$PM_{2.5}$ Model Protocol

Liberty-Clairton Nonattainment Area

Allegheny County Health Department
Air Quality Program

October 15, 2007

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1.0 OVERVIEW

This section explains the official designations for particulate matter 2.5 microns or less ($PM_{2.5}$) in Allegheny County and need to carry out an attainment demonstration for the Liberty-Clairton Nonattainment Area according to this protocol. Stakeholders for the $PM_{2.5}$ protocol are also discussed.

1.1 $PM_{2.5}$ Designations

EPA issued final $PM_{2.5}$ area designations on December 17, 2004, which became final on April 5, 2005.

Designations for $PM_{2.5}$ were based on several factors, including 2001-2003 monitored data, proximity to metropolitan areas, census populations, types of emissions, and others. Five counties in the Pittsburgh metropolitan area (MSA)[1] and portions of adjacent counties were designated as the Pittsburgh-Beaver Valley nonattainment area. Additionally, the Liberty-Clairton area was designated as a separate area within Allegheny County.

The Liberty-Clairton Area includes the Boroughs of Glassport, Liberty, Lincoln, Port Vue, and the City of Clairton. Appendix A provides maps of the Southwestern PA designation areas, including close-ups of the Liberty-Clairton Area.

1.2 Stakeholders

The PA Dept. of Environmental Protection (DEP) will model the Pittsburgh-Beaver Valley nonattainment area, while the Allegheny County Health Department (ACHD) will model the Liberty-Clairton Area. A final attainment demonstration for the Liberty-Clairton Area will be submitted to the PA DEP, on behalf of the ACHD, for submittal to the U.S. Environmental Protection Agency (EPA) Region 3 office.

All contractual assistance for the development of Liberty-Clairton Area modeling will be under the direction of the ACHD. ACHD staff, the ACHD Criteria Subcommittee (subcommittee of the Air Advisory Committee), and the ACHD $PM_{2.5}$ Modeling Workgroup have participated in the development of this protocol.

The Criteria Subcommittee members include persons from industry, environmental advocacy organizations, environmental consultation companies, and the general public.

Sullivan Environmental Inc. has been selected as the meteorological consultant for this modeling demonstration. Additional support for the dispersion modeling has not been contracted at the time of this protocol.

[1] The Pittsburgh Metropolitan Statistical Area (MSA) encompasses Allegheny, Armstrong, Beaver, Butler, Fayette, Washington, and Westmoreland counties, according to the U.S. Census Bureau, November 2004.

2.0 PROBLEM STATEMENT

This section explains the nature of the $PM_{2.5}$ problem and provides a conceptual design for the Liberty-Clairton Area. Monitored data results are also given.

2.1 Modeling Area

The Liberty-Clairton Area is made up of complex river valley terrain, approximately 3 miles wide by 5 miles long. It includes a 4-mile winding portion of the Monongahela River and is bordered by the Youghiogheny River to the east. The area includes rural land, densely populated residential areas, and industrial facilities.

River valleys lie at 718 feet in elevation (MSL), while adjacent hilltops can be greater than 1250 feet. 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.

The Liberty-Clairton Area is presumably impacted by regional, urban excess, and localized $PM_{2.5}$. Source apportionment results based on speciated data can be found in the report *Allegheny County PM2.5 Source Apportionment Results using the Positive Matrix Factorization Model (PMF Version 1.1).*[2]

2.2 Monitored Data

The Federal Reference Method (FRM) $PM_{2.5}$ monitor at Liberty is located atop a school at high elevation near the center of the Liberty-Clairton area. The FRM monitor at Clairton is located atop a school at low elevation in the western portion of the area. Both are violating the annual $PM_{2.5}$ standard of 15 µg/m³. The Liberty monitor is also in violation of the 24-hour standard of 65 µg/m³. FRM monitors located to the west and to the south of the area have monitored attainment of both standards. Appendix B contains details of monitor sites and data.

