the calculations must therefore be performed according to EPA guidance by spreadsheet or other tools. Excel will be used for the attainment calculations for this local analysis.

The sources modeled with the refined LAA modeling will include the following

- Near-field sources: U. S. Steel (USS) Mon Valley Works (Clairton, Irvin, ET Plants)
- Distant sources: Shenango, Allegheny Ludlum, McConway & Torley

These sources are the same sources that were modeled as PiG sources and tracked with the Particulate Source Apportionment Technology (PSAT) in CAMx. Primary PM_{2.5} impacts from these sources have been subtracted from the regional/widespread contributions of the CAMx impacts. The refined modeling will lump the AERMOD impacts from these sources into a new component called local primary material (LPM), to be summed with the non-LPM CAMx impacts according to the SANDWICH reconstruction method to generate the final design values at Liberty.

Meteorological inputs will be extracted from WRF using the Mesoscale Model Interface Program (MMIF) for prognostic site-specific data at each source location. This is consistent with the CAMx modeling, using the same meteorological inputs but for different models.

Some assumptions will also be made for this refined modeling to better account for non-steady state conditions for the model scenario, including the use of the alternative BLP/AERMOD approach for buoyant lines and an expanded receptor grid to represent the Liberty monitor site.

¹¹ Chemical Speciation Network (<https://www3.epa.gov/ttnamti1/speciepg.html>)

¹² Sulfate, Adjusted Nitrate, Derived Water, Inferred Carbon Hybrid material balance approach

3 MODEL SELECTION

This section outlines the model selection for the Liberty local area analysis. Modeling is designed to conform to the Guideline on Air Quality Models (U.S. EPA, 2017).

3.1 Model Selection

The AERMOD modeling system version 18081, including the latest versions of preprocessors and related programs, will be used for the local source modeling.

The attainment demonstration will utilize the most recent version of the AERMOD modeling system (version 18081). AERMOD is the preferred model for near-field regulatory modeling applications. Besides AERMOD itself, the current regulatory components include:

- AERMET (v. 18081), the meteorological preprocessor for AERMOD
- AERMAP (v. 18081), the terrain preprocessor for AERMOD

The non-regulatory components of AERMOD that will be employed in this modeling demonstration are:

- BPIPPRIME (v. 04274), the building parameter preprocessor for AERMOD
- MMIF (v. 3.4), the prognostic meteorological preprocessor for dispersion models
- AERSURFACE (v. 13016), the surface characteristics processor

The AERMOD modeling system flowchart is shown below in Figure 3-1.

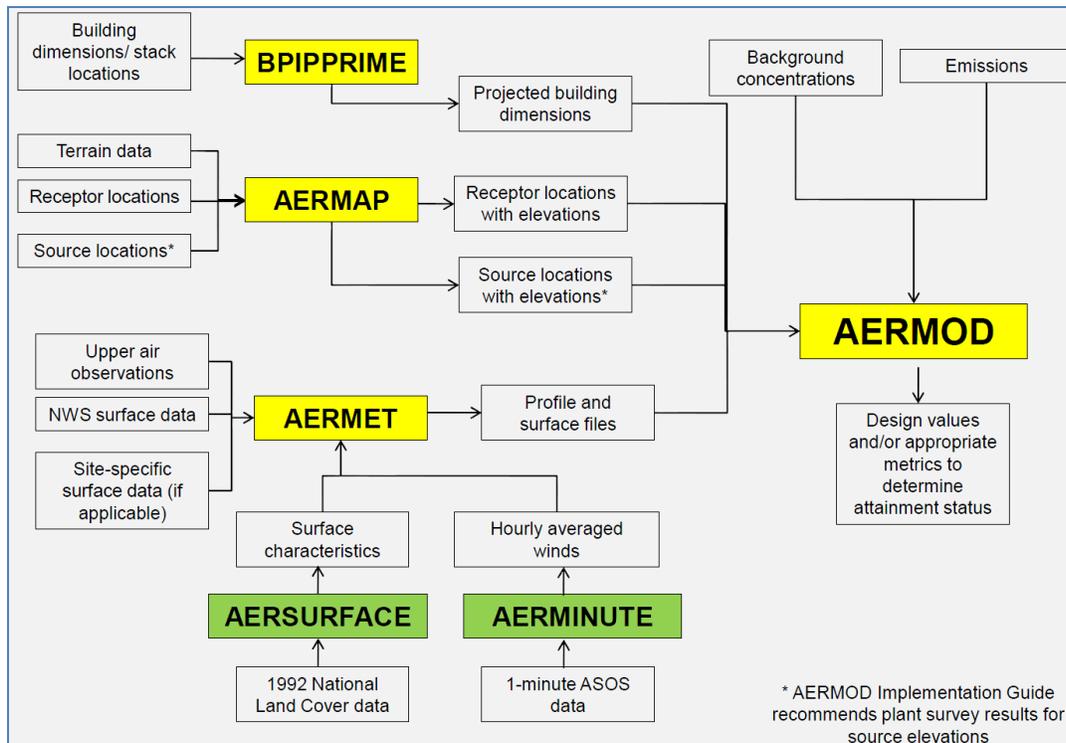


Figure 3-1. AERMOD Modeling System

With the use of MMIF data, neither the AERSURFACE nor AERMINUTE preprocessor is used, since all surface characteristics and wind data are generated by the WRF model. (AERSURFACE will however be used for determination of rural or urban modeling options.) MMIF also allows for the extraction of either AERMOD-ready or AERMET-ready files. Based on current MMIF guidance (U.S. EPA, 2018d), the use of AERMET-files is preferred and will be used for this demonstration.

Emissions inputs will be based on actual emissions for the base case 2011 and projected future case 2021 scenarios. Background concentrations will not be used, as the CAMx-based impacts without LPM will represent the background component of PM_{2.5} at Liberty. Additionally, not shown in Figure 3-1, the alternative modeling approach using BLP-based plume rises in conjunction with AERMOD volume sources will also be employed.

3.2 Model Year

While three years of prognostic data are preferred for regulatory applications, only one year of data was available based on the WRF/CAMx configuration. The year 2011 will therefore be selected as the meteorological year for AERMET/AERMOD, with emissions projected to year 2021 for the future (control) case. ACHD deemed 2011 to be an appropriate year to represent typical meteorological conditions for the area for the weighted timeframe (2009-2013) as well as more recent years (see Appendix B of the SIP). MMIF data will be derived from the WRF 1.33 km and 0.444 km domains as site-specific data for the sources modeled, combined via post-processing.

4 MODELING PROCEDURES

ACHD will prepare and run AERMOD in order to adequately simulate the impacts of primary $PM_{2.5}$ at the Liberty monitor site. These local source impacts will then be combined with the regional CAMx impacts without the local source influences. This section describes the procedures for inputs, preprocessing, model configuration, and post-processing to be used for the modeling demonstration.

4.1 Modeling Domain

The domain for AERMOD (specifically for AERMAP terrain preprocessing) should be appropriate to account for terrain influencing the modeled area. The modeling domain will be set to a 12 x 12 km rectangle centered on the Liberty monitor, shown in orange in Figure 4-1 below.



Figure 4-1. Modeling Domain for the Liberty Area

Terrain is similar throughout most of Allegheny County, with the most variation in elevation in the river valleys. The 12 x 12 km setting should be sufficient to encompass elevations in the near-field area around Liberty and to generate the correct critical hill heights with AERMAP.

4.2 Geophysical Data

Terrain and land use processing will include the most recent data available for use in the AERMOD system. This includes the following:

- USGS NED¹³ terrain data, 0.3 (10 m) arc-second resolution
- MRLC NLCD¹⁴ 1992 land cover data, 1 arc-second (30 m) resolution

A contour map of NED 1 arc-second (30 m resolution) terrain data for all of Allegheny County is shown in Figure 4-2, with contours shown in black and white (rivers shown in blue). A close up of terrain for the Liberty area is shown in Figure 4-3.

The NLCD 1992 land cover map for Allegheny County is shown in Figure 4-4. Note that for MMIF meteorological output, the AERSURFACE preprocessor is not used since MMIF generates surface characteristics specific to each grid cell based on NLCD land cover.

¹³ United States Geological Survey (USGS) National Elevation Dataset (NED) (<https://viewer.nationalmap.gov/launch/>)

¹⁴ Multi-Resolution Land Characteristics (MRLC) National Land Cover Database (NLCD) (<https://www.mrlc.gov/>)



Figure 4-2. NED Terrain Data for Allegheny County

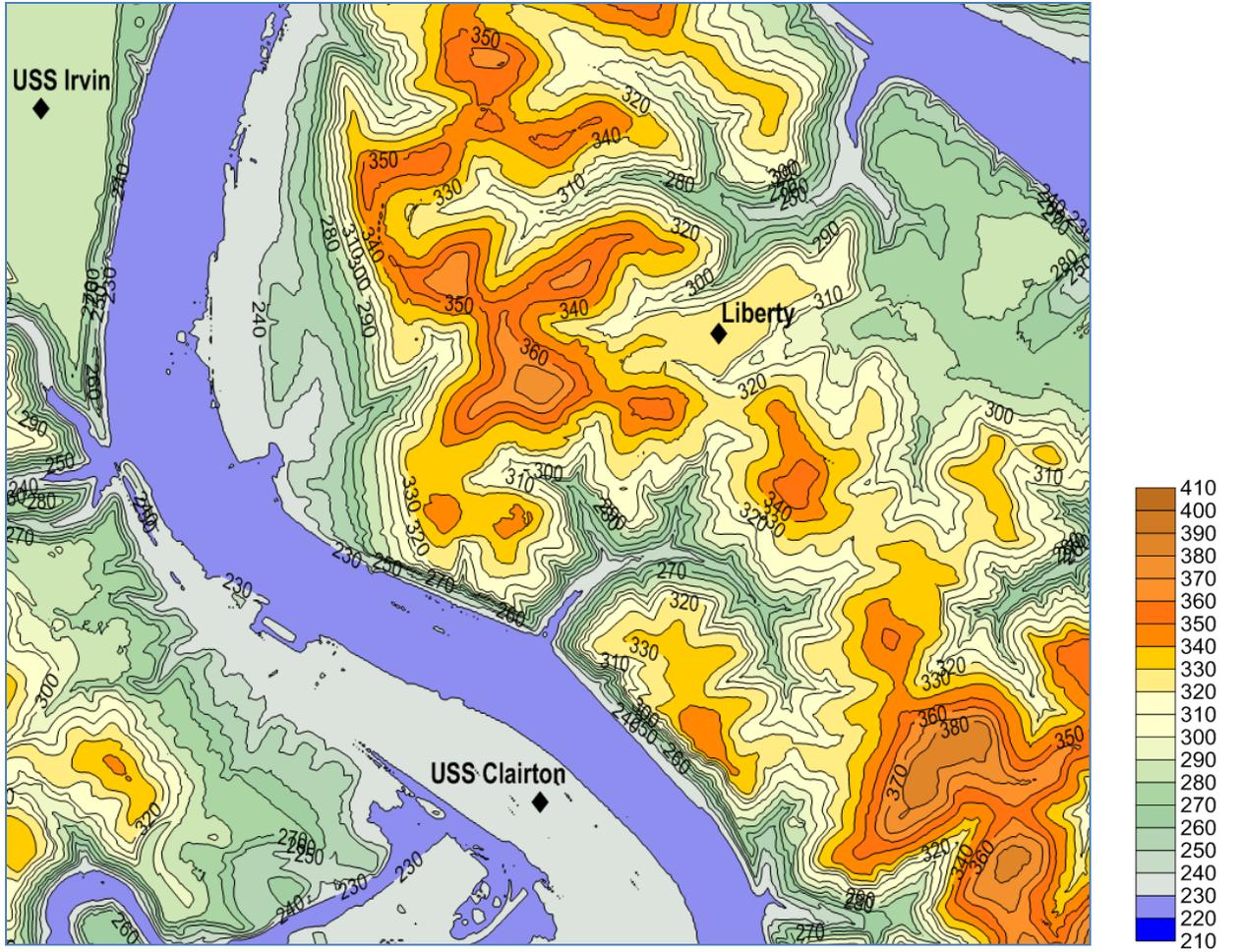


Figure 4-3. Close-Up of Terrain Contours, Liberty Area

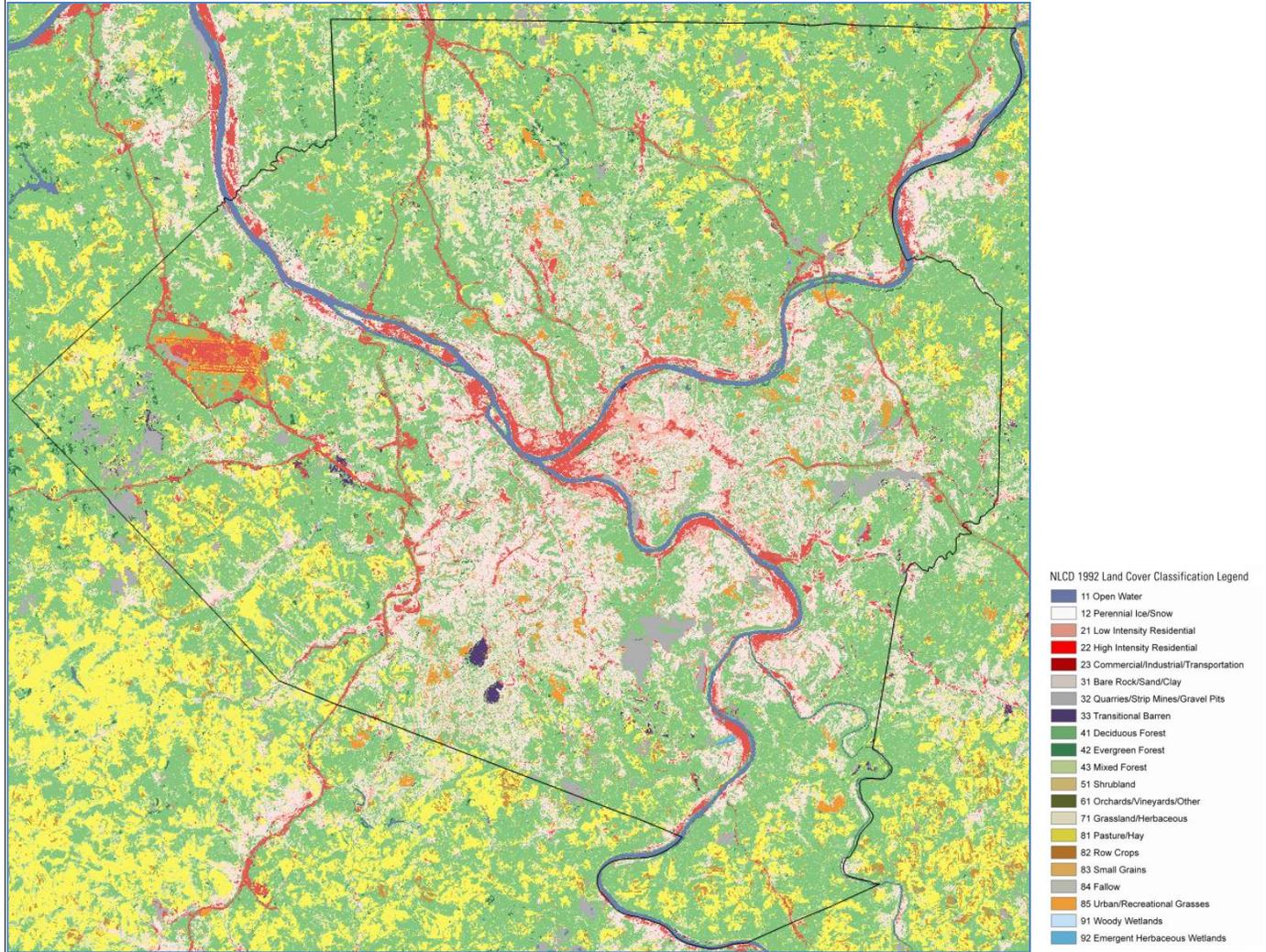


Figure 4-4. NLCD 1992 Land Cover for Allegheny County

4.3 Urban/Rural Determination

For determination of the urban or rural option in AERMOD, the Auer technique (Auer, 1978) was used to determine the urban and rural components of land cover for an area. Land cover within a 3 km circle surrounding the U. S. Steel Clairton Plant (the largest source in the Liberty near-field area) is shown in Figure 4-5. The statistics for urban and rural land cover were generated by AERSURFACE to determine the counts of each land cover type within the area, given in Table 4-1.