Results from the Liberty $PM_{2.5}$ speciation monitor show that carbons, ammonia, and some trace elements are higher in the Liberty-Clairton Area than in other monitored areas by 4 to 5 µg/m³. An in-depth analysis of speciated $PM_{2.5}$ components in Allegheny County can be found in the report *$PM_{2.5}$ Chemical Speciation and Related Comparisons at Lawrenceville and Liberty: 18-Month Results.*[3]

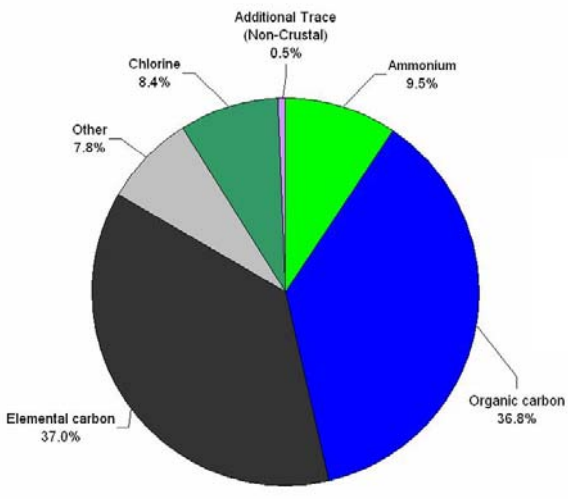


Figure 2.2. Liberty $PM_{2.5}$ Excess Species Pie Chart

[2] Report can be found online at http://www.achd.net/airqual/pubs/pdf/pmf0106.pdf
[3] Report can be found online at http://www.achd.net/airqual/pubs/pdf/speciation_report.pdf

3.0 SELECTION CRITERIA

This section outlines the models, the species of $PM_{2.5,}$ and the years to be modeled for the Liberty-Clairton Area. The final EPA $PM_{2.5}$ Implementation Rule was published in March 2007. The final EPA $PM_{2.5}$ Modeling Guidance was published in April 2007.

3.1 Models Selection

The PaDEP is using CMAQ modeling for PM-2.5 as developed by the Mid-Atlantic NorthEast Visibility Union. The same modeling results will be used for the Liberty/Clairton area. However, a more detailed analysis is necessary for the Liberty/Clairton area due to localized emissions impacting communities located nearby. In this process, a local dispersion model will be used to more precisely locate and represent the impact of local emissions, the regional model CMAQ will be used for the remaining sources.

The EPA-preferred CALPUFF modeling system will be used to create near-field and some long-range transport simulations of the Liberty-Clairton area. CALPUFF Version 5.8 (dated June 29, 2007) is the most recently EPA-approved version for regulatory applications. CALPUFF was selected as the dispersion model for the Liberty-Clairton Area based on the complex terrain and strong temperature inversions that are characteristic to the area. CALPUFF also has the ability to model buoyant line sources that are resident to the area.

The CALPUFF modeling system is comprised of CALMET (meteorological model), CALPUFF (dispersion model), geophysical data preprocessors, meteorological data preprocessors, and several postprocessors such as CALPOST. The CALPro GUI (dated June 29, 2007) comprises CALPUFF and associated preprocessors and postprocessors in a central interface and will be utilized as the modeling software.[4]

The CALMET meteorological model employs the use of gridded multi-layer wind fields. Data from the PSU/NCAR Mesoscale Model Generation 5 (MM5) will be used for prognostic wind field data. Regional modeling will also be required for background values for the Liberty-Clairton domain. This will be performed using the Community Multiscale Air Quality (CMAQ) model. Regional impacts from CMAQ will be combined with the near-field impacts and long-range transport from CALPUFF during post-processing.

3.2 Regional Modeling

The Pennsylvania Department of Environmental Protection or its contractor will complete modeling for the Pittsburgh-Beaver Valley Nonattainment Area, likely using the regional reactive model CMAQ. The results of this modeling will be the basis of the modeling completed for the Liberty-Clairton attainment demonstration.

The regional results will provide a hourly concentrations by major $PM_{2.5}$ component for each 12 x 12 km grid cell. This will represent the background value for each cell, which will then be combined with the impacts from the CALPUFF model simulations. Sample hourly CMAQ results for major species for base year 2002 and projected year 2009 are shown in the tables in Appendix G.

[4] CALPUFF can be downloaded at: http://www.src.com/calpuff/download/download.htm

3.3 $PM_{2.5}$ Components

Analysis of speciated $PM_{2.5}$ data in Southwestern PA indicates that the Liberty-Clairton Area excess is composed mainly of primary components of $PM_{2.5}$. Therefore, emission inputs for the CALPUFF modeling will consist of primary filterable and condensable $PM_{2.5}$. Secondary formation of $PM_{2.5}$ from sulfur dioxide, nitrogen oxides, and volatile organic compounds (VOCs) will be excluded from the Liberty-Clairton modeling. Therefore, CMAQ modeled results will be used for all secondary components, and a combination of CMAQ (for background) and CALPUFF modeled results will be used for primary components.

3.4 Modeling Year

The availability of MM5 and CMAQ data is the limiting factor in the Liberty-Clairton modeling timeframe. Data is available for the area for the year 2002, based on MANE-VU regional modeling. Hence, 2002 will be the modeled year for the Liberty-Clairton modeling. Modeling will focus on annual concentrations, but selected short-term modeling periods may reveal specific meteorological scenarios and control techniques.

4.0 CALPUFF MODELING PROCEDURE

This section delineates the procedures for preprocessing, model simulations, and postprocessing required for the Liberty-Clairton modeling demonstration.

4.1 Domain Settings

Since nested domains are not possible in the current version of CALPUFF/CALMET, separate domains for long-range transport and near-field impacts will be used at different resolutions. Results from these domains will be combined in postprocessing with the regional CMAQ background results.

Common domain settings can be shared for CALPUFF, CALMET, and most associated preprocessor programs. These include:

- Projection: Universal Transverse Mercator (UTM)
- Zone: 17, Northern
- Datum: North American 1983
- Continent/Region: North America/Continental US (CONUS), NAR-C
- Base Time Zone: Eastern U.S. (GMT -05:00)
- Grid Type: Cartesian, referenced to lower left corner
- Grid Spacing:
  - 1 km for long-range transport grid
  - 100 m for near-field impact grid
- Grid Dimensions:
  - 140 x 140 km for long-range transport grid
  - 20 x 20 km for near-field impact grid