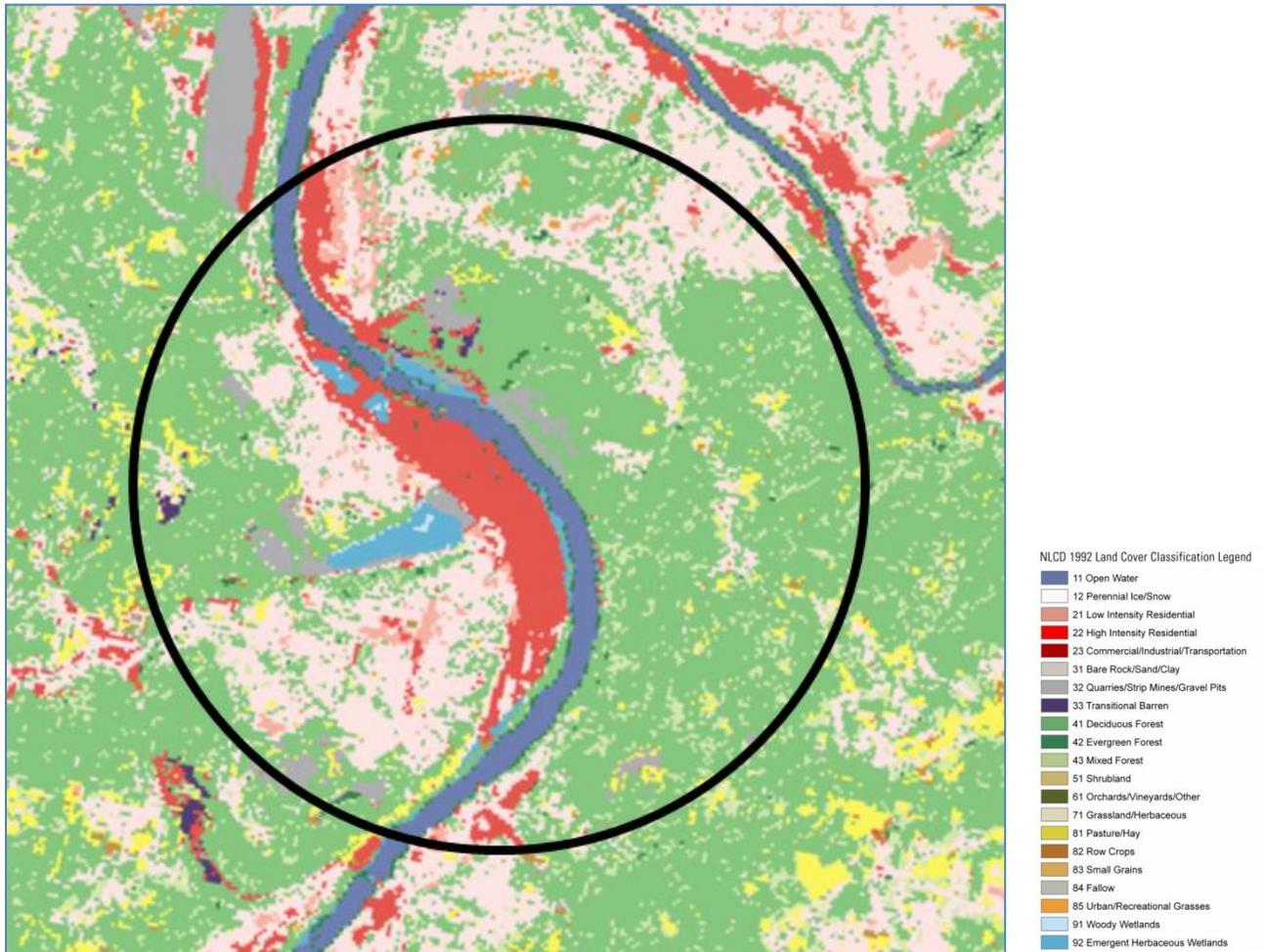


Figure 4-5. Land Cover Surrounding the U. S. Steel Clairton Plant, at 3 km Radius

Table 4-1. Land Cover Counts for Clairton/Liberty Area, 3 km Radius

CATEGORY	LAND COVER DESCRIPTION	COUNT
21	Low Intensity Residential	25933
22	High Intensity Residential	1768
23	Commercial/Industrial/Transp	5181
32	Quarries/Strip Mines/Gravel	2822
33	Transitional	397
	Urban Subtotal	36101
11	Open Water	2892
41	Deciduous Forest	55440
42	Evergreen Forest	937
43	Mixed Forest	7991
81	Pasture/Hay	6376
82	Row Crops	1036
85	Urban/Recreational Grasses	699
91	Woody Wetlands	38
92	Emergent Herbaceous Wetlands	715
	Rural Subtotal	76124
	Total	112225

The land cover types in Table 4-1 show that rural land cover is the most dominant type for the 3 km area, comprising 68% of the land cover counts. AERMOD will therefore utilize the rural setting for processing.

4.4 Meteorological Inputs

The AERMOD meteorological preprocessor AERMET 18081 (U.S. EPA, 2018b) will be run with the following settings.

- Meteorological year: 2011
- MMIF version 3.4 (Brashers and Emery, 2018) inputs for multiple facility locations
 - o 0.444 km resolution MMIF onsite, upper air, and surface characteristics inputs (U. S. Steel facility locations)
 - o 1.33 km resolution MMIF inputs (all other source locations)
- Bulk Richardson low-level delta_T and solar radiation for stable boundary layer
- Low wind option ADJ_U* for stable boundary layer
- 0.0 m/s wind speed threshold, based on MMIF guidance (U.S. EPA, 2018d)

For more discussion on the MMIF inputs and configuration, see Appendix C of this protocol.

4.5 Sources and Source Types

The following sources will be modeled in AERMOD as the primary PM_{2.5} (LPM) sources:

- U. S. Steel Mon Valley Works
 - o Clairton Plant
 - o Irvin Plant
 - o Edgar Thomson Plant
- Shenango
- ATI Allegheny Ludlum
- McConway & Torley

The U. S. Steel plants are an integrated steel mill, connected by pipeline and railroads throughout the Mon Valley. The Shenango, ATI Allegheny Ludlum, and McConway & Torley facilities are distant sources for Liberty, located several miles away. They are included in the PM_{2.5} model design as LPM sources due to potential source/receptor impacts near their locations, and they are included in this demonstration only to account for all possible contributions of primary PM_{2.5}.

Only primary filterable and condensable PM_{2.5} emissions will be modeled. The modeled source inventory used for the AERMOD sources is given in Appendix B of this protocol.

Types of sources will be assigned as follows:

- Stacks/towers: point sources, including building parameters for point sources with downwash
- Ambient-temperature process fugitives: volume sources
- Pile erosion sources: area sources
- Coke oven (buoyant) battery fugitives: line volume sources with BLP/AERMOD hybrid approach

Specific facility-based road and mobile source fugitives will be modeled as volumes based on EPA haul roads methodologies (U.S. EPA, 2012). Note that there may be some double-counting with the CAMx results for these sources, but potential effects are considered to be negligible at the Liberty monitor.

4.6 Receptor Grid

Based on PM_{2.5} modeling guidance (U.S. EPA, 2014), an expanded-scale receptor grid is appropriate for localized PM_{2.5}, with several receptors placed near a monitor in order to assess concentration gradients. Receptors should also be located in areas that are appropriate for Federal Reference Method (FRM) monitor placement.

The Liberty monitor spatial scale is a neighborhood-scale site for PM_{2.5}, which can be representative of an area of reasonably homogenous conditions within a range of 0.5 to 4.0 km.¹⁵ Homogeneity refers to concentrations, as well as land use and land surface characteristics.

For this demonstration, a Cartesian grid within a 500-m radius of the Liberty site and within 50 ft elevation of the flagpole height of the monitor will be used to represent the Liberty monitored concentrations. As a result, receptors will capture concentration gradients at the minimum of the

¹⁵ 40 CFR Part 58 Appendix D, for pollutants in general, a spatial scale of representativeness is described in terms of the physical dimensions of the air parcel nearest to a monitoring site throughout which actual pollutant concentrations are reasonably similar.

neighborhood-scale extent and without encompassing regions that are not suitable to represent the Liberty FRM monitor.

Figure 4-6 below shows the receptor grid to be used for the modeling, with the U. S. Steel Clairton location shown to the south. The red circle indicates the 500-m radius, and black lines indicate the CAMx grid cells of the 1.33 km domain (see more in the Combination of Local and Regional Impacts section).

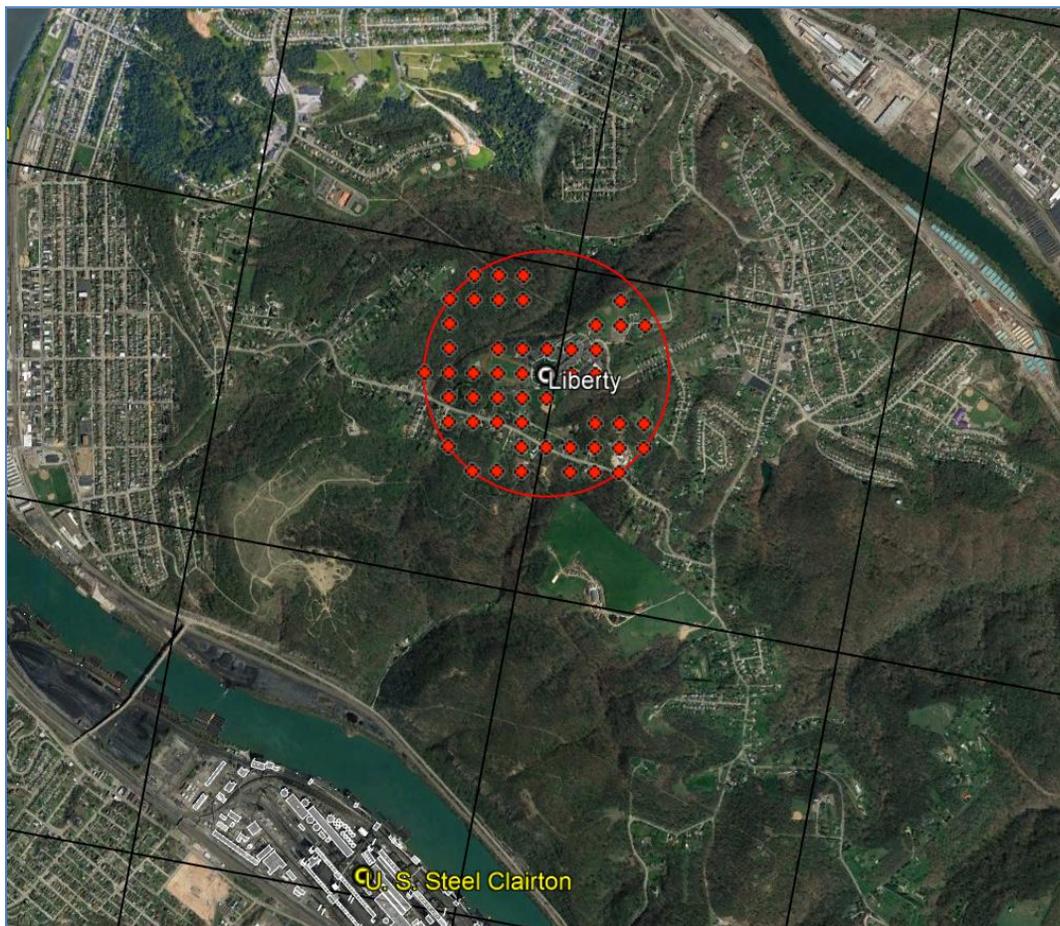


Figure 4-6. Receptor Grid for the Liberty Area

Figure 4-7 shows a close-up of the Liberty receptor grid, with the property of the South Allegheny High School (the location of the Liberty monitor) also shown in blue.

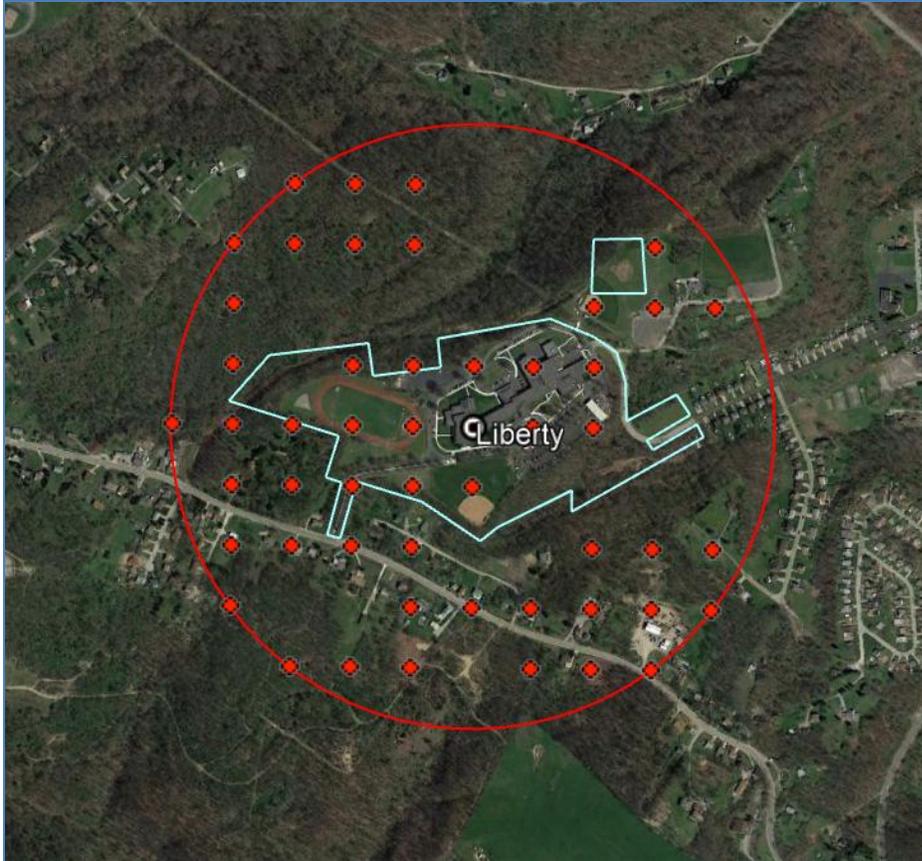


Figure 4-7. Close-Up of the Liberty Receptor Grid, with Property Boundaries

The close-up map in Figure 4-7 shows that the receptor grid is essentially the high school property, adjacent residences, and other nearby locations that could be suitable for FRM placement within 500 m.

The expanded-scale receptor approach also likely provides an adequate simulation of non-steady state conditions in the Liberty area for the following reasons:

- For a proper simulation of non-steady state conditions in complex terrain, there is a degree of forgiveness needed for both time and space with a steady-state model such as AERMOD. AERMOD is designed to produce straight-line concentrations on an hourly basis, which may be limited for some non-steady state situations.
- In addition to limitations with the model, there is a degree of uncertainty with meteorological data supplied to AERMOD, using any type of meteorological data. Inaccuracies in wind speeds or directions can lead to substantial variations in spatial impacts.
- Even with multiple MMIF data sets (and with multiple-level profiles), meteorological parameters are assumed to be constant for each hour from each starting point throughout the complex terrain. High-resolution sub-hourly wind fields (such as with a Lagrangian puff or computational fluid dynamic (CFD) model) may be more appropriate for this situation, but AERMOD with MMIF meteorology was chosen as the best-available regulatory approach at this time.

- Merged plumes may be physically larger in real-life than modeled, especially in extremely stagnant conditions with elevated pollutant periods (lasting longer than an hour). A larger receptor grid can help to account for more wide-spread impacts near the monitor.

Coinciding with the expanded-scale receptor approach, a maximum-exposure basis will also be used for the demonstration. The highest hourly modeled concentration from any receptor in the expanded-scale grid will be used as the hourly localized impact for each site, and corresponding 24-hour averages will be based on composite averages of the maximum hourly concentrations. The Liberty monitor is therefore represented as the worst-case of any receptor at any hour.

The AERMOD terrain preprocessor AERMAP version 18081 (U.S. EPA, 2018c) will be run with the following settings to generate the receptor grids:

- Domain
 - SW corner: 590000.0, 4457900.0
 - NE corner: 602100.0, 4469700.0
 - UTM zone 17, NAD83 datum
- Elevations based on 10 m resolution USGS NED data
- Total of 51 receptors
- Flagpole receptor for the Liberty monitor
 - Flagpole height of 9 m above ground level (building roof + probe height)

4.7 AERMOD Configuration

AERMOD 18081 (U.S. EPA, 2018a) will be run with the following settings:

- Calculate concentration values (CONC)
- Regulatory DEFAULT options:
 - Includes stack-tip downwash
 - Accounts for elevated terrain effects
 - Uses calms processing routine
 - Uses missing data processing routine
 - No exponential decay
- RURAL dispersion only
- Pollutant type: OTHER (since specific processing routines are not needed)
- Time period: 1-hour averaging, for 8760 total hours for the period (year: 2011)
- Accepts FLAGPOLE receptor heights
- BPIPRM building downwash parameters for POINT sources (U.S. EPA, 1993)
- No wet or dry depletion/deposition
- Meteorological data can include TEMP substitutions
- Multiple AERMOD runs, post-processed
- Source types:
 - POINT sources for stacks
 - VOLUME sources for non-buoyant fugitive sources
 - AREA sources for pile erosion
 - LINE VOLUME sources for buoyant fugitives (varying-height)
- HOUREMIS for buoyant line volume sources
- Haul Road methodology (U.S. EPA, 2012) for road/vehicle emissions

4.8 CAMx Configuration

For the regional (non-LPM) impacts, CAMx version 6.30 (Ramboll Environ, 2016a) was run with the following settings:

- Modeled year: 2011
- Weather Research and Forecasting (WRF)¹⁶ version 3.7.1 mesoscale meteorological inputs (extracted by MMIF)
- 36/12/4/1.33 km resolution nested grid structure
 - o 1.33 km domain focused on Allegheny County
 - o Additional 444 m resolution WRF grid (for MMIF only, at U. S. Steel locations)
- Particulate Source Appointment Technology (PSAT) for source group tracking
- Emissions based on 2011 MARAMA Alpha2¹⁷ and NEI v6.2 Modeling Platform¹⁸
- Emissions modeling based on the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system¹⁹

The CAMx results without the localized primary impacts include emissions from all sources and sectors, for PM_{2.5} and all precursors, except for PM_{2.5} from the LPM sources listed in the Sources and Source Types section above.

More information can be found in the WRF and CAMx modeling protocols (Ramboll Environ, 2016b; 2017a), model performance evaluations (Ramboll Environ, 2016c; 2017b), and Technical Support Document (Ramboll Environ, 2018) as provided in the SIP Appendices F, G, and I. (Note: the AERMOD configuration that was included in the CAMx model performance evaluation did not use the same design as outlined in this protocol with refined source types.)

4.9 Combination of Local and Regional Impacts

The CAMx modeling was configured with tracking for specific source groups, allowing for the apportionment of both wide-scale regional and local (LPM) contributions. Regional impacts from CAMx without LPM are essentially PM_{2.5} background for the Liberty area, both primary and secondary in nature, without the localized primary excess.

The CAMx grid cells corresponding with the Liberty monitor will be used for the non-LPM component of PM_{2.5} at Liberty. Figure 4-8 shows the numbered CAMx 1.33 km resolution grid cells containing or adjacent to the Liberty site.

¹⁶ <https://www.mmm.ucar.edu/weather-research-and-forecasting-model>

¹⁷ <http://www.marama.org/technical-center/emissions-inventory/2011-inventory-and-projections>

¹⁸ <https://www.epa.gov/air-emissions-modeling/2011-version-6-air-emissions-modeling-platforms>

¹⁹ <https://www.cmascenter.org/smoke/>



Figure 4-8. CAMx 1.33 km Grid Cells, Liberty Area

Since Liberty falls near the border of two CAMx grid cells (18042 and 18043),²⁰ averages of the two grid cells will be used in combination with the AERMOD impacts. Modeled species will be averaged by major species on a daily (24-hour calendar day) basis.

The regional (non-LPM) CAMx and local (LPM) AERMOD impacts will be combined as follows:

- For the annual attainment test, quarterly averages and modeled RRFs will be calculated separately for regional species and for local. LPM is treated as new component in the SANDWICH reconstruction of species.
- For the 24-hour attainment test, since the test is based on quarterly high days and not quarterly averages, the impacts can be combined in two ways:
 - Option 1: similar to the annual test, quarterly high-day averages would be calculated separately for regional and local components. High days for each quarter would be ranked by component, with the RRFs used for high-day local and high-day regional components.

²⁰ CAMx grid cells were numbered according to geographic x-y coordinates used by the model.