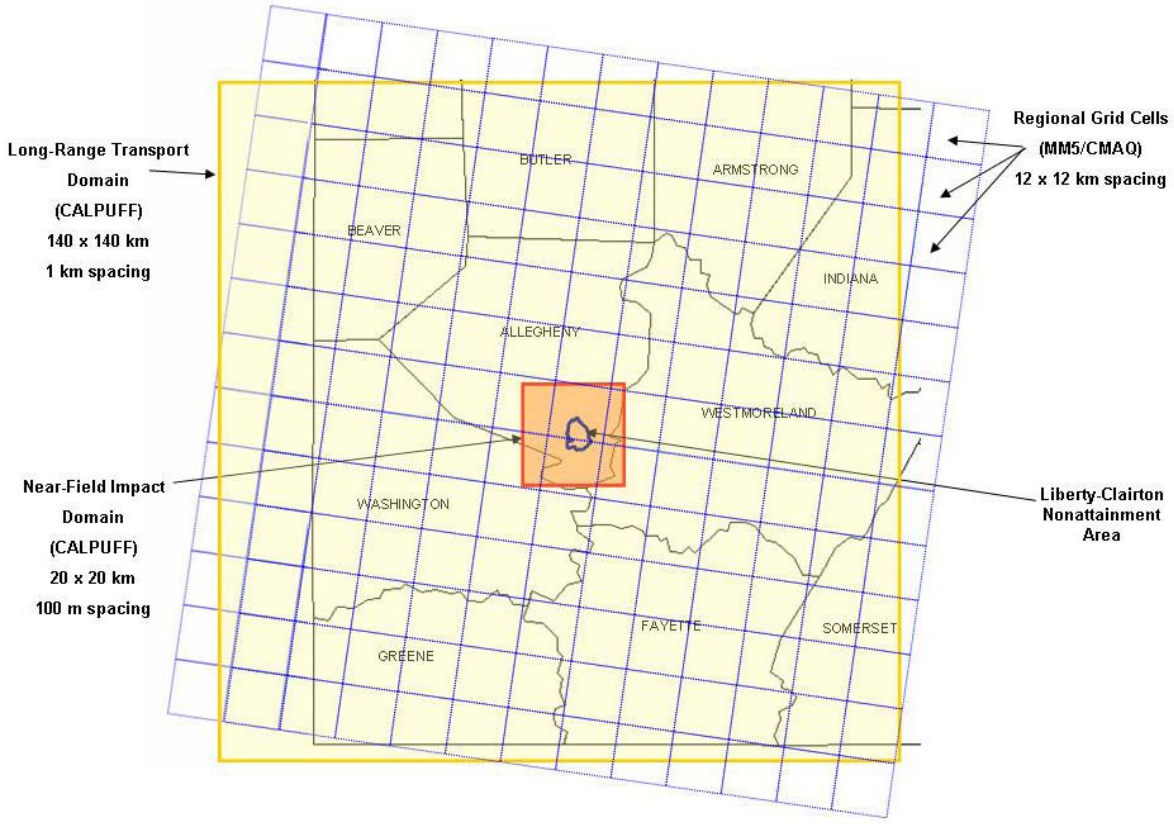


Figure 4.1. Modeling Domains

The near-field domain will be centered on the Liberty Monitor, allowing for equidistant movement of puffs around maximum monitored concentration point. The long-range transport domain will match the extent of the MM5 data as supplied by the regional modelers.

Data files from different datum references can be used for geophysical inputs since the preprocessors are able to convert to one consistent datum. Contour plotting with software such as Surfer® should be used to reveal errors that may exist in gridded data.

For the long-range modeling applications, Lambert Conformal coordinates are recommended for domains in which the earth's curvature may be significant (greater than 200 km). For purposes of post-processing Liberty-Clairton results, UTM will be datum to be used for the gridded and discrete receptor coordinates within the long-range transport and near-field domains.

4.2 Geophysical Preprocessing

Geophysical preprocessing for CALMET includes the programs TERREL, CTGCOMP, CTGPROC, and MAKEGEO. The following settings should be used for these:

- Coastline: none
- Terrain Files:
  - USGS30, 7.5' DEMs in and adjacent to the Liberty-Clairton Area
  - USGS90, 1° DEMs outside the vicinity of the Liberty-Clairton Area
- Discrete Receptors: only for Liberty and Clairton nearby receptors
- Land Use Files:
  - USGS NLCD 1992 land use (by state)

The use of 7.5' DEM terrain and NLCD 1992 land use data provide data points at every 30 meters within the near-field domain (100 meter resolution). Since the resolution of the long-range transport domain is 1 km, the use of 1° DEM terrain data at 90-meter resolution is sufficient.

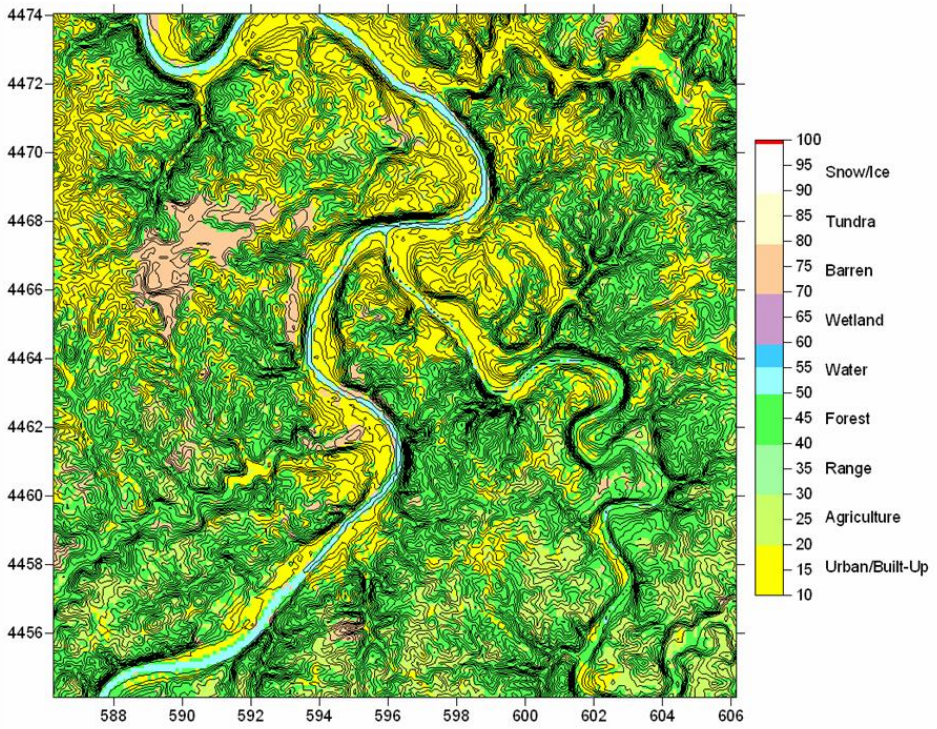


Figure 4.2. Near-Field CALMET Domain at 100 m Resolution

Land use files are periodically updated by the USGS. NLCD 2001 land use data would provide a more accurate depiction of the Liberty-Clairton Area. However, The CTGPROC preprocessor code will not accept NLCD 2001 at the time of this protocol.

4.3 Meteorological Preprocessing

Meteorological preprocessing for CALMET includes SMERGE, READ62, PXTRACT, and PMERGE. The following inputs should be used for these preprocessors:

- Period: Jan.1-Dec. 31, 2002, Local Standard Time (LST)
- Surface Data: DATSAV3 (TD-9956), converted to SAMSON
- Upper Air Data: NCDC FSL or MM5
- Top Pressure: must equal or exceed top of vertical domain
- Precipitation Data: TD-3240

Airports near the Liberty-Clairton Area include the Pittsburgh International Airport (Code: PIT, WBAN: 94823) and the Allegheny County Airport (Code: AGC, WBAN: 14762). Upper air and precipitation data is not available for the Allegheny County Airport.

Several local surface data sites have been evaluated for use in the modeling demonstration. Local surface data to be included are the Liberty site, operated by the ACHD Air Quality Program, and the Clairton site, operated by US Steel on Clairton Coke Works property. Photographs and wind roses of 2002 data for key sites are shown are shown in Appendix C.

For the long-range transport domain, the following inputs will be used
- PIT Airport surface and precipitation data
- PIT Airport and/or MM5 for hourly upper air data

For the near-field domain, the following inputs will be used:
- AGC Airport, Liberty, and Clairton surface data
- PIT Airport precipitation data
- PIT Airport and/or MM5 for hourly upper air data

Raw surface from the U.S. Steel Clairton site is incomplete, containing no data from Jan.1 – Aug. 11, 2002. A regression analysis based on additional years of data from Clairton, Liberty, and historical met sites may be used to substitute or “back-fill” missing data for 2002 at Clairton. Details of the regression analysis will be given in the final report by the meteorological contractor.

Since surface data from local meteorological sites only provide wind speed, wind direction, and temperature, airport data will be substituted for other meteorological variables. During hours where local temperature is lower than airport dew point temperature, relative humidity will be corrected to 100% in the surface data files.

Surface characteristics such as albedo and surface roughness can vary by season. Therefore, CALMET files will be processed on a seasonal basis with varying surface characteristics for the near-field domain. Adjustments will also be made to anthropogenic heat flux in grid cell areas where combustion sources emit large amounts of heat. Appendix D shows default average surface parameters (all-season) and high anthropogenic heat flux areas.

4.4 Prognostic Meteorology

Data for prognostic meteorology will be extracted from 2002 MM5 results. The PSU/NCAR Mesoscale Model Generation 5 (MM5) is a limited-area, non-hydrostatic, terrain-following sigma-coordinate model designed to simulate or predict mesoscale atmospheric circulation. Modeled surfaces near the ground closely follow the terrain, and the higher-level sigma surfaces tend to approximate isobaric surfaces. The vertical and horizontal resolution and domain size are variable.