- Option 2: quarterly high-day averages would be based on total (regional + local) impacts, with daily regional CAMx and local AERMOD impacts summed (paired by day). High days for each quarter would be ranked by total impacts.

The method that leads to the highest 24-hour design value will be used as the final 24-hour projection for Liberty.

- For the model performance evaluation, daily modeled impacts will be based on total impacts (similar to option 2 above for the 24-hour attainment test) for comparison to daily monitored data. If hourly data are used for any comparison in the model performance, modeled impacts would also be based on the total of regional and local components.

4.10 Liberty Attainment Test Calculations

This section describes the steps used to calculate the Liberty attainment tests (design values) for the refined local analysis (LAA). The attainment test calculations will be given in the local area analysis section of Appendix I of the SIP.

Two AERMOD simulations will be run for each source: one for base case emissions (2011), and one for future projected case emissions (2021). The AERMOD local impacts (LPM) from all sources will then be summed via post-processing for each case and used to derive modeled relative response ratios (RRFs). The RRFs will be used in combination with speciation monitored results that are “split” into local and regional components. The regional species will be represented by the averages of the surrounding Pittsburgh MSA²¹ sites.

The CSN speciation data used for the attainment tests are adjusted by the SANDWICH methodology (U.S. EPA, 2014, Abt Associates, 2014) and are included with the SMAT-CE software. Corrections made by ACHD to the CSN SANDWICH data are summarized below. (More details on SANDWICH data corrections and assumptions are given in the technical support document of Appendix I of the SIP.)

- Concentrations of salt (NaCl) at Liberty were incorrectly calculated by the SANDWICH method and were replaced by the average available concurrent (measured on the same day) salt concentrations from the three regional MSA sites.
- For CSN samples with missing concurrent FRM mass (for Liberty or the regional sites), the CSN total gravimetric mass were substituted for the missing FRM. Additionally, quarters with a minimum of 8 valid samples (>50% data completeness) were used for the calculations. The use of substituted CSN masses and a minimum of 8 samples allowed for more quarters to be used over the 2009-2013 timeframe.

Assumptions that were made in the SANDWICH average quarterly reconstruction of the species are summarized as follows:

- Nitrate is based on retained estimations (provided by EPA with the SANDWICH data)
- Ammonium is derived from sulfate and nitrate concentrations and degree of neutralization (DON) of sulfate (with DON held constant from base to future case)

²¹ Metropolitan Statistical Area. For CSN, these sites are Lawrenceville (Allegheny Co.), Florence (Washington Co.), and Greensburg (Westmoreland Co.)

- Particle-bound water (PBW) is derived from sulfate, nitrate, and ammonium concentrations
- Organic carbon mass by mass balance (OCMmb) is based on FRM gravimetric mass minus other species
- Alternative method (without aluminum) is used for crustal component calculations
- Blank (passive) mass of 0.5 $\mu\text{g}/\text{m}^3$ is included in each quarterly composition of species

To split the Liberty monitored species into local and regional components for the annual design value, the following steps will be taken:

- 1) Weighted average quarterly values will be calculated for the Liberty FRM concentrations for 2009-2013. Weighted averages are the averages of each 3-year period within 2009-2013, with the weighted base year 2011 included in each of the 3-year averages.
- 2) Quarterly CSN major species averages will be calculated for 2009-2013 from valid calendar quarters from each of the four CSN sites in the Pittsburgh MSA. Indirect species (ammonium, PBW, OCMmb) are calculated from the quarterly averages of the other species.
- 3) The average of the Lawrenceville, Florence, and Greensburg quarterly species averages will be used for the regional component of $\text{PM}_{2.5}$. The regional species averages will be subtracted from the Liberty quarterly species averages to determine the excess component for Liberty. If any negative values are present for the Liberty excess, values are corrected to zero, and the regional species are recalculated by subtracting the corrected excess species averages from the Liberty total component before the local/regional split (from step 2).
- 4) The indirect species will be recalculated for the regional component for consistency with SANDWICH methodology, also accounting for any corrections made to the excess from step 3. The Liberty local (LPM) component is then calculated from the differences of the total non-blank mass (step 2) and the sum of the recalculated regional species. LPM is one lumped species that contains any excess primary material, with the regional containing all other species.
- 5) Relative compositions (fractions of total mass) of the Liberty LPM and regional species from step 4 will be then be used to calculate weighted compositions from the weighted quarterly concentrations. The weighted compositions will be projected to future case by the quarterly modeled RRFs by species (AERMOD for LPM, CAMx for non-LPM).
- 6) Indirect species will then be recalculated from the projected species, and all species are summed by quarter (including blank mass). Quarterly totals are then averaged to generate an annual future case design value.

To split the Liberty monitored species into local and regional components for the 24-hour design value, the following steps will be taken (some steps are similar to those used for the annual design value):

- 1) Liberty 24-hour FRM concentrations will be sorted into the top 8 days per quarter²² per year for 2009-2013, for a total of 160 high days.
- 2) Quarterly CSN major species high-day averages of the top 3 days per quarter per year will be calculated for 2009-2013 from valid calendar quarters from each of the four CSN sites in the Pittsburgh MSA. Indirect species (ammonium, PBW, OCMmb) are calculated from the quarterly high-day averages of the other species.
- 3) The average of the Lawrenceville, Florence, and Greensburg quarterly species high-day averages will be used for the regional component of PM_{2.5}. The regional species averages will be subtracted from the Liberty quarterly species high-day averages to determine the excess component for Liberty. If any negative values are present for the Liberty excess, values are corrected to zero, and the regional species are recalculated by subtracting the corrected excess species averages from the Liberty total component before the local/regional split (from step 2).
- 4) The indirect species will be recalculated for the regional component for consistency with SANDWICH methodology, also accounting for any corrections made to the excess from step 3. The Liberty local (LPM) component is then calculated from the differences of the total non-blank mass (step 2) and the sum of the recalculated regional species. LPM is one lumped species that contains any excess primary material, with the regional containing all other species.
- 5) Relative compositions (fractions of total mass) of the Liberty LPM and regional species from step 4 will be then be used to project the high days by the modeled RRFs by species (AERMOD for LPM, CAMx for non-LPM) to projected future case high-day compositions. Indirect species will be recalculated from the projected species for each high day, and all species are summed by high day (including blank mass).
- 6) The projected high days will then be re-ranked per year, since future high days can differ from base case (depending on the controls in the plan). The future case 24-hour design value is determined by the weighted average of the projected yearly 98th percentiles over the 5-year timeframe (average of the 3-year averages).

Based on the CAMx modeling design and the above procedures for the LAA, there may be some locally-formed secondary PM_{2.5} that is apportioned to the regional component and not to the LPM component. Examination of the different source apportionment groups from CAMx shows that the majority of the local excess is primary in nature, and the sensitivity modeling (see the precursor demonstration in Appendix I of the SIP) shows that secondary ammonium or VOC are insignificant contributors to PM_{2.5} at Liberty. Therefore, the discrepancy should be minimal for secondary PM_{2.5} with the split of local/regional impacts.

Additionally, the LAA will include different configurations of modeled source type and parameters by local and regional component for some processes. For example, battery fugitives are modeled as varying-height line volume sources (using the alternative approach in Appendix H of the SIP) for the AERMOD LPM component but are modeled as fixed-height point sources for the CAMx regional component (SO₂, NO_x, NH₃, VOC). Similar to above, it is assumed that any inconsistencies will lead to negligible effects on the results, with the most important impacts due to primary PM_{2.5}.

²² Based on the PM_{2.5} modeling guidance (U.S. EPA, 2014), about the top 10% of days will be used as high days. This can differ based on monitor frequency, data recovery, etc. For the Liberty FRM, the top 8 days will be used. For the CSN sites, the top 3 days will be used. For the modeling, the top 10 days will be used.

5 EVALUATION OF RESULTS

This section describes a range of model testing methodologies potentially available to adequately evaluate the performance of an air quality modeling system. Model performance is based on analysis of the modeled predictions against available measurements at air quality monitor(s). Statistical measures and methods used in this analysis are similar to the techniques recommended by EPA and used in the evaluation of other model demonstrations (U.S. EPA, 2014; ENVIRON, 2012).

A comprehensive, multi-layered approach to model performance can include up to four components, viewed conceptually as follows:

- **Operational:** tests the ability of the model to estimate concentrations. This evaluation examines whether the measurements are properly represented by the model predictions but does not necessarily ensure that the model is getting “the right answer for the right reason”;
- **Diagnostic (or scientific):** tests the ability of the model to get the right answer for the right reason;
- **Mechanistic (or dynamic):** tests the ability of the model to predict the response of concentrations to changes in variables such as emissions and meteorology; and
- **Probabilistic:** takes into account the uncertainties associated with model predictions and observations.

The operational component will be the focus of the performance evaluation, while elements of the other components can also be included in the analysis. Table 5-1 lists a core set of statistical performance measures that can be used to evaluate model performance results. Following Table 5-1 are additional statistical metrics and analyses that will be used for the model evaluation. Since there is only one model configuration outlined in this protocol, composite performance measure (CPM) and model comparison measure (MCM) will not be used for comparison between different model cases/options.

Like described previously for the combination of regional and local results, impacts will be combined on a daily basis for the model performance statistics. Hourly impacts may also be used in the model performance analysis.

Note that model results are used in a relative manner for $PM_{2.5}$, scaling down monitored data by response ratios rather than comparing absolute concentrations to air quality standards. Negative or positive bias can be consistent in base and future model cases and do not always indicate poor performance.

Table 5-1. Core Statistical Measures for Air Quality Model Evaluation

Statistical Measure	Mathematical Expression	Notes
Mean Bias (MB)	$\frac{1}{n} \sum_1^n (M - O)$	Reported as concentration (e.g., µg/m³)
Mean (Gross) Error (ME)	$\frac{1}{n} \sum_1^n M - O $	Reported as concentration, absolute values
Root Mean Square Error (RMSE)	$\sqrt{\frac{\sum_1^n (M - O)^2}{n}}$	Reported as concentration
Normalized Mean Bias (NMB)	$\frac{\sum_1^n (M - O)}{\sum_1^n (O)}$	Reported as unitless (or %)
Normalized Mean Error (NME)	$\frac{\sum_1^n M - O }{\sum_1^n (O)}$	Reported as unitless (or %), absolute values
(Mean) Fractional Bias (FB)	$\frac{1}{n} \left(\frac{\sum_1^n (M - O)}{\sum_1^n \left(\frac{M + O}{2} \right)} \right)$	Reported as unitless (or %)
(Mean) Fractional Error (FE)	$\frac{1}{n} \left(\frac{\sum_1^n M - O }{\sum_1^n \left(\frac{M + O}{2} \right)} \right)$	Reported as unitless (or %), absolute values
Standard Deviation (σ)	$\sqrt{\frac{1}{n} \sum_1^n (X - \bar{X})^2}$	Reported as concentration \bar{X} = arithmetic average
Correlation Coefficient (r)	$\frac{1}{(n - 1)} \sum_1^n \left(\left(\frac{O - \bar{O}}{\sigma_o} \right) * \left(\frac{M - \bar{M}}{\sigma_m} \right) \right)$	Unitless \bar{M}, \bar{O} = arithmetic averages

M = modeled (predicted) concentration at each time/location (1 through *n*)
O = observed (monitored) concentration at each time/location (1 through *n*)
X = modeled or observed concentration at each time/location (1 through *n*)
n = number of paired concentrations

Additional metrics used in the evaluation are described below.

Fractional factor of two (FF2): the ratio of the number of modeled concentrations within a factor of two of observed concentrations compared to the total number of modeled concentrations.

Geometric correlation coefficient (r_g): standard correlation coefficient computed using the natural log of the modeled and measured concentrations, calculated in equation (1):

$$r_g = \frac{\sum(\ln(x) - \overline{\ln(x)})(\ln(y) - \overline{\ln(y)})}{\sqrt{\sum(\ln(x) - \overline{\ln(x)})^2} \sqrt{\sum(\ln(y) - \overline{\ln(y)})^2}} \quad (1)$$

Geometric mean (μ_g): the n^{th} root of the product of n numbers, calculated in equation (2). The geometric mean is used to evaluate a general expected value with dampened outlier influence.

$$\mu_g = \left(\prod_{i=1}^n c_i \right)^{1/n} \quad (2)$$

Geometric mean variance (VG): a measure of the precision of the dataset. A perfect model would result in $VG = 1$. VG is calculated in equation (3), where c_o and c_p are the observed and predicted concentrations, respectively:

$$VG = e^{\left(\left(\ln\left(\frac{c_o}{c_p}\right) \right)^2 \right)} \quad (3)$$

Robust highest concentration (RHC): a comparison of modeled and observed concentrations at upper end of a frequency distribution, calculated using equation (4):

$$RHC = c_n + (\bar{c} - c_n) \ln\left(\frac{3n-1}{2}\right) \quad (4)$$

where c_n is the n^{th} highest concentration and \bar{c} is the average of the $(n-1)$ highest concentrations, and n is set to 26 as a threshold value

Graphical displays also facilitate quantitative and qualitative comparisons between predictions and measurements. Graphical displays can include the following:

- Quantile-quantile (Q-Q) plots: a series of ranked pairings of predicted and observed concentration, where any rank of the predicted concentration is plotted against the same ranking of the observed concentration. Q-Q plots are used to evaluate a model's ability to represent the frequency distribution of the observed concentrations.
- Time series and scatter plots: concentrations matched in time for each monitoring location. Time series plots are helpful to understand the response of the model during specific measured time periods. Scatter plots show the correlation during all time periods between predicted and observed.

- Temporal distribution plots: concentrations shown by averages over selected time periods, such as hour of the day (diurnal), month, season, etc. Temporal plots show average patterns in time for groups of concentrations instead of for each concentration.
- Goal plots: provides a visual display of statistical metrics such as bias and error along with respective benchmarks (goals or criteria). For example, model results showing bias and/or error within a box (or “goal”) indicate good model performance.

Table 5-2 below lists benchmarks for 24-hour PM_{2.5} model performance statistics, based on previous photochemical modeling applications (Emery et al, 2017). The “goal” benchmarks are considered to be the best performance that a model can achieve, while the “criteria” benchmarks are considered to be average or reasonable performance.

Table 5-2. Model Performance Benchmarks for 24-Hour PM_{2.5}

Metric	Goal	Criteria
Fractional Bias (FB)	<±30%	<±60%
Fractional Error (FE)	<50%	<75%
Normalized Mean Bias (NMB)	<±10%	<±30%
Normalized Mean Error (NME)	<35%	<50%
Correlation Coefficient (r)	>0.70	>0.40

Base case (2011) model performance results for the refined local modeling with AERMOD (combined with CAMx regional impacts) will be given in Appendix G of the SIP.

Monitored data used for comparison to modeled results will be identical to data available on EPA databases, with missing data excluded from the analysis. In order to remove missing periods (hourly or daily), monitored and modeled concentrations are first sorted on a time-paired basis, and then hours with missing data (monitored or modeled) are removed. This excludes periods of unknown concentrations and also ensures the same number of samples for the comparisons.

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APPENDICES

APPENDIX A – Monitored Data

The figures and tables below show the PM_{2.5} annual and 24-hour design values for 3-year periods from 2000 through 2017. (Note: preliminary monitored data for the first half of 2018 (Jan. through June) show trends similar to the first half of 2017.)

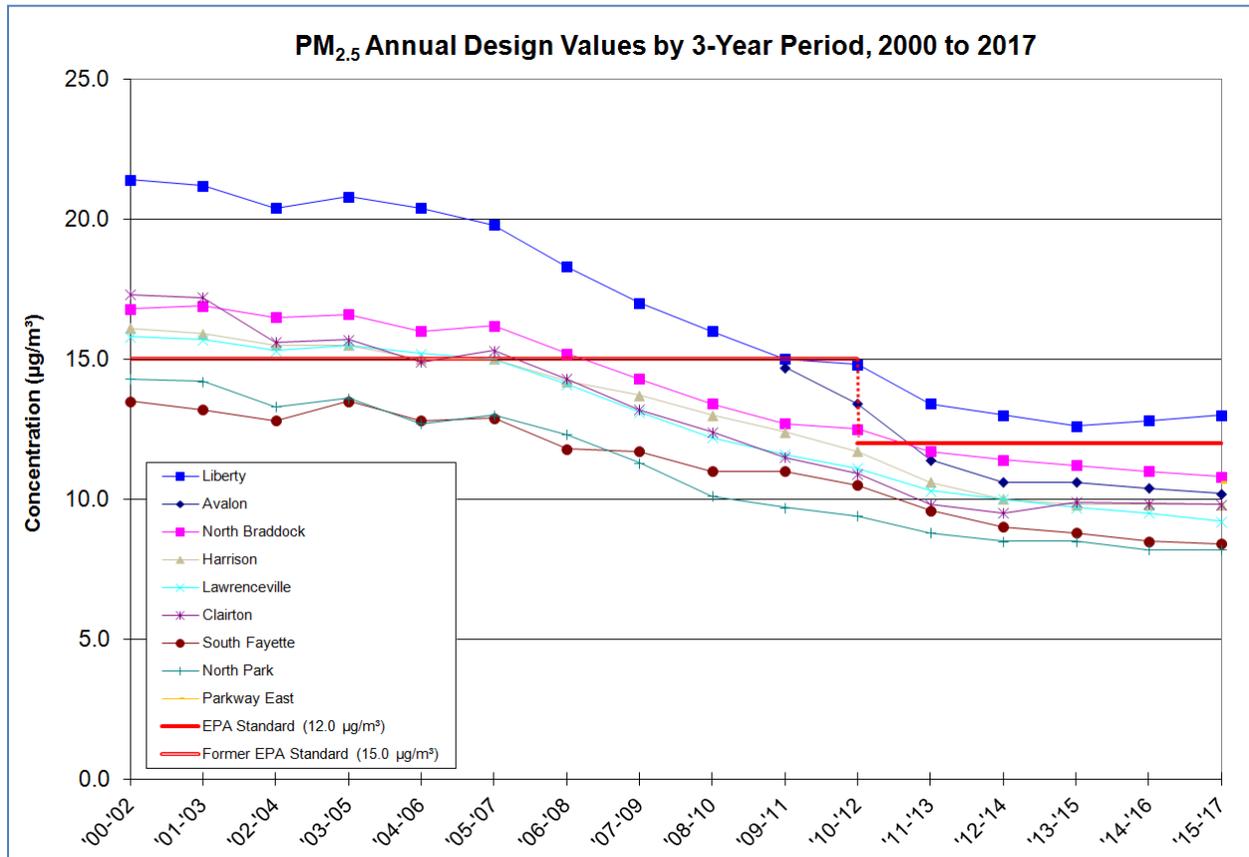


Figure A-1. Annual Design Value Trends, 2000-2017

Table A-1. Annual Design Values, 2000-2017

Site	'00-'02	'01-'03	'02-'04	'03-'05	'04-'06	'05-'07	'06-'08	'07-'09	'08-'10	'09-'11	'10-'12	'11-'13	'12-'14	'13-'15	'14-'16	'15-'17
Liberty	21.4	21.2	20.4	20.8	20.4	19.8	18.3	17.0	16.0	15.0	14.8	13.4	13.0	12.6	12.8	13.0
Avalon										14.7	13.4	11.4	10.6	10.6	10.4	10.2
North Braddock	16.8	16.9	16.5	16.6	16.0	16.2	15.2	14.3	13.4	12.7	12.5	11.7	11.4	11.2	11.0	10.8
Harrison	16.1	15.9	15.5	15.5	15.0	15.0	14.2	13.7	13.0	12.4	11.7	10.6	10.0	9.8	9.8	9.8
Lawrenceville	15.8	15.7	15.3	15.5	15.2	15.0	14.1	13.1	12.2	11.6	11.1	10.3	10.0	9.7	9.5	9.2
Clairton	17.3	17.2	15.6	15.7	14.9	15.3	14.3	13.2	12.4	11.5	10.9	9.8	9.5	9.9	9.8	9.8
South Fayette	13.5	13.2	12.8	13.5	12.8	12.9	11.8	11.7	11.0	11.0	10.5	9.6	9.0	8.8	8.5	8.4
North Park	14.3	14.2	13.3	13.6	12.7	13.0	12.3	11.3	10.1	9.7	9.4	8.8	8.5	8.5	8.2	8.2
Parkway East																10.6
EPA Standard (12.0 µg/m³)											12.0	12.0	12.0	12.0	12.0	12.0
Former EPA Standard (15.0 µg/m³)	15.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0						