MM5 data has been prepared for 2002 in the Northeastern United States by states in the Mid-Atlantic/Northeast States Visibility Union (MANE-VU) during early work for Regional Haze State Implementation Plans (SIPs) for these states. This same data will be used by the member states in preparation of their $PM_{2.5}$ SIPs. PA DEP has indicated that they will use this data in their SIPs, including the Pittsburgh-Beaver Valley SIP.

For consistency with the regional modeling for the Pittsburgh-Beaver Valley SIP, ACHD will use the same meteorological data and process it through CALMET for use in the CALPUFF model. The MM5 grid cells are set at 12 km spacing. ACHD will use the existing grid and the subset of meteorological data appropriate for the modeling domains. Appendix E shows MANE-VU MM5 and CMAQ maps and configurations for Southwestern Pennsylvania.

Additional meteorological data will be included in the CALMET processing of data. This includes surface, upper air, and precipitation data from the Greater Pittsburgh Airport (PIT), surface data from the Allegheny County Airport, and surface data from ACHD air quality or other monitoring sites. CALMET will create a three-dimensional wind and temperature gridded fields for use in CALPUFF.

4.5 Meteorological Simulation

CALMET will be used for the meteorological simulation. ACHD will begin by using only the MM5 data in CALMET and review the CALMET-created wind fields for representative wind characterization. Meteorological site data will be added, with limited range of effectiveness, until sufficiently accurate representative wind fields are structured for each hour across the modeling domain.

Meteorological data processed through CALMET will result in two gridded meteorological domains: a long-range transport domain (140 x 140 km, 1 km receptor spacing) and a near-field impact domain (20 x 20 km, 100 m receptor spacing), with each domain containing 11 vertical layers of meteorological data. Data used to create these grids will come from 12-km spaced MM5 data already processed for multi-state regional modeling, combined with local airport and local meteorological tower data. The steps of meteorological data preparations are:

a) Quality-assure MM5 grid points from MANE-VU MM5 meteorological data processed for 2002.
b) Reformat observed data as necessary to prepare for CALMET runs.
c) Review results for model input parameters such as albedo and surface roughness from the preprocessor programs. Identify values for model inputs such as bias and mixing height constants; use default values if unknown.
d) Compare meteorological data from CALMET run to observed data. Identify specific days to run during data preparation tests, including days of high concentration and representation of various meteorological conditions.
e) Make a first run through CALMET using only MM5 and terrain data, using the days selected in (d).
f) Evaluate results against observed data.

g) Review airflow information surrounding the USS Clairton coke works. Using heat information from the plant, identify a proper representation of air movement near and above the plant.
h) Review and determine use of observed meteorological data for subsequent test runs.
i) Make subsequent test runs, with selected observed data files and adjusted meteorological parameters. Analyze results, and recommend modifications to meteorological parameters with each run.
j) Make full year runs with final meteorological parameters and chosen observed data sets.

CALMET runs will be performed by season to allow for seasonally-adjusted surface parameters. For modeling purposes, seasons are defined as follows:

- Winter: Dec. – Feb.
- Spring; Mar. -May
- Summer: June - July
- Autumn: Sept. - Nov.

For a complete year of CALMET data for year 2002, a total of five files are needed as input to CALPUFF, since the winter season is split between Jan.-Feb. and December.

Key variables in CALMET are needed to assign bias, radii of influence, and many other options. Table 4.5 below lists CALMET variable assignments based on preliminary modeling and meteorological analyses.