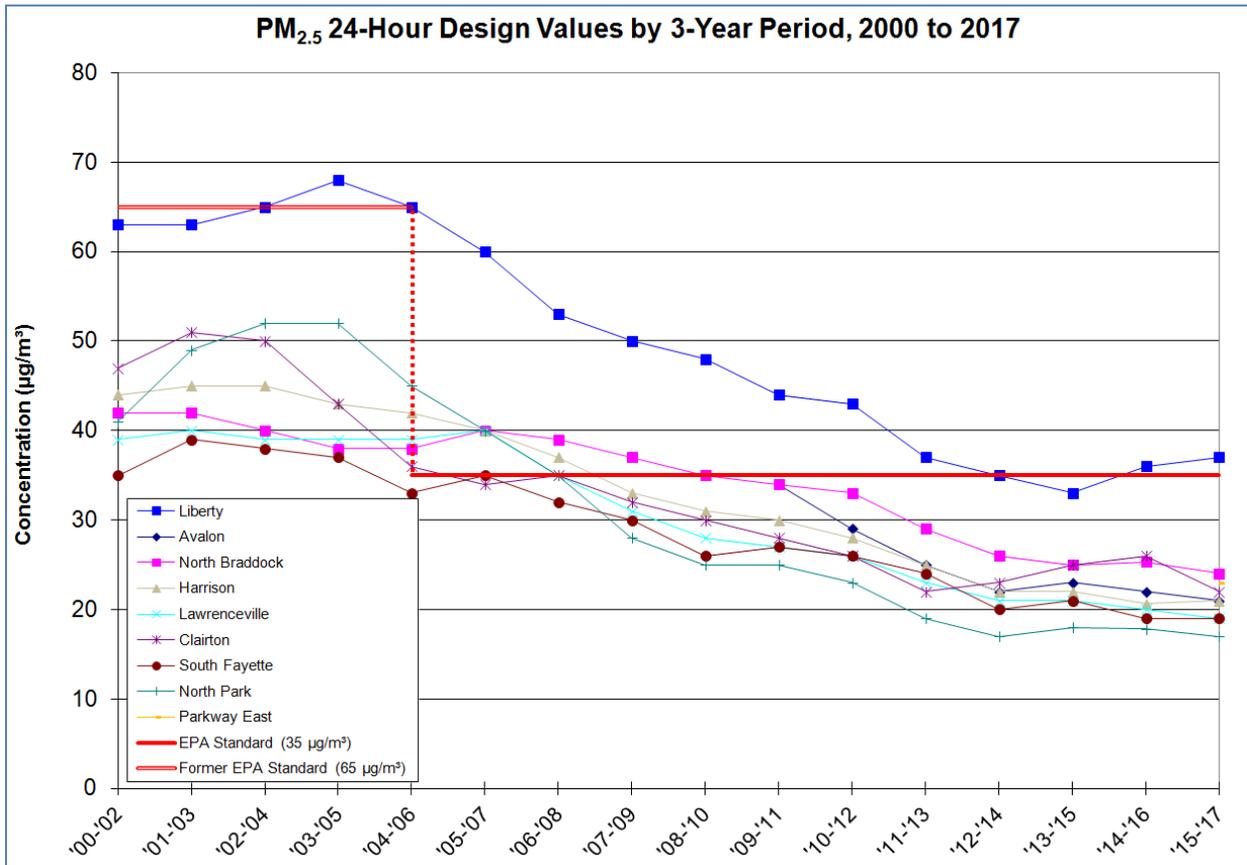


Figure A-2. 24-Hour Design Value Trends, 2000-2017

Table A-2. 24-Hour Design Values, 2000-2017

Site	'00-'02	'01-'03	'02-'04	'03-'05	'04-'06	'05-'07	'06-'08	'07-'09	'08-'10	'09-'11	'10-'12	'11-'13	'12-'14	'13-'15	'14-'16	'15-'17
Liberty	63	63	65	68	65	60	53	50	48	44	43	37	35	33	36	37
Avalon										34	29	25	22	23	22	21
North Braddock	42	42	40	38	38	40	39	37	35	34	33	29	26	25	25	24
Harrison	44	45	45	43	42	40	37	33	31	30	28	25	22	22	21	21
Lawrenceville	39	40	39	39	39	40	35	31	28	27	26	23	21	21	20	19
Clairton	47	51	50	43	36	34	35	32	30	28	26	22	23	25	26	22
South Fayette	35	39	38	37	33	35	32	30	26	27	26	24	20	21	19	19
North Park	41	49	52	52	45	40	35	28	25	25	23	19	17	18	18	17
Parkway East																23
EPA Standard (35 µg/m³)					35	35	35	35	35	35	35	35	35	35	35	35
Former EPA Standard (65 µg/m³)	65	65	65	65												

APPENDIX B – Sources Modeled

This appendix provides the emissions and source parameters used for the sources modeled with AERMOD, by facility/process and model ID. More details on the source inventories and revisions will be given in Appendix D of the SIP.

Below is a key of the abbreviations used in the tables, with a description of each parameter and the corresponding unit.

Parameter	Description	Unit
UTMx	UTM x-coordinate	meters
UTMy	UTM y-coordinate	meters
ELEV	Elevation	meters
HEIGHT	Stack height	meters
TEMP	Stack exit velocity	meters/second
VEL	Stack exit temperature	Kelvin
DIAM	Stack diameter	meters
BLDG	Building downwash parameters included (yes/no)	n/a
REL HEIGHT	Release height above ground (volume or area)	meters
INIT SY	Initial lateral dimension of volume (σ_y)	meters
INIT SZ	Initial vertical dimension of volume (σ_z)	meters
BASE RATE	Base case (2011) emission rate	grams/second
PROJ RATE	Projected future case (2021) emission rate	grams/second

U. S. Steel Clairton Plant point, non-buoyant volume, and area source parameters are given in Tables B-1 through B-3, respectively.

Table B-1. U. S. Steel Clairton Point Sources

SOURCE	ID	UTMx	UTMy	ELEV	HEIGHT	TEMP	VEL	DIAM	BLDG	BASE RATE	PROJ RATE
Quench Tower 1	CLQNCH1	595964.0	4461731.0	231	30.48	358.49	3.54	6.80	YES	1.676500	0.634830
Quench Tower 5	CLQNCH5	595472.0	4462078.0	231	30.48	358.49	3.54	7.10	YES	0.684100	0.000000
Quench Tower 7	CLQNCH7	595430.0	4462047.0	231	37.18	362.77	2.99	8.81	YES	1.973100	0.000000
Quench Tower B	CLQNCHB	595460.0	4462374.0	231	41.15	368.55	4.30	9.51	YES	1.313800	0.497510
Quench Tower C	CLQNCHC	595622.0	4462186.0	231	50.00	378.00	3.66	12.67	YES	--	0.667790
Quench Tower 5A	CLQNCH5A	595223.0	4462366.0	231	50.00	378.00	3.66	12.67	YES	--	0.392580
Quench Tower 7A	CLQNCH7A	595188.0	4462316.0	231	50.00	378.00	3.66	12.67	YES	--	0.763340
PEC Baghouse 1-3, Module 1	CLPEC1A	595865.8	4461872.2	231	24.99	324.83	18.81	0.91	YES	0.012000	0.012000
PEC Baghouse 1-3, Module 2	CLPEC1B	595861.1	4461877.2	231	24.99	324.83	18.81	0.91	YES	0.012000	0.012000
PEC Baghouse 1-3, Module 3	CLPEC1C	595856.4	4461882.4	231	24.99	324.83	18.81	0.91	YES	0.012000	0.012000
PEC Baghouse 1-3, Module 4	CLPEC1D	595863.6	4461874.4	231	24.99	324.83	18.81	0.91	YES	0.012000	0.012000
PEC Baghouse 1-3, Module 5	CLPEC1E	595858.8	4461879.7	231	24.99	324.83	18.81	0.91	YES	0.012000	0.012000
PEC Baghouse 13-15, Module 1	CLPEC13A	595324.7	4462210.5	231	24.99	324.83	18.23	0.91	YES	0.015800	0.015800
PEC Baghouse 13-15, Module 2	CLPEC13B	595320.3	4462215.5	231	24.99	324.83	18.23	0.91	YES	0.015800	0.015800
PEC Baghouse 13-15, Module 3	CLPEC13C	595315.9	4462220.4	231	24.99	324.83	18.23	0.91	YES	0.015800	0.015800
PEC Baghouse 13-15, Module 4	CLPEC13D	595317.9	4462218.0	231	24.99	324.83	18.23	0.91	YES	0.015800	0.015800
PEC Baghouse 13-15, Module 5	CLPEC13E	595322.6	4462212.8	231	24.99	324.83	18.23	0.91	YES	0.015800	0.015800
PEC Baghouse 19-20, Module 1	CLPEC19A	595320.0	4462206.4	231	24.99	304.83	17.94	0.91	YES	0.018800	0.018800
PEC Baghouse 19-20, Module 2	CLPEC19B	595315.5	4462211.3	231	24.99	304.83	17.94	0.91	YES	0.018800	0.018800
PEC Baghouse 19-20, Module 3	CLPEC19C	595311.0	4462216.5	231	24.99	304.83	17.94	0.91	YES	0.018800	0.018800
PEC Baghouse 19-20, Module 4	CLPEC19D	595313.0	4462214.0	231	24.99	304.83	17.94	0.91	YES	0.018800	0.018800
PEC Baghouse 19-20, Module 5	CLPEC19E	595317.7	4462208.8	231	24.99	304.83	17.94	0.91	YES	0.018800	0.018800
PEC Baghouse B, Module 1	CLPECBA	595439.6	4462430.5	231	15.54	324.83	13.79	1.22	YES	0.030000	0.030000
PEC Baghouse B, Module 2	CLPECBB	595435.9	4462433.4	231	15.54	324.83	13.79	1.22	YES	0.030000	0.030000
PEC Baghouse B, Module 3	CLPECBC	595420.8	4462445.6	231	15.54	324.83	13.79	1.22	YES	0.030000	0.030000
PEC Baghouse B, Module 4	CLPECBD	595432.5	4462436.1	231	15.54	324.83	13.79	1.22	YES	0.030000	0.030000
PEC Baghouse B, Module 5	CLPECBE	595428.6	4462439.3	231	15.54	324.83	13.79	1.22	YES	0.030000	0.030000
PEC Baghouse B, Module 6	CLPECBF	595424.5	4462442.6	231	15.54	324.83	13.79	1.22	YES	0.030000	0.030000
PEC Baghouse B, Module 7	CLPECBG	595436.0	4462425.7	231	15.54	324.83	13.79	1.22	YES	0.030000	0.030000
PEC Baghouse B, Module 8	CLPECBH	595432.2	4462428.7	231	15.54	324.83	13.79	1.22	YES	0.030000	0.030000
PEC Baghouse B, Module 9	CLPECBI	595428.7	4462431.5	231	15.54	324.83	13.79	1.22	YES	0.030000	0.030000
PEC Baghouse B, Module 10	CLPECBJ	595424.3	4462435.1	231	15.54	324.83	13.79	1.22	YES	0.030000	0.030000
PEC Baghouse B, Module 11	CLPECBK	595420.3	4462438.2	231	15.54	324.83	13.79	1.22	YES	0.030000	0.030000
PEC Baghouse B, Module 12	CLPECBL	595416.8	4462441.3	231	15.54	324.83	13.79	1.22	YES	0.030000	0.030000
PEC Baghouse C	CLPECC	595678.0	4462007.0	231	30.00	328.20	16.79	2.49	YES	--	0.015900
Battery 1 Underfiring	CLCOMB1	595871.0	4461845.0	231	68.58	526.49	7.59	2.44	YES	0.187200	0.187200
Battery 2 Underfiring	CLCOMB2	595866.0	4461852.0	231	68.58	534.27	7.71	2.44	YES	0.339200	0.339200
Battery 3 Underfiring	CLCOMB3	595742.0	4461989.0	231	68.58	539.27	7.38	2.44	YES	0.253700	0.253700
Battery 13 Underfiring	CLCOMB13	595389.0	4462164.0	231	68.58	535.38	4.48	3.05	YES	0.208700	0.208700
Battery 14 Underfiring	CLCOMB14	595380.0	4462174.0	231	68.58	536.49	4.30	3.05	YES	0.210000	0.210000
Battery 15 Underfiring	CLCOMB15	595253.0	4462318.0	231	68.58	541.49	4.48	3.05	YES	0.395300	0.395300
Battery 19 Underfiring	CLCOMB19	595273.0	4462117.0	231	76.20	519.27	3.72	4.72	YES	0.327800	0.327800
Battery 20 Underfiring	CLCOMB20	595258.0	4462134.0	231	76.20	542.05	4.27	4.72	YES	0.358800	0.358800
B Battery Underfiring	CLCOMBB	595477.0	4462406.0	231	96.01	515.38	5.06	4.95	YES	0.251000	0.251000
C Battery Underfiring	CLCOMBC	595768.0	4462126.0	231	98.14	503.20	5.81	3.66	YES	--	1.052600
Boiler 1	CLBLR1	595004.0	4462714.0	231	57.91	457.60	29.56	2.67	YES	0.517500	0.517500
Boiler 2	CLBLR2	594989.0	4462717.0	231	57.91	437.05	21.94	2.13	YES	0.215000	0.215000
Boiler R1	CLBLRR1	594892.0	4462604.0	231	50.29	524.27	7.47	2.59	YES	0.016600	0.016600
Boiler R2	CLBLRR2	594892.0	4462604.0	231	50.29	524.27	7.47	2.59	YES	0.011600	0.011600
Boiler T1	CLBLRT1	594845.0	4462563.0	231	26.52	544.27	9.05	1.46	YES	0.030500	0.030500
Boiler T2	CLBLRT2	594837.0	4462569.0	231	26.52	543.16	9.05	1.46	YES	0.029300	0.029300
SCOT Incinerator	CLSCOT	595575.0	4462036.0	231	45.72	638.16	17.43	1.17	YES	0.079200	0.079200
Misc. Flaring	CLFLARE	595554.0	4462083.0	231	8.26	1273.00	20.00	0.63	NO	0.000003	0.000003

Table B-2. U. S. Steel Clairton Volume Sources (Non-Buoyant)

SOURCE	ID	UTMx	UTMy	ELEV	REL HEIGHT	INIT SY	INIT SZ	BASE RATE	PROJ RATE
Cooling Tower, Fan 1	CLCOOL1	595464.2	4462313.2	231	44.20	5.02	10.28	0.581140	0.581140
Cooling Tower, Fan 2	CLCOOL2	595457.6	4462322.7	231	44.20	5.02	10.28	0.581140	0.581140
Cooling Tower, Fan 3	CLCOOL3	595451.2	4462331.5	231	44.20	5.02	10.28	0.581140	0.581140
Cooling Tower, Fan 4	CLCOOL4	595444.7	4462340.4	231	44.20	5.02	10.28	0.581140	0.581140
Cooling Tower, Fan 5	CLCOOL5	595438.3	4462349.1	231	44.20	5.02	10.28	0.581140	0.581140
#1 Pulverizers	CLPULV1	595943.0	4461998.0	231	9.00	2.33	8.37	0.000101	0.000101
#2 Pulverizers	CLPULV2	595579.0	4462373.0	231	3.65	2.33	3.40	0.000017	0.000017
Blasting - Black Beauty	CLBLKBTY	595835.0	4461406.0	231	6.10	2.33	5.67	0.001671	0.001671
Boom Conveyor, Segment 1	CLBOOM1	594267.0	4463101.0	231	5.50	2.33	2.56	0.000190	0.000190
Boom Conveyor, Segment 2	CLBOOM2	594421.0	4463005.0	231	5.50	2.33	2.56	0.000190	0.000190
Coke Pile, Load/Unload	CLCOKEP	595085.0	4461671.0	231	6.10	2.33	2.84	0.000316	0.000316
Coal Bins/Bunkers, Segment 1	CLBUNK1	595858.0	4461835.0	231	18.25	2.33	8.48	0.000065	0.000065
Coal Bins/Bunkers, Segment 2	CLBUNK2	595334.0	4462256.0	231	18.40	2.33	8.56	0.000065	0.000065
Coal Bins/Bunkers, Segment 3	CLBUNK3	595313.0	4462162.0	231	21.25	2.33	9.88	0.000065	0.000065
Coal Bins/Bunkers, Segment 4	CLBUNK4	595606.0	4462239.0	231	28.55	2.33	13.28	0.000065	0.000065
Ball Mill 1-3	CLBALL1	595858.0	4461835.0	231	18.25	2.33	8.48	0.000118	0.000118
Ball Mill 13-15	CLBALL13	595334.0	4462256.0	231	18.40	2.33	8.56	0.000150	0.000150
Ball Mill 19-20	CLBALL19	595313.0	4462162.0	231	21.25	2.33	9.88	0.000167	0.000167
Ball Mill B	CLBALLB	595606.0	4462239.0	231	28.55	2.33	13.28	0.000083	0.000083
Ball Mill C	CLBALLC	595606.0	4462239.0	231	28.55	2.33	13.28	--	0.000575
Continuous Unloading #1	CLUNLD1	595826.0	4462163.0	231	10.00	2.33	4.65	0.000547	0.000547
Continuous Unloading #2	CLUNLD2	595365.0	4462576.0	231	10.00	2.33	4.65	0.000690	0.000690
Pedestal Crane Unloader	CLPED	595153.0	4462670.0	231	6.10	2.33	2.84	0.000049	0.000049
Clamshell Unloader	CLCLAM	594032.0	4463306.0	231	6.10	2.33	2.84	0.000037	0.000037
Screen Station 1 (1-3)	CLSCR1	595768.0	4461988.0	231	7.50	2.33	3.49	0.001556	0.001556
Screen Station 2 (13-15, 19-20)	CLSCR2	595229.0	4462312.0	231	12.40	2.33	5.77	0.004180	0.004180
Screen Station 3 (B)	CLSCR3	595685.0	4462051.0	231	7.50	2.33	3.49	0.005115	--
Screen Station 4 (B/C)	CLSCR4	595700.0	4462085.0	231	8.00	2.33	3.72	--	0.008630
Coal Transfer, Tower 1	CLCOALT1	595988.0	4461954.0	231	9.00	2.33	4.19	0.000247	0.000247
Coal Transfer, Tower 2	CLCOALT2	595770.0	4462190.0	231	9.00	2.33	4.19	0.000247	0.000247
Coal Transfer, Tower 3	CLCOALT3	595655.0	4462289.0	231	9.00	2.33	4.19	0.000247	0.000247
Coal Transfer, Tower 4	CLCOALT4	595480.0	4462454.0	231	9.00	2.33	4.19	0.000247	0.000247
Coal Transfer, Tower 5	CLCOALT5	595215.0	4462632.0	231	9.00	2.33	4.19	0.000247	0.000247
Coke Transfer 1-3, B, C - Segment 1	CLCOKET1	595844.0	4461883.0	231	6.10	2.33	2.84	0.002877	0.002877
Coke Transfer 1-3, B, C - Segment 2	CLCOKET2	595596.0	4462200.0	231	6.10	2.33	2.84	0.002877	0.004315
Coke Transfer 13-15, 19-20	CLCOKET3	595331.0	4462196.0	231	6.10	2.33	2.84	0.007013	0.007013
By-Product, Tar/Liquor/Pitch - Segment 1	CLTAR1	595411.0	4462269.0	231	6.10	2.33	2.84	0.030305	0.030305
By-Product, Tar/Liquor/Pitch - Segment 2	CLTAR2	595514.0	4462136.0	231	6.10	2.33	2.84	0.030305	0.030305
By-Product (Cooler/Pumphouse Sumps)	CLSUMP	595364.0	4462306.0	231	6.10	2.33	2.84	0.015646	0.015646
By-Product (Tar Storage Tanks)	CLTANK	595356.0	4462436.0	231	8.10	3.26	3.77	0.000149	0.000149
Aeration Basins - WWTP	CLAERBN	595158.0	4462533.0	231	7.50	5.35	3.49	0.032093	0.032093
Motor Vehicles and Roads, Segment 1	CLROAD1	595738.0	4461596.0	231	2.55	6.98	2.37	0.017053	0.017053
Motor Vehicles and Roads, Segment 2	CLROAD2	595795.0	4461036.0	231	2.55	6.98	2.37	0.017053	0.017053
Motor Vehicles and Roads, Segment 3	CLROAD3	596031.0	4461518.0	231	2.55	6.98	2.37	0.017053	0.017053
Motor Vehicles and Roads, Segment 4	CLROAD4	595989.0	4461695.0	231	2.55	6.98	2.37	0.017053	0.017053
Motor Vehicles and Roads, Segment 5	CLROAD5	595943.0	4461926.0	231	2.55	6.98	2.37	0.017053	0.017053
Motor Vehicles and Roads, Segment 6	CLROAD6	595390.0	4462452.0	231	2.55	6.98	2.37	0.017053	0.017053
Motor Vehicles and Roads, Segment 7	CLROAD7	594913.0	4462537.0	231	2.55	6.98	2.37	0.017053	0.017053
Motor Vehicles and Roads, Segment 8	CLROAD8	595185.0	4462261.0	231	2.55	6.98	2.37	0.017053	0.017053
Motor Vehicles and Roads, Segment 9	CLROAD9	595437.0	4461976.0	231	2.55	6.98	2.37	0.017053	0.017053
Motor Vehicles and Roads, Segment 10	CLROAD10	594747.0	4462629.0	231	2.55	6.98	2.37	0.017053	0.017053
Motor Vehicles and Roads, Segment 11	CLROAD11	594409.0	4462859.0	231	2.55	6.98	2.37	0.017053	0.017053
Motor Vehicles and Roads, Segment 12	CLROAD12	593930.0	4463233.0	231	2.55	6.98	2.37	0.017053	0.017053
Tug Boat Exhaust, Segment 1	CLTUG1	594222.0	4463159.0	231	3.05	2.33	1.42	0.039818	0.039818
Tug Boat Exhaust, Segment 2	CLTUG2	595312.0	4462606.0	231	3.05	2.33	1.42	0.039818	0.039818
Tug Boat Exhaust, Segment 3	CLTUG3	595863.0	4462126.0	231	3.05	2.33	1.42	0.039818	0.039818

Table B-3. U. S. Steel Clairton Area Sources

SOURCE	ID	UTMx	UTMy	VERTEX	ELEV	REL HEIGHT	BASE RATE (per m ²)	PROJ RATE (per m ²)
Coke Storage/Erosion (Peters Creek)	CLEROS1	594891.0	4461579.0	1	231	6.1	0.0000001119	0.0000001119
		594847.0	4461711.0	2	231	6.1		
		595204.0	4461836.0	3	231	6.1		
		595249.0	4461705.0	4	231	6.1		
Coke Storage/Erosion (South Yard)	CLEROS2	595726.0	4460737.0	1	231	6.1	0.0000003663	0.0000003663
		595781.0	4460960.0	2	231	6.1		
		595848.0	4460943.0	3	231	6.1		
		595794.0	4460722.0	4	231	6.1		

U. S. Steel Clairton Plant buoyant line (battery) volume source coordinates, elevations, and emission rates are given in Table B-4, with the line parameters used for the BLP calculations given in Table B-5.

Batteries were modeled by segments of each battery line, by adjacent line volume source methodology (equidistant segments). The number of segments for each line is as follows:

- Batteries 1-3: 21 segments
- Batteries 13-15: 19 segments
- Batteries 19-20: 18 segments
- B Battery: 6 segments
- C Battery: 7 segments

Additional parameters, specific to each segment, were assigned as follows:

- Release height: varying by hour (based on BLP-based plume rises + battery height)
- Initial lateral dimension (σ_y): based on width of building by segment
 - o Batteries 1-3: 6.70 m
 - o Batteries 13-15: 6.51 m
 - o Batteries 19-20: 6.51 m
 - o B Battery: 7.77 m
 - o C Battery: 7.77 m
- Initial vertical dimension (σ_z): varying by hour, release height/4.3

Table B-4. U. S. Steel Clairton Buoyant Line Volumes

SOURCE	ID	UTMx	UTMy	ELEV	BASE RATE	PROJ RATE
Batteries 1-3 Fugitives Seg 1	CLB01S01	595737.1	4461971.8	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 2	CLB01S02	595746.2	4461961.5	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 3	CLB01S03	595755.3	4461951.3	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 4	CLB01S04	595764.4	4461941.0	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 5	CLB01S05	595773.5	4461930.8	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 6	CLB01S06	595782.6	4461920.6	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 7	CLB01S07	595791.7	4461910.3	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 8	CLB01S08	595800.8	4461900.1	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 9	CLB01S09	595809.9	4461889.9	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 10	CLB01S10	595819.0	4461879.6	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 11	CLB01S11	595828.1	4461869.4	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 12	CLB01S12	595837.2	4461859.2	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 13	CLB01S13	595846.3	4461848.9	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 14	CLB01S14	595855.4	4461838.7	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 15	CLB01S15	595864.6	4461828.5	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 16	CLB01S16	595873.7	4461818.2	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 17	CLB01S17	595882.8	4461808.0	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 18	CLB01S18	595891.9	4461797.7	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 19	CLB01S19	595901.0	4461787.5	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 20	CLB01S20	595910.1	4461777.3	231	0.044144	0.043979
Batteries 1-3 Fugitives Seg 21	CLB01S21	595919.2	4461767.0	231	0.044144	0.043979
Batteries 13-15 Fugitives Seg 1	CLB13S01	595276.1	4462317.8	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 2	CLB13S02	595285.4	4462307.4	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 3	CLB13S03	595294.7	4462296.9	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 4	CLB13S04	595304.1	4462286.5	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 5	CLB13S05	595313.4	4462276.0	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 6	CLB13S06	595322.7	4462265.6	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 7	CLB13S07	595332.0	4462255.1	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 8	CLB13S08	595341.3	4462244.7	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 9	CLB13S09	595350.7	4462234.2	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 10	CLB13S10	595360.0	4462223.8	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 11	CLB13S11	595369.3	4462213.3	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 12	CLB13S12	595378.6	4462202.9	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 13	CLB13S13	595387.9	4462192.5	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 14	CLB13S14	595397.3	4462182.0	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 15	CLB13S15	595406.6	4462171.6	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 16	CLB13S16	595415.9	4462161.1	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 17	CLB13S17	595425.2	4462150.7	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 18	CLB13S18	595434.6	4462140.2	231	0.057614	0.057432
Batteries 13-15 Fugitives Seg 19	CLB13S19	595443.9	4462129.8	231	0.057614	0.057432

Table B-4. U. S. Steel Clairton Buoyant Line Volumes – continued

SOURCE	ID	UTMx	UTMy	ELEV	BASE RATE	PROJ RATE
Batteries 19-20 Fugitives Seg 1	CLB19S01	595234.2	4462249.3	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 2	CLB19S02	595243.6	4462238.8	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 3	CLB19S03	595252.9	4462228.4	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 4	CLB19S04	595262.2	4462217.9	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 5	CLB19S05	595271.5	4462207.5	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 6	CLB19S06	595280.8	4462197.0	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 7	CLB19S07	595290.1	4462186.5	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 8	CLB19S08	595299.4	4462176.1	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 9	CLB19S09	595308.7	4462165.6	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 10	CLB19S10	595318.0	4462155.1	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 11	CLB19S11	595327.3	4462144.7	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 12	CLB19S12	595336.6	4462134.2	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 13	CLB19S13	595345.9	4462123.8	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 14	CLB19S14	595355.2	4462113.3	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 15	CLB19S15	595364.5	4462102.8	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 16	CLB19S16	595373.8	4462092.4	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 17	CLB19S17	595383.1	4462081.9	231	0.079216	0.079023
Batteries 19-20 Fugitives Seg 18	CLB19S18	595392.4	4462071.4	231	0.079216	0.079023
B Battery Fugitives Seg 1	CLBBS01	595521.4	4462332.4	231	0.072687	0.072110
B Battery Fugitives Seg 2	CLBBS02	595532.5	4462319.9	231	0.072687	0.072110
B Battery Fugitives Seg 3	CLBBS03	595543.7	4462307.5	231	0.072687	0.072110
B Battery Fugitives Seg 4	CLBBS04	595554.8	4462295.0	231	0.072687	0.072110
B Battery Fugitives Seg 5	CLBBS05	595565.9	4462282.6	231	0.072687	0.072110
B Battery Fugitives Seg 6	CLBBS06	595577.1	4462270.2	231	0.072687	0.072110
C Battery Fugitives Seg 1	CLBCS01	595668.6	4462167.0	231	--	0.090777
C Battery Fugitives Seg 2	CLBCS02	595679.7	4462154.5	231	--	0.090777
C Battery Fugitives Seg 3	CLBCS03	595690.8	4462142.1	231	--	0.090777
C Battery Fugitives Seg 4	CLBCS04	595701.9	4462129.6	231	--	0.090777
C Battery Fugitives Seg 5	CLBCS05	595713.0	4462117.1	231	--	0.090777
C Battery Fugitives Seg 6	CLBCS06	595724.1	4462104.7	231	--	0.090777
C Battery Fugitives Seg 7	CLBCS07	595735.2	4462092.2	231	--	0.090777

Table B-5. U. S. Steel Clairton Buoyant Line Parameters

Buoyant Line Source	ID	Elev (m)	UTMx (m) nw	UTMy (m) nw	UTMx (m) se	UTMy (m) se
US STEEL CLAIRTON Batteries 1-3	CLBATT1_3	231	595732.5	4461976.9	595922.9	4461762.9
US STEEL CLAIRTON Batteries 13-15	CLBATT13_15	231	595271.4	4462323.0	595453.0	4462119.6
US STEEL CLAIRTON Batteries 19-20	CLBATT19_20	231	595229.6	4462254.5	595393.9	4462069.8
US STEEL CLAIRTON B Battery	CLBATTB	231	595515.8	4462338.6	595585.5	4462260.7
US STEEL CLAIRTON C Battery	CLBATTC	231	595663.0	4462173.2	595739.9	4462086.9
Buoyant Line Source (cont.)	ID	Avg Bldg (Line) Length (m)	Avg Bldg Ht (m)	Avg Bldg Width (m)	Avg Line Width (m)	Spacing (m)
US STEEL CLAIRTON Batteries 1-3	CLBATT1_3	287.0	8.5	13.7	1.0	0.0
US STEEL CLAIRTON Batteries 13-15	CLBATT13_15	273.0	8.8	14.0	1.0	0.0
US STEEL CLAIRTON Batteries 19-20	CLBATT19_20	247.0	10.5	14.0	1.0	0.0
US STEEL CLAIRTON B Battery	CLBATTB	106.0	15.1	16.7	1.0	0.0
US STEEL CLAIRTON C Battery	CLBATTC	115.0	15.1	16.7	1.0	0.0
Buoyant Line Source (cont.)	ID	Exit Temp (K)	Amb Temp (K)	Exit Vel (m/s)	Avg Line Buoyancy (m ⁴ /s ³)	Release Ht (m)
US STEEL CLAIRTON Batteries 1-3	CLBATT1_3	1184.83	284.27	3.05	6520.3	8.5
US STEEL CLAIRTON Batteries 13-15	CLBATT13_15	1184.83	284.27	3.05	6202.2	8.8
US STEEL CLAIRTON Batteries 19-20	CLBATT19_20	1184.83	284.27	3.05	5611.5	10.5
US STEEL CLAIRTON B Battery	CLBATTB	1184.83	284.27	3.05	2408.2	15.1
US STEEL CLAIRTON C Battery	CLBATTC	1184.83	284.27	3.05	2612.6	15.1

Tables B-6 through B-9 show the point and volume source parameters used for the U. S. Steel Edgar Thomson and Irvin Plants. These facilities, while part of the same integrated mill as the Clairton Plant (U. S. Steel Mon Valley Works), are further away from the Liberty monitor than the Clairton Plant. (Irvin is about 3 km to the WNW, and Edgar Thomson is about 8 km to the NNE.)

Table B-6. U. S. Steel Edgar Thomson Point Sources

SOURCE	ID	UTMx	UTMy	ELEV	HEIGHT	TEMP	VEL	DIAM	BLDG	BASE RATE	PROJ RATE
Riley Boiler 1	ETRB1	597057.0	4471990.0	225	49.17	672.04	7.86	4.22	YES	2.570700	2.570700
Riley Boiler 2	ETRB2	597042.0	4471996.0	225	49.17	672.04	7.86	4.22	YES	2.669000	2.669000
Riley Boiler 3	ETRB3	597027.0	4472001.0	225	49.17	672.04	7.86	4.22	YES	2.439900	2.439900
Blast Furnace 1 Stoves	ETBF1STV	597180.0	4472051.0	225	79.42	464.82	7.97	3.28	YES	1.629100	1.629100
Casthouse Baghouse (4 comps)	ETCASTB	597131.0	4471997.0	225	27.43	394.26	10.00	3.60	YES	0.040282	0.040282
Blast Furnace 3 Stoves	ETBF3STV	597014.0	4472084.0	225	57.05	522.59	9.84	2.59	YES	1.691800	1.691800
BFG Flare	ETBFGF	597166.0	4471984.0	225	66.00	1273.00	20.00	0.92	YES	0.299670	0.299670
BOP Mixer Baghouse, Module 1	ETMIX1	596463.3	4472314.5	228	21.64	327.44	22.91	0.73	YES	0.010230	0.010230
BOP Mixer Baghouse, Module 2	ETMIX2	596466.0	4472313.7	228	21.64	327.44	22.91	0.73	YES	0.010230	0.010230
BOP Mixer Baghouse, Module 3	ETMIX3	596462.3	4472311.6	228	21.64	327.44	22.91	0.73	YES	0.010230	0.010230
BOP Mixer Baghouse, Module 4	ETMIX4	596465.2	4472310.8	228	21.64	327.44	22.91	0.73	YES	0.010230	0.010230
BOP Mixer Baghouse, Module 5	ETMIX5	596461.4	4472308.7	228	21.64	327.44	22.91	0.73	YES	0.010230	0.010230
BOP Mixer Baghouse, Module 6	ETMIX6	596464.4	4472307.8	228	21.64	327.44	22.91	0.73	YES	0.010230	0.010230
BOP Mixer Baghouse, Module 7	ETMIX7	596460.7	4472305.8	228	21.64	327.44	22.91	0.73	YES	0.010230	0.010230
BOP Mixer Baghouse, Module 8	ETMIX8	596463.5	4472304.9	228	21.64	327.44	22.91	0.73	YES	0.010230	0.010230
BOP Mixer Baghouse, Module 9	ETMIX9	596459.7	4472302.9	228	21.64	327.44	22.91	0.73	YES	0.010230	0.010230
BOP Mixer Baghouse, Module 10	ETMIX10	596462.7	4472302.1	228	21.64	327.44	22.91	0.73	YES	0.010230	0.010230
BOP Mixer Baghouse, Module 11	ETMIX11	596459.2	4472300.0	228	21.64	327.44	22.91	0.73	YES	0.010230	0.010230
BOP Mixer Baghouse, Module 12	ETMIX12	596462.0	4472299.2	228	21.64	327.44	22.91	0.73	YES	0.010230	0.010230
BOP Vessel F&R Scrubber, Stack 1	ETSCR1	596571.9	4472271.8	228	55.17	321.88	17.54	3.05	YES	2.002200	2.002200
BOP Vessel F&R Scrubber, Stack 2	ETSCR2	596588.3	4472257.7	228	55.17	321.88	17.54	3.05	YES	2.002200	2.002200
BOP Secondary Baghouse, Module 1	ETSEC1	596411.1	4472401.5	228	14.63	322.10	10.00	3.60	YES	0.009652	0.009652
BOP Secondary Baghouse, Module 2	ETSEC2	596411.0	4472398.0	228	14.63	322.10	10.00	3.60	YES	0.009652	0.009652
BOP Secondary Baghouse, Module 3	ETSEC3	596411.1	4472394.7	228	14.63	322.10	10.00	3.60	YES	0.009652	0.009652
BOP Secondary Baghouse, Module 4	ETSEC4	596410.9	4472391.2	228	14.63	322.10	10.00	3.60	YES	0.009652	0.009652
BOP Secondary Baghouse, Module 5	ETSEC5	596410.9	4472387.5	228	14.63	322.10	10.00	3.60	YES	0.009652	0.009652
BOP Secondary Baghouse, Module 6	ETSEC6	596410.9	4472384.1	228	14.63	322.10	10.00	3.60	YES	0.009652	0.009652
BOP Secondary Baghouse, Module 7	ETSEC7	596410.8	4472380.2	228	14.63	322.10	10.00	3.60	YES	0.009652	0.009652
BOP Secondary Baghouse, Module 8	ETSEC8	596410.8	4472376.7	228	14.63	322.10	10.00	3.60	YES	0.009652	0.009652
BOP Secondary Baghouse, Module 9	ETSEC9	596410.7	4472373.3	228	14.63	322.10	10.00	3.60	YES	0.009652	0.009652
BOP Secondary Baghouse, Module 10	ETSEC10	596410.7	4472369.6	228	14.63	322.10	10.00	3.60	YES	0.009652	0.009652
BOP Railcar Unloading Baghouse	ETUNLD	596443.3	4472403.6	228	12.19	294.27	10.00	0.70	YES	0.004030	0.004030
BOP Transfer Tower Baghouse	ETTRAN	596422.5	4472201.2	228	32.61	294.27	10.00	1.60	YES	0.002017	0.002017
LMF Baghouse, Module 1	ETLMFB1	596603.2	4472432.3	229	20.42	351.97	10.94	0.73	YES	0.004871	0.004871
LMF Baghouse, Module 2	ETLMFB2	596596.5	4472433.9	229	20.42	351.97	10.94	0.73	YES	0.004871	0.004871
LMF Baghouse, Module 3	ETLMFB3	596604.2	4472435.7	229	20.42	351.97	10.94	0.73	YES	0.004871	0.004871
LMF Baghouse, Module 4	ETLMFB4	596597.3	4472437.2	229	20.42	351.97	10.94	0.73	YES	0.004871	0.004871
LMF Baghouse, Module 5	ETLMFB5	596605.1	4472439.2	229	20.42	351.97	10.94	0.73	YES	0.004871	0.004871
LMF Baghouse, Module 6	ETLMFB6	596598.2	4472440.6	229	20.42	351.97	10.94	0.73	YES	0.004871	0.004871

Table B-7. U. S. Steel Edgar Thomson Volume Sources

SOURCE	ID	UTMx	UTMy	ELEV	REL HEIGHT	INIT SY	INIT SZ	BASE RATE	PROJ RATE
BF1 Material/Slag Handling	ETBF1SLG	597224.0	4472002.0	228	6.10	2.33	2.84	0.012318	0.012318
BF1 Casthouse (Roof + Fume) Seg a	ETCAST1A	597195.6	4472010.1	225	27.13	7.07	12.62	0.490120	0.490120
BF1 Casthouse (Roof + Fume) Seg b	ETCAST1B	597190.4	4471995.9	225	27.13	7.07	12.62	0.490120	0.490120
BF1 Breakdown	ETBF1BRK	597206.5	4472031.4	226	52.50	1.86	24.42	0.079443	0.079443
BF3 Material/Slag Handling	ETBF3SLG	597095.2	4472077.2	228	6.10	1.86	2.84	0.010695	0.010695
BF3 Casthouse (Roof + Fume) Seg a	ETCAST3A	597072.8	4472065.3	225	30.78	6.13	14.32	0.497160	0.497160
BF3 Casthouse (Roof + Fume) Seg b	ETCAST3B	597078.3	4472046.3	225	30.78	6.13	14.32	0.497160	0.497160
BF3 Breakdown	ETBF3BRK	597066.5	4472083.8	226	43.80	2.74	19.30	0.079443	0.079443
BOP Process Fuel Use (Roof Monitor) Seg 1	ETBOP1	596533.9	4472311.0	228	53.11	5.12	24.70	0.023003	0.023003
BOP Process Fuel Use (Roof Monitor) Seg 2	ETBOP2	596536.9	4472321.6	228	53.11	5.12	24.70	0.023003	0.023003
BOP Process Fuel Use (Roof Monitor) Seg 3	ETBOP3	596539.9	4472332.1	228	53.11	5.12	24.70	0.023003	0.023003
BOP Process Fuel Use (Roof Monitor) Seg 4	ETBOP4	596543.0	4472342.7	228	53.11	5.12	24.70	0.023003	0.023003
BOP Process Fuel Use (Roof Monitor) Seg 5	ETBOP5	596546.0	4472353.3	228	53.11	5.12	24.70	0.023003	0.023003
BOP Process Fuel Use (Roof Monitor) Seg 6	ETBOP6	596549.1	4472363.9	228	53.11	5.12	24.70	0.023003	0.023003
BOP Process Fuel Use (Roof Monitor) Seg 7	ETBOP7	596552.1	4472374.4	228	53.11	5.12	24.70	0.023003	0.023003
BOP Process Fuel Use (Roof Monitor) Seg 8	ETBOP8	596555.1	4472385.0	228	53.11	5.12	24.70	0.023003	0.023003
Continuous Casting/LMF (Roof Mon) Seg 1	ETCCLMF1	596609.7	4472367.6	228	51.16	4.79	23.79	0.001919	0.001919
Continuous Casting/LMF (Roof Mon) Seg 2	ETCCLMF2	596612.4	4472377.5	228	51.16	4.79	23.79	0.001919	0.001919
Continuous Casting/LMF (Roof Mon) Seg 3	ETCCLMF3	596615.0	4472387.5	228	51.16	4.79	23.79	0.001919	0.001919
Continuous Casting/LMF (Roof Mon) Seg 4	ETCCLMF4	596617.7	4472397.5	228	51.16	4.79	23.79	0.001919	0.001919
Continuous Casting/LMF (Roof Mon) Seg 5	ETCCLMF5	596620.3	4472407.4	228	51.16	4.79	23.79	0.001919	0.001919
BF Fugitives (Misc. Comb.) Seg 1	ETBFMC1	597248.0	4471879.0	225	18.00	5.74	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 2	ETBFMC2	596873.9	4472180.3	228	18.00	8.76	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 3	ETBFMC3	596891.7	4472174.1	228	18.00	8.76	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 4	ETBFMC4	596909.4	4472167.9	228	18.00	8.76	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 5	ETBFMC5	596927.2	4472161.7	228	18.00	8.76	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 6	ETBFMC6	596945.0	4472155.5	228	18.00	8.76	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 7	ETBFMC7	596962.8	4472149.3	228	18.00	8.76	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 8	ETBFMC8	596980.6	4472143.1	228	18.00	8.76	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 9	ETBFMC9	596998.4	4472136.9	228	18.00	8.76	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 10	ETBFMC10	597016.1	4472130.7	228	18.00	8.76	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 11	ETBFMC11	597091.9	4472159.3	228	18.00	8.80	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 12	ETBFMC12	597109.6	4472152.8	228	18.00	8.80	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 13	ETBFMC13	597127.4	4472146.4	228	18.00	8.80	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 14	ETBFMC14	597145.2	4472139.9	228	18.00	8.80	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 15	ETBFMC15	597163.0	4472133.5	228	18.00	8.80	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 16	ETBFMC16	597180.8	4472127.1	228	18.00	8.80	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 17	ETBFMC17	597198.6	4472120.6	228	18.00	8.80	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 18	ETBFMC18	597216.4	4472114.2	228	18.00	8.80	8.37	0.004220	0.004220
BF Fugitives (Misc. Comb.) Seg 19	ETBFMC19	597234.2	4472107.8	228	18.00	8.80	8.37	0.004220	0.004220
Cooling Tower / BFCE Recycle	ETCOOL1	596485.1	4472243.7	228	20.42	2.11	9.50	0.011311	0.011311
Cooling Tower / BOP	ETCOOL2	596575.1	4472241.0	228	15.24	1.52	7.09	0.014231	0.014231
Cooling Tower / Caster	ETCOOL3	596761.2	4472390.9	228	15.24	1.05	7.09	0.006478	0.006478
Cooling Tower / WSAC (Mold Water)	ETCOOL4	596979.0	4472046.0	228	9.14	0.82	4.25	0.074842	0.074842
Roads & Misc. Combustion	ETROAD	596941.9	4472066.8	225	2.55	6.98	2.37	0.068928	0.068928
Storage Piles	ETSTOR	597037.4	4472151.3	225	6.10	7.94	2.84	0.010014	0.010014

Table B-8. U. S. Steel Irvin Point Sources

SOURCE	ID	UTMx	UTMy	ELEV	HEIGHT	TEMP	VEL	DIAM	BLDG	BASE RATE	PROJ RATE
Boiler #1	IRBLR1	593149.0	4465476.0	287	19.50	635.38	10.23	1.10	YES	0.045860	0.045860
Boiler #2	IRBLR2	593171.0	4465165.0	287	21.94	537.05	8.00	1.28	YES	0.053949	0.053949
Boilers #3-4	IRBLR3	593419.0	4465596.0	287	22.86	644.26	9.70	1.42	YES	0.029060	0.029060
80" Mill Reheat Furnace 1	IR80IN1	593177.0	4465871.0	287	20.00	710.38	29.43	1.98	YES	0.117270	0.117270
80" Mill Reheat Furnace 2	IR80IN2	593178.0	4465884.0	287	20.00	710.38	29.43	1.98	YES	0.116760	0.116760
80" Mill Reheat Furnace 3	IR80IN3	593179.0	4465896.0	287	20.00	710.38	29.43	1.98	YES	0.109440	0.109440
80" Mill Reheat Furnace 4	IR80IN4	593180.0	4465909.0	287	20.00	710.38	29.43	1.98	YES	0.178070	0.178070
80" Mill Reheat Furnace 5	IR80IN5	593181.0	4465923.0	287	20.00	710.38	29.43	1.98	YES	0.161300	0.161300
80" Mill Reheat Waste Stack 6	IR80INW	593243.0	4465922.0	287	28.34	710.38	29.43	1.82	YES	0.169170	0.169170
#1 Galv Line Preheat	IRGALV1	593352.0	4465406.0	287	25.30	944.26	9.48	1.42	YES	0.014944	0.014944
#2 Galv Line Preheat	IRGALV2	593350.0	4465386.0	287	26.82	944.26	2.66	1.37	YES	0.010730	0.010730
HPH Annealing Furnaces (seg a)	IRHPH_A	593328.6	4465585.5	287	21.33	527.60	10.00	0.76	YES	0.007587	0.007587
HPH Annealing Furnaces (seg b)	IRHPH_B	593325.2	4465553.5	287	21.33	527.60	10.00	0.76	YES	0.007587	0.007587
HPH Annealing Furnaces (seg c)	IRHPH_C	593321.8	4465521.6	287	21.33	527.60	10.00	0.76	YES	0.007587	0.007587
HPH Annealing Furnaces (seg d)	IRHPH_D	593318.4	4465489.8	287	21.33	527.60	10.00	0.76	YES	0.007587	0.007587
HPH Annealing Furnaces (seg e)	IRHPH_E	593315.3	4465457.8	287	21.33	527.60	10.00	0.76	YES	0.007587	0.007587
HPH Annealing Furnaces (seg f)	IRHPH_F	593311.6	4465425.9	287	21.33	527.60	10.00	0.76	YES	0.007587	0.007587
HPH Annealing Furnaces (seg g)	IRHPH_G	593308.2	4465394.0	287	21.33	527.60	10.00	0.76	YES	0.007587	0.007587
Open Coil Annealing	IROCA	593335.0	4465243.0	287	21.33	310.94	10.52	2.96	YES	0.031390	0.031390
Continuous Annealing	IRCONTA	593341.0	4464903.0	287	36.57	513.72	10.52	1.07	YES	0.014038	0.014038
Peach Tree Flare A&B	IRPTF	592868.0	4464808.0	333	18.28	1273.00	20.00	0.63	NO	0.023717	0.023717
COG Flares 1-3	IRCOGF	593237.0	4464601.0	287	8.99	1273.00	20.00	0.63	NO	0.014341	0.014341
64" Pickling Line (Descaler)	IR64PKL	593213.0	4465111.0	287	15.54	328.15	12.41	0.76	YES	0.005787	0.005787
84" Pickling Line (Descaler)	IR84PKL	593130.1	4465287.6	287	35.05	327.59	10.36	1.37	YES	0.015871	0.015871
Cold Reduction Mill	IRCOLD	593397.0	4465193.0	287	26.82	312.04	12.71	6.86	YES	0.870700	0.870700

Table B-9. U. S. Steel Irvin Volume Sources

SOURCE	ID	UTMx	UTMy	ELEV	REL HEIGHT	INIT SY	INIT SZ	BASE RATE	PROJ RATE
Cooling Tower HPH	IRCOOL1	593359.0	4465916.0	287	10.06	1.60	4.68	0.002275	0.002275
Cooling Tower North Water Treatment	IRCOOL2	593006.0	4465719.0	293	10.36	1.30	4.82	0.002158	0.002158
Miscellaneous NG Combustion (segment 1)	IRMISC1	593181.0	4464880.0	287	17.00	2.33	7.91	0.009603	0.009603
Miscellaneous NG Combustion (segment 2)	IRMISC2	593230.0	4465326.0	287	17.00	2.33	7.91	0.009603	0.009603
Miscellaneous NG Combustion (segment 3)	IRMISC3	593275.0	4465778.0	287	17.00	2.33	7.91	0.009603	0.009603
Roads/Vehicles (segment 1)	IRROAD1	593146.0	4466074.0	287	2.55	6.98	2.37	0.000303	0.000303
Roads/Vehicles (segment 2)	IRROAD2	593167.0	4464665.0	287	2.55	6.98	2.37	0.000303	0.000303

Tables B-10 through B-12 shows the point source parameters used for the distant sources (Allegheny Ludlum, McConway & Torley, Shenango). These sources are several kilometers away from the Liberty monitor. They were included in the AERMOD modeling in order to account for all background primary PM_{2.5} impacts, since they were tracked as local primary (LPM) sources separately from the CAMx regional sources.

AERMOD source characterization for the distant sources was not refined like with the U. S. Steel sources and did not include the use of volume or area sources, building downwash parameters, etc. All source parameters were identical to the CAMx inputs, with some smaller sources aggregated into one source (such as plant-wide fugitives, cooling towers, etc.)

The Cheswick power plant is an additional large source of primary PM_{2.5} located in the northeastern portion of Allegheny County (about 9 km to the southwest of Allegheny Ludlum). Since emissions are

from a tall stack (552 ft) and not near the immediate impact zone of any surrounding PM_{2.5} monitor, it was not included in the local source tracking or AERMOD modeling but was included in the CAMx regional component. Previous screening results with AERMOD for this source have shown minimal impacts of primary pollutants in southeastern Allegheny County that do not contribute to nonattainment (see the SO₂ SIP for more information (ACHD, 2017)).

Table B-10. Allegheny Ludlum Sources

SOURCE	BASE ID	PROJ ID	UTMx	UTMy	ELEV	HEIGHT	TEMP	VEL	DIAM	BLDG	BASE RATE	PROJ RATE
#1 A&P LINE, SHOTBLAST	LUD01	LUD01	607692.8	4496079.5	233	3.05	295.37	10.06	0.91	NO	0.097519	0.097519
#1-2 A&P ANNEALING FCE / CAR BOTTOM FURNACES 1-4	LUD02	LUD02	607323.9	4495839.9	233	19.81	295.37	0.03	0.03	NO	0.018411	0.022240
#2 A&P LINE, KOLENE DESCALING	LUD03	LUD03	607692.8	4496079.5	233	16.76	313.71	3.05	1.31	NO	0.007767	0.007767
#3 B&P LINE PREHEATER NG	LUD04	--	607692.8	4496079.5	233	15.24	295.37	0.03	0.03	NO	0.004027	--
#3 B&P LINE, SHOTBLAST / #3 B&P, NEW SHOT BLAST	LUD05	LUD04	607692.8	4496079.5	233	3.05	295.37	9.33	0.49	NO	0.207410	0.207410
#3 DEPT. BOILERS / #3 DEPT. BOILERS, NG	LUD06	LUD05	607692.8	4496079.5	233	6.10	449.82	5.70	2.13	NO	0.012945	0.012945
1-3 PICKLE ACID SCRUBBING / #1-3 PICKLE ACID SCRUBBER	LUD07	LUD06	607601.3	4496027.1	233	21.30	310.99	15.20	1.22	NO	0.050054	0.050054
AMER. HORIZ LADLE PREHEAT 1-3 NG	LUD08	--	607692.8	4496079.5	233	12.19	295.37	0.03	0.03	NO	0.000015	--
AOD - CANOPY BAGHOUSE / CASTER PREHEAT / TORCH CUTTERS	LUD09	LUD08	607692.8	4496079.5	233	22.55	366.48	3.41	3.05	NO	0.158790	0.159690
AOD - UNCAPTURED	LUD10	LUD09	607692.8	4496079.5	233	22.55	295.37	0.03	0.03	NO	0.004890	0.004890
AOD MOLD PREHEATERS 1-24	LUD11	LUD10	607724.8	4496265.4	233	39.62	295.37	0.03	0.03	NO	0.000299	0.000299
AOD VESSEL PREHEATER / AOD VESSEL PRHTR NG	LUD12	--	607692.8	4496079.5	233	12.19	295.37	0.03	0.03	NO	0.000748	--
BELL ANNEAL FCES. 1-6 / NG	LUD13	--	607380.4	4495853.0	233	23.42	295.37	0.03	0.03	NO	0.000748	--
BLOOM HORIZ PREHEATERS	LUD14	LUD11	607760.1	4496220.4	233	42.00	295.37	0.03	0.03	NO	0.006904	0.006904
CASTER TUNDISH PREHEAT / PREHEATERS 1,2 NG	LUD15	--	607692.8	4496079.5	233	22.55	366.48	3.41	3.05	NO	0.000898	--
CONTINUOUS CASTER / TORCH CUT-OFF BAGHOUSE	LUD16	LUD12	607692.8	4496079.5	233	22.55	366.48	11.19	3.05	NO	0.001536	0.001536
EAF 1 - CANOPY / AOD CANOPY BAGHOUSE	LUD17	LUD13	607702.7	4496090.8	233	22.86	366.99	2.54	5.18	NO	1.099200	1.099200
EAF 1 - CANOPY / EAF 1 CANOPY - UNCAPTURED	LUD18	LUD14	607702.7	4496090.8	233	3.05	295.37	0.03	0.03	NO	0.036534	0.036534
EAF 1 - MELTING (33 & 34 DEC) / MELTING - DEC BAGHOUSE	LUD19	LUD15	607715.7	4496072.1	233	22.86	366.99	2.54	5.18	NO	0.030780	0.030780
EAF 2 - CANOPY / CANOPY BAGHOUSE	LUD20	LUD16	607646.0	4496273.1	233	18.59	366.99	3.41	3.05	NO	0.098957	0.098957
EAF 2 - CANOPY / CANOPY UNCAPTURED	LUD21	LUD17	607646.0	4496273.1	233	3.05	295.37	0.03	0.03	NO	0.150280	0.150280
EAF 2 -- MELTING (31 & 32DEC) / MELTING - DEC BAGHOUSE	LUD22	LUD18	607694.2	4496098.4	233	25.60	366.99	2.76	4.27	NO	0.039123	0.039123
HORIZ EAF LADLE PREHEATER / AOD VESSEL PREHEAT	LUD23	LUD20	607692.8	4496079.5	233	12.19	295.37	0.03	0.03	NO	0.000748	0.001511
HOT BAND NORMALIZER	LUD24	LUD21	607702.7	4496090.8	233	2.30	1393.99	3.56	1.83	NO	0.017548	0.017548
HOT STRIP UNIVERSAL MILL	LUD25	--	607692.8	4496079.5	233	21.34	338.71	15.24	2.44	NO	0.269190	--
LOFTUS SOAK PITS / LOFTUS SOAK PITS 13-16 NG	LUD26	LUD24	607254.9	4495754.5	233	38.10	810.99	3.46	1.22	NO	0.012082	0.012082
LOFTUS SOAK PITS / LOFTUS SOAK PITS 17-20 NG	LUD27	LUD25	607236.4	4495746.5	233	38.10	810.99	3.46	1.22	NO	0.012082	0.012082
LOFTUS SOAK PITS / LOFTUS SOAK PITS 21-23 NG	LUD28	LUD26	607211.1	4495738.4	233	38.10	810.99	2.57	1.22	NO	0.009781	0.009781
LOFTUS SOAK PITS / LOFTUS SOAK PITS 9-12, NG	LUD29	LUD27	607277.6	4495761.5	233	38.10	810.99	3.43	1.22	NO	0.012082	0.012082
MISC FUGS, COOLING TWRS, STRIP DRYING	LUD30	LUD28	607692.8	4496079.5	233	3.05	295.37	0.03	0.03	NO	0.659360	0.739200
NO. 3 DEPT WET GRINDER	LUD31	LUD29	607692.8	4496079.5	233	10.67	293.15	15.24	0.91	NO	0.005466	0.005466
PLATE BURNERS / TORCH CUTTERS	LUD32	--	607692.8	4496079.5	233	12.19	294.26	15.24	1.22	NO	0.042172	--
RUST REHEAT FURNACE, NG	LUD33	--	607341.6	4495841.3	233	38.10	810.92	16.52	1.52	NO	0.158790	--
SALEM REHEAT FURNACE, NG	LUD34	--	607411.1	4495839.0	233	38.10	810.92	15.64	2.44	NO	1.207300	--
SLAB GRINDERS / HRF GRINDER	LUD35	LUD22	607692.8	4496079.5	233	12.19	310.93	19.60	1.22	NO	0.159650	0.044876
TANDEM MILL / 56 INCH TANDEM MILL	LUD36	LUD30	607626.4	4495913.5	233	12.19	294.26	30.48	1.22	NO	1.455000	1.455000
TANDEM MILL PREHEATER / #3 B&P LINE PREHEAT	LUD37	LUD31	607692.8	4496079.5	233	15.24	295.37	0.03	0.03	NO	0.000748	0.004775
UNITED MILL	LUD38	LUD32	607692.8	4496079.5	233	12.19	294.26	30.48	1.22	NO	0.285260	0.285260
VERT. EAF LADLE PREHEATRS NG	LUD39	LUD33	607692.8	4496079.5	233	12.19	295.37	0.03	0.03	NO	0.000374	0.000374
Z MILL / HRF ROUGHING, FINISHING	LUD40	LUD23	607692.8	4496079.5	233	10.67	294.26	15.24	0.91	NO	0.066065	0.326950
ACTIVE HOT BOXES 1-3	--	LUD07	607100.4	4495847.8	233	28.34	295.37	0.03	0.03	NO	--	0.002383
EMERGENCY GENERATORS 1-4	--	LUD19	607123.3	4495667.2	233	12.50	295.37	0.03	0.03	NO	--	0.001064
WALKING BEAM FURNACE 1	--	LUD34	607111.0	4495698.1	233	50.29	765.36	10.97	3.35	NO	--	0.049660
WALKING BEAM FURNACE 2	--	LUD35	607118.9	4495677.1	233	50.29	765.36	10.97	3.35	NO	--	0.050849

Table B-11. McConway & Torley Sources

SOURCE	BASE ID	PROJ ID	UTMx	UTMy	ELEV	HEIGHT	TEMP	VEL	DIAM	BLDG	BASE RATE	PROJ RATE
CLEANING AND FINISHING / AIR ARC TABLES BAGHOUSE	MC01	MC01	588111.0	4481386.9	224	12.80	293.15	8.99	1.52	NO	0.008156	0.008156
CLEANING AND FINISHING / SHOT BLAST BAGHOUSE	MC02	MC02	588111.0	4481386.9	224	10.06	293.15	13.35	1.16	NO	0.013605	0.013605
CORE MAKING / H-80 AND A-12 CORE MACH	MC03	--	588111.0	4481386.9	224	4.88	295.37	2.04	1.37	NO	0.002877	--
MISC FUGS, CORE MAKING, CLEANING, HANDLING	MC04	MC05	588111.0	4481386.9	224	3.05	295.37	0.03	0.03	NO	0.286490	0.076011
MOLD AND SAND HANDLING / CASTING SHAKEOUT	MC05	MC06	588111.0	4481386.9	224	8.53	293.15	12.19	1.01	NO	0.066731	0.002877
MOLD AND SAND HANDLING / SAND HANDLING AND PREP	MC06	MC07	588111.0	4481386.9	224	8.53	293.15	33.22	1.01	NO	0.006242	0.030693
MOLD AND SAND HANDLING / SAND RECLAIM	MC07	MC08	588111.0	4481386.9	224	9.45	293.15	18.44	1.35	NO	0.010356	0.010356
STEEL MAKING / ELECTRIC ARC FURNACE-BH3A	MC08	--	587992.7	4481463.7	224	7.62	367.39	19.05	0.84	NO	0.069759	--
STEEL MAKING / ELECTRIC ARC FURNACE-BH7	MC09	--	588043.7	4481527.6	224	5.49	426.39	11.69	1.14	NO	0.313240	--
STEEL MAKING / STOPPER ROD / LADLE PREHEAT	MC10	MC10	588111.0	4481386.9	224	4.88	295.37	6.71	1.37	NO	1.778900	0.016463
LECTROMELT OT FURNACE	--	MC04	588111.0	4481386.9	224	6.10	295.37	0.03	0.03	NO	--	0.136190
STEEL MAKING / ELECTRIC ARC FURNACE-BH11	--	MC09	587980.4	4481397.8	224	18.90	367.39	19.05	0.84	NO	--	0.020644

Table B-12. Shenango Sources

SOURCE	ID	UTMx	UTMy	ELEV	HEIGHT	TEMP	VEL	DIAM	BLDG	BASE RATE
#1-4 PACKAGE BOILERS	SHEN01	578300.9	4483067.8	220	15.24	449.66	20.33	0.91	NO	0.367350
BATTERY S1 FUGITIVES	SHEN02	578075.6	4483295.2	220	10.36	644.26	3.05	0.46	NO	0.028519
BATTERY S1 FUGITIVES / BATTERY S-1 SOAKING	SHEN03	578075.6	4483295.2	220	12.50	1366.48	6.10	0.46	NO	0.001254
BATTERY S-1 UNDERFIRE / BATTERY S-1 UNDERFIRE	SHEN04	578137.2	4483244.8	220	76.20	590.21	9.02	2.59	NO	0.704700
COAL HANDLING & EROSION	SHEN05	578127.0	4483228.4	220	15.24	294.26	3.05	0.27	NO	0.046163
COKE HANDLING & COKE/COAL EROSION	SHEN06	578127.0	4483228.4	220	7.62	294.26	3.05	0.27	NO	0.065775
COOLING TOWERS / WET SURFACE COOLER #1	SHEN07	578127.0	4483228.4	220	9.14	294.26	3.05	0.27	NO	0.028275
EMERGENCY FLARE / COG RELEASES UNFLARED	SHEN08	578091.1	4483271.0	220	14.02	295.37	4.39	0.58	NO	0.001133
EMERGENCY FLARE / EMGNCY FLARE-COG FLARING	SHEN09	578091.1	4483271.0	220	14.02	1272.99	20.00	0.58	NO	0.043338
LIGHT OIL TRUCK AND BARGE	SHEN10	578127.0	4483228.4	220	6.10	294.26	3.05	0.27	NO	0.000006
MAIN (BLEEDER) FLARE	SHEN11	578211.4	4483202.3	220	30.48	1272.99	20.00	0.61	NO	0.001144
MISC FUGS, COOLING TWRS	SHEN12	578127.0	4483228.4	220	3.05	294.26	0.03	0.03	NO	0.205170
PEC BAGHOUSE	SHEN13	578118.0	4483380.0	220	45.72	295.37	19.41	3.05	NO	0.033933
QUENCH TOWER, BATTERY S-1	SHEN14	578162.7	4483238.4	220	17.07	338.55	4.33	4.57	NO	1.209100
S-1 PUSHING FUGITIVES / S-1 PUSHING FUGITIVES	SHEN15	578082.4	4483300.8	220	10.36	1033.15	1.59	1.59	NO	0.024170
SULFEROX VENT / SULFEROX VENT	SHEN16	578080.1	4483114.3	220	17.68	329.10	14.54	0.20	NO	0.038873
TAR DECANter SLUDGE RECYL	SHEN17	578127.0	4483228.4	220	7.62	294.26	3.05	0.27	NO	0.000009

Note: Shenango was closed permanently in 2016, with emissions for base case (2011) only.

APPENDIX C – MMIF Configuration

MMIF meteorological data will be used for this demonstration as the most appropriate available meteorological inputs to AERMET. MMIF guidance (U.S. EPA, 2018d) includes recommendations for some settings for MMIF, while allowing for user selection for other settings (Brashers and Emery, 2018). See the SO₂ SIP for the 2010 NAAQS (ACHD, 2017) for a detailed analysis of MMIF for regulatory modeling.

MMIF Output Mode

AERMET-ready output files will be selected for the MMIF processing. As such, MMIF data are used for onsite, upper air, and surface characteristic inputs, processed through AERMET to generate AERMOD-ready meteorological files. This is the recommended approach and allows for other options such as ADJ_U*.

MMIF Vertical Layers

The following vertical layers will be selected for MMIF, with TOP structure:

20 30 40 60 80 100 125 150 175 200 250 300 350 400 450 500 600 700 800 900 1000 1500 2000 2500 3000 3500 4000 5000

These layers are slightly different than the recommended lowest layers up to 100 m but allow for more characterization in-valley, specifically for the 10 m level winds.

Mixing Height

The user has three different options for mixing heights supplied by MMIF:

- WRF (no recalculation of mixing heights)
- MMIF (MMIF-recalculated mixing heights)
- AERMET (allow AERMET to calculate mixing heights)

The AERMET option will be selected for mixing height, allowing for AERMET calculation of mixing height along with ADJ_U* processing. (Note: ADJ_U* can affect several interdependent variables in the boundary layer parameters file (.sfc), including mixing height. Also, turbulence parameters are not included with MMIF, so ADJ_U* is appropriate for use.) The use of AERMET-based mixing heights was deemed to be the best complement for MMIF to AERMOD, more consistent with the overall methodology for the AERMOD modeling system.

MMIF Upper Levels

Based on comparisons to measured sodar and multi-level tower data, wind speeds at upper levels (above 50 m) were found to contain a high bias. This is based on airport/plateau wind speeds built into the WRF and not translating into lower wind speeds to represent localized in-valley flow. (See more details in the SO₂ SIP (ACHD, 2017).)

To eliminate this bias, only surface wind speeds up to the 50 m layer will be used from the supplied MMIF onsite data. This technique forces AERMOD, which extrapolates hourly data based on any/all supplied measurements, to more realistically calculate the upper levels wind speeds. This may also be a

more AERMET-like approach for wind speed, putting more emphasis on AERMET than WRF for vertical profiles.

Wind Speed Threshold

A wind speed threshold of 0.0 m/s will be selected for Stage 1 AERMET processing of MMIF data, as recommended by the MMIF guidance. This allows for all wind speeds generated by the WRF model to be used in the profile (.pfl) file, but a minimum speed of 0.28 m/s is substituted for any hour below this minimum in the boundary layer parameters file (.sfc). The use of MMIF therefore contains no missing or calms data for any hour.

Post-Processing

As mentioned in earlier sections of this document, the use of multiple meteorological data sets requires post-processing. CALPOST will be used for the post-processing (see Appendix D of this protocol).

MMIF Cells

The MMIF cells to be used for site-specific meteorology for each facility location are shown geographically in Figure C-1. The U. S. Steel locations lie within the 444 m resolution WRF grid, while the others fall within the 1.33 km resolution grid.



Figure C-1. MMIF Locations used for the Modeling

Figure C-2 shows surface level (10 m) wind roses for the U. S. Steel MMIF locations, as extracted from the 0.444 km resolution WRF domain. (MMIF wind roses from the distant sources in the 1.33 km domain are not shown.) Valley channeling is evident from the wind directions, with lower wind speeds also present at the in-valley locations (Clairton, Edgar Thomson).

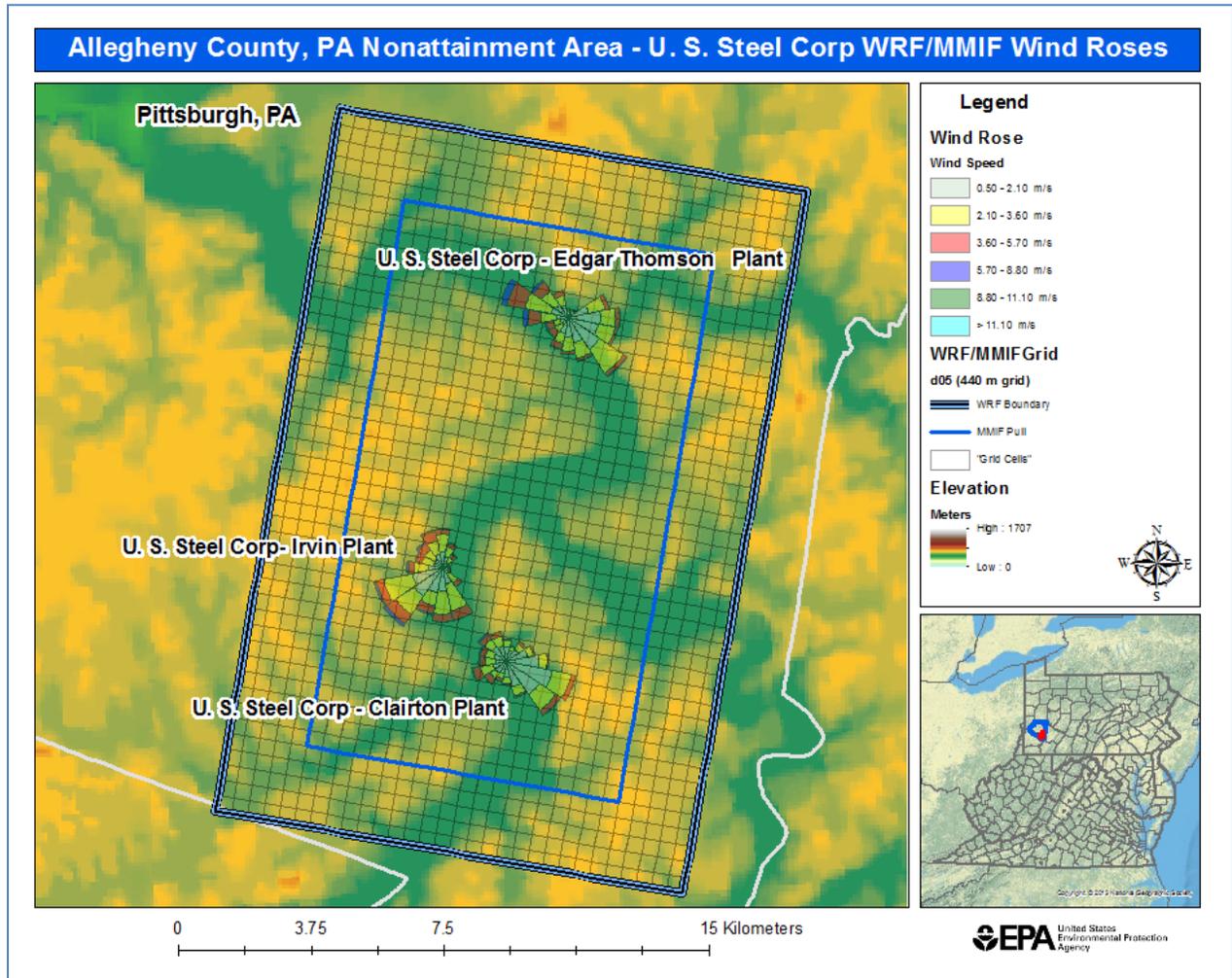


Figure C-2. Wind Roses for MMIF 2011 Surface Level (10 m) Data, U. S. Steel Locations²³

²³ Figure was originally used in the alternative modeling request from EPA Region 3 to the EPA Model Clearinghouse (see Appendix H of the SIP).

APPENDIX D – Post-Processing

For post-processing results from different runs (e.g., using different MMIF cells), the CALPUFF modeling system post-processors will be used.

This requires three steps/programs:

- AER2CAL (version 1.21): converts AERMOD post files to CALPUFF format. The AERMOD post files (using the POSTFILE keyword) are in unformatted binary format, with the 1-hour averages for each discrete receptor.
- CALSUM (version 7.0.0): sums the hourly impacts from different runs, matched in time/space.
- CALPOST (version 7.1.0): processes the impacts, generating the impact totals in summary and plot formats.

AER2CAL and CALSUM are related programs with no regulatory status. CALPOST is no longer part of a preferred modeling system (with CALPUFF), but there is no preferred post-processor available with AERMOD. These CALPUFF tools are publicly available and show equivalent results to AERMOD.

To test the equivalence of the default AERMOD processing to the CALPOST post-processing, individual test sources were run in AERMOD and then post-processed and summed with CALPOST. Results were identical between AERMOD (with all sources in one run) and CALPOST, except for some slight differences ($\pm 0.01 \mu\text{g}/\text{m}^3$) due to CALPOST rounding the impacts to five significant figures, while AERMOD keeps five decimal places.

APPENDIX E – BLP Plume Rise Methodology

This appendix describes the methodology used to generate plume rises from BLP for use in AERMOD. (For more information on the BLP/AERMOD hybrid approach, see Appendix H of the SIP.)

The steps taken to use BLP plume rises for AERMOD volume sources are as follows:

1. Modify the BLP code so that plume rises are explicitly generated as hourly output data. Changes to the BLP code do not alter the line source algorithms, only adding the output of plume rise data as a model option.
2. Reformat the MMIF meteorological data corresponding to the facility with buoyant line sources into PCRAMMET ASCII format (the format used by BLP). This follows the procedure outlined in the AERMOD/BLP technical support document (Paumier, 2016). For this demonstration, only the Clairton Plant battery fugitives are characterized as buoyant line volumes.
 - a. Convert stability conditions (based on Monin-Obukhov lengths and surface roughness) into Pasquill-Gifford stability classes (1 through 6, or A through F). This conversion is based on the AERMOD subroutine LTOPG (LSTAB).
 - b. Convert wind directions to flow vectors (wind flowing toward). For mixing height, use the maximum of the convective and mechanical heights for each hour as both the urban and rural mixing height for BLP.
 - c. Since BLP cannot accept missing data, fill any missing hours using interpolation, persistence, and professional judgment. (With the current low wind speed handling procedures for MMIF, there are no calms/missing hours with MMIF.)
3. Run the modified BLP code (named “BLPRISE” by ACHD) for the buoyant line sources. The BLP inputs include line dimensions, exit velocity, and buoyancy parameter F' . Only the plume rises generated by BLP are utilized after this step.
4. Using the generated plume rises for each line, calculate hourly release heights as plume rises added to the building height. Equidistant (adjacent, or exact) line volume sources were created to represent segments of the line, and each volume source was then assigned the hourly release heights. An HOUREMIS file will be used for the height-varying data for the buoyant volume sources.

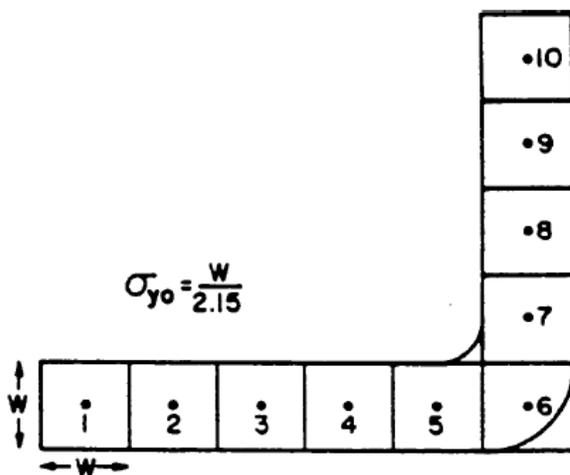
The BLPRISE fortran code is included in Appendix H of the SIP, with modifications from the BLP code highlighted in yellow. The code was modified only to generate output that was not automatically created by BLP version 99176.

Initial lateral dimensions (σ_{y0}) and initial vertical dimensions (σ_{z0}) for each volume source will be based on the suggested procedures for volume and line sources, from Table 3-2 of the AERMOD User's Guide (U.S. EPA, 2018a), shown below:

Type of Source	Procedure for Obtaining Initial Dimension	
(a) Initial Lateral Dimension (σ_{y0})		
Single Volume Source	$\sigma_{y0} =$	length of side divided by 4.3
Line Source Represented by Adjacent Volume Sources (see Figure 1-8 (a) in EPA, 1995a)	$\sigma_{y0} =$	length of side divided by 2.15
Line Source Represented by Separated Volume Sources (see Figure 1-8(b) in EPA, 1995a)	$\sigma_{y0} =$	center to center distance divided by 2.15
(b) Initial Vertical Dimension (σ_{z0})		
Surface-Based Source ($h_e \sim 0$)	$\sigma_{z0} =$	vertical dimension of source divided by 2.15
Elevated Source ($h_e > 0$) on or Adjacent to a Building	$\sigma_{z0} =$	building height divided by 2.15
Elevated Source ($h_e > 0$) not on or Adjacent to a Building	$\sigma_{z0} =$	vertical dimension of source divided by 4.3

Initial lateral dimensions are constant for each hour, based on the width of the battery divided by 2.15. Initial vertical dimensions vary by hour, based on the hourly-varying released heights divided 4.3.

The locations used for the volumes are based on the adjacent (or exact) representation of a line source by multiple volume sources, from Figure 1-8 from Section 1.2.2 of the ISC Model User's Guide, Volume II (U.S. EPA, 1995), shown below:



Several transitional plume rises and distances are created with each hour of plume rise data from BLPRISE. Final plume rise can occur very close to the line or a few kilometers from the line, depending on stability and wind conditions. Terrain could be theoretically impacted during transitional plume rises before final plume rise is reached (but BLP was a simple-terrain model).

However, after examination of the transitional plume rises in relation to the sources and terrain for this demonstration, the use of final plume rise is appropriate. Hours with little plume rise generally reach final plume rise over a short distance (within the property fenceline), and hours with elevated plume rise quickly reach heights above surrounding terrain over short transitional distances. Additionally, the highest rises and distances occur during convective unstable/neutral conditions, with good dispersion and low monitored concentrations. Some of these plume rises may seem unrealistic, but they may also be considered as measures of atmospheric conditions, analogous to extremely low Monin-Obukhov lengths or mixing heights.

Figure E-1 shows the hourly average (diurnal) release heights from BLPRISE for each line, along with hourly average mixing heights and stability classes. Stability classes are shown with a different y-axis, cycling from very stable conditions (class=6) to very unstable conditions (class=1), with neutral conditions (class=4) occurring during the day/night transitions.

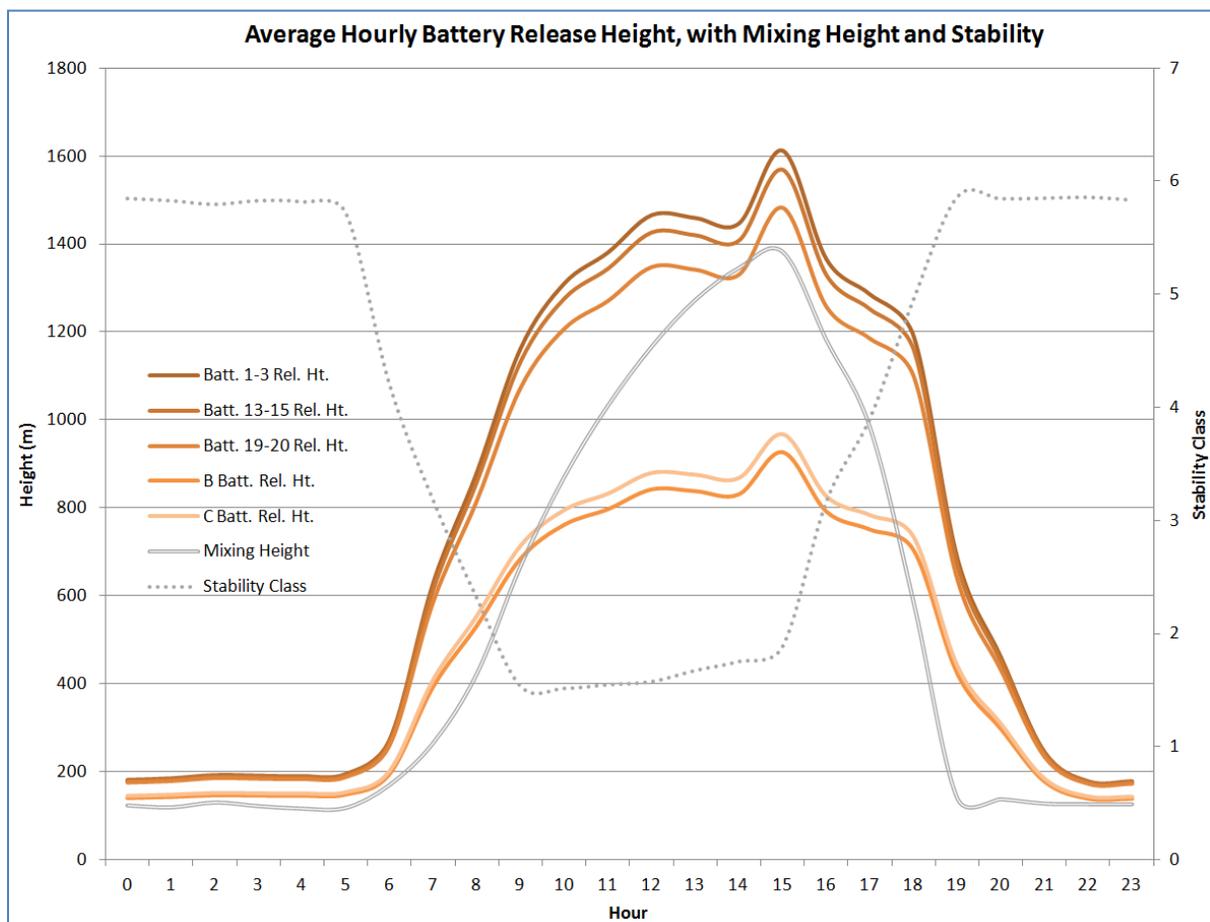


Figure E-1. Average Hourly Height (Battery Release Height, Mixing Height) and Stability Class

Plume rises from BLPRISE are a function of stabilities and mixing heights for each hour. On an average basis, the thermal buoyancy of each line is effectively forcing the modeled plumes upward and into the mixing layer. As a result, AERMOD is provided with more appropriate starting heights for the dispersion of battery fugitives in complex terrain.

Additive buoyancy from parallel lines will not be used, with each line modeled separately for the hybrid method and corresponding impacts combined via post-processing (see Appendix D of this protocol). Buoyancy will be calculated from emissions-based heat flux only, with surface-based heat transfer not considered (due to potential double-counting).

Figure E-2 shows the location of each U. S. Steel Clairton Plant buoyant line source (shown in red) modeled in this demonstration. The center coordinate of each corresponding volume source are indicated by dots within the line.

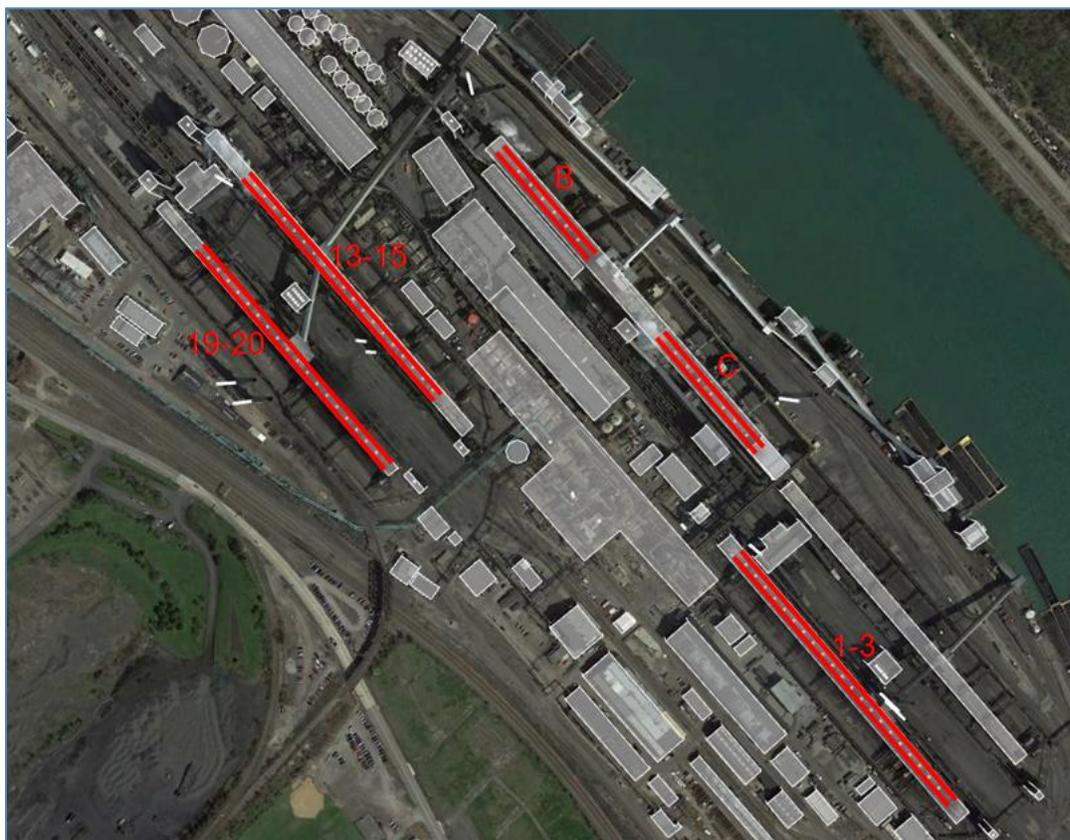


Figure E-2. U. S. Steel Clairton Plant Battery Lines

Line parameters are based on physical dimensions, flow, and temperatures of the line. The F' buoyancy term, based on the original BLP formulation, is given in Figure E-3 (Schulman and Scire, 1980). Appendix B of this protocol provides the parameters of each line modeled, with emissions and line parameters assumed to be constant for each hour.

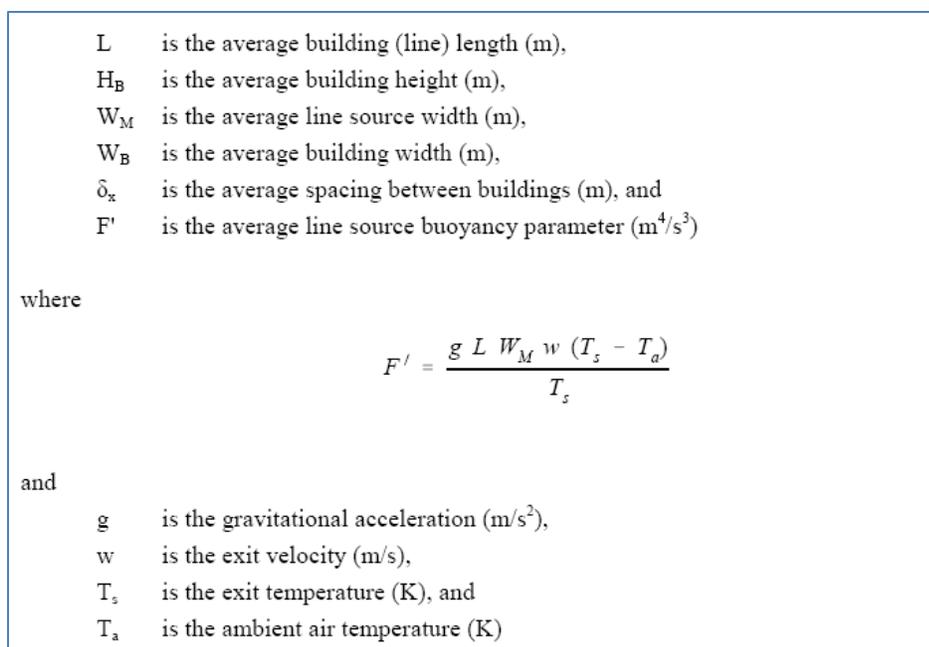


Figure E-3. Line Buoyancy F' Term

Battery height, length, and width are based on the actual physical dimensions of each battery. Line length is equal to the physical length of the line, while line width is based on an “equivalent” diameter of the various fugitive release points along the line (estimated as an average of 1.0 m). Exit velocity is based on calculated flows for each line (Layland and Mersch, 1985) along with observations of visible fugitive emissions (estimated as an average of 10 ft/s (or 3.05 m/s) collectively for the line emissions). Note that all values for the line parameters (and emissions) are considered to be constant for each hour, which assumes some “smoothing” for the line buoyancy calculations needed for steady-state modeling.

Ambient temperature is estimated as an average of year-round temperature for the Pittsburgh area (about 52 °F, or 284.27 K). Exit temperatures are based on the fugitive emission temperatures from all processes associated with the coking. The methodology for calculating the exit temperatures by process is described as follows:

- Charging and leaks (topside/door): calculated as the midpoint of the surface temperature (an average of 350 °F for door and top surfaces (Layland and Mersch, 1985)) and the temperature of hot coke 1800 °F (AISE, 1999), for an average of 1075 °F. It is assumed that that leaks are cooled by ambient air quicker than other processes (such as pushing, where the ovens and coke are exposed when the doors are off).
- For pushing (including pre-push, controlled (PEC), and uncontrolled pushing): a temperature of 1800 °F, equal to that of hot coke. The general range of coking is 1650-2000 °F, with a range of 1900-2000 °F for the actual skin of coke inside a coke oven chamber (AISE, 1999). It is assumed that that the 1800 °F temperature inherently includes some immediate heat loss and that pushing retains more heat from the oven and block of coke than other sources (such as leaks).
- For the hot cars (aka travel or quench cars): calculated as the midpoint of the temperature of “resting” coke in the car (1500 °F) (AISE, 1999) and the pushing temperature (1800 °F), for an average of 1650 °F during traveling from pushing to quenching.

- For soaking: calculated as the average of measured temperatures during stack testing (1273 °F) (ATS, 1995).

The calculated temperatures are then weighted by the corresponding fractions of each process to total battery fugitive emissions. PM_{10} emissions, used collectively for PM since $PM_{2.5}$ is a fraction of PM_{10} , for year 2011 (base year of the SIP) are used for the weighted calculation. The percentages of battery fugitive PM_{10} emissions by process are as follows: charging/leaks (13%), pushing (73%), hot cars (10%), and soaking (4%). The weighted average exit temperature is calculated as 1673 °F (1184.83 K).

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