TABLE 4.5. CALMET Variable Values

CALMET Variable	*Selected Value*	*Rationale*
NOOBS	1	Use MM5 upper air data
NPSTA	-1	Use MM5 precipitation data (to consider wet deposition)
IEXTRP	-4	Using MM5 for upper levels, extrapolate observed surface winds aloft to account for valley wind effects based on BIAS.
ZFACE	0.,20.,40.,80.,160.,320.,640., 1000.,1500.,2000.,2500.,3000.	Define 11 cell face heights (m) in vertical grid
BIAS	-1, -1, -1, -1, .5, .8, 1, 1, 1, 1, 1	Heavily weight surface observations below valley wall height of 200m and then increase weighting of upper air observations above valley wall.
RMIN2	-1	Not used since NOOBS=1; IEXTRP=-1
IPROG	14	Use MM5 as a first guess but allow CALMET to adjust for terrain
TERRAD	0.5	Using formula of terrain ridge to ridge distance divided by 2 plus some small factor
R1 & R2	1.5	This adjustment is data dependent and projected wind patterns will be compared to observed wind flows (feedback mechanism)
RMAX1 & RMAX2	1.5	This adjustment dependent on met data sites relative to terrain valley/ridge features
ITPROG	1	Use surface stations and MM5 for upper air
IRHPROG	1	Use MM5 relative humidity
SIGMAP	12	Set radius to the MM5grid spacing

4.6 Emissions Inputs

Emissions inputs will be based on calculated actual emissions data for sources affecting the Liberty-Clairton Area. Types of sources should be modeled as such:

- Stacks: point sources
- Ambient-Temperature Fugitives: area or volume sources
- Quench Towers: point or short buoyant line sources
- Coke Oven Batteries: buoyant (BLP) line sources
- Significant roads: non-buoyant line sources

For the base inventory, the ACHD will begin with the NEI inventory as prepared for the MANE-VU regional $PM_{2.5}$ modeling effort. All sources in Allegheny County and significant sources outside Allegheny County will be reviewed for their influence on the non-attainment area.

The MANE-VU inventory lists 1439 point sources for Allegheny County. Preliminary runs will be made of individual sources and groups of sources to determine if these sources create a gradient of concentrations across the CMAQ grid cell (that matches the near-field domain), i.e. that the source results in a significantly higher concentration at one receptor point than another. Sources with no gradient that are not targeted with local controls will be removed from the CALPUFF inventory. The intent in the CALPUFF modeling is to find the variance of concentrations to add or subtract that gradient from the full CMAQ model.

Sources will be reviewed for emissions and source parameter errors. MANE-VU has corrected some source inputs, but since the accuracy of source emissions and parameters become more sensitive to a finer grid, it may be necessary to further refine these sources. Recent stack tests may be incorporated to better characterize emission rates and stack parameters.

For consistency with CMAQ modeled results, sources with erred parameters will be subtracted from the regional results, based on average CALPUFF results that closely matches that CMAQ grid cell, then added according to corrected CALPUFF average results. This is discussed more in the model simulation and postprocessing sections that follow.

The MANE-VU emission inventory contains a number of area sources. ACHD will evaluate these sources to determine whether they are spread evenly across the County and therefore would not be responsive to the CALPUFF model. Also, ACHD will review the effect of these sources within the Liberty/Clairton non-attainment domain.

Allowable vs. Actual Emissions

The regional model is based on 2002 actual emissions for its modeling runs. This is necessary because the formation of some $PM_{2.5}$ components such as sulfates and nitrates depend on the ambient mix of chemicals. Thus, an actual emission inventory, rather than an allowable emission inventory, is needed. The CALPUFF modeling of the Liberty-Clairton Area must be consistent with the CMAQ modeling, so modeling will also be based on 2002 actual emissions using the inventory. This is different from most local regulatory dispersion modeling applications, where allowable or potential emissions are used.

In developing a control strategy, a procedure must be developed to calculate expected actual emissions from the control strategy. For those sources with a control strategy set by the Pittsburgh-Beaver Valley SIP demonstration and modeled in the attainment run for that model, the ACHD will use the same emission rates for the CALPUFF modeling runs. For those sources whose emissions have changed by the ACHD control strategy for the Liberty-Clairton Area, or changed due to other expected source changes, emission rates will be adjusted to represent

actual emission rates in the attainment year by evaluating actual operating levels and actual fuel use over the most recent two years.

Appendix F contains sources potentially affecting the Liberty-Clairton $PM_{2.5}$ Nonattainment Area, lying within the nonattainment area or adjacent municipalities.

4.7 Receptor Grid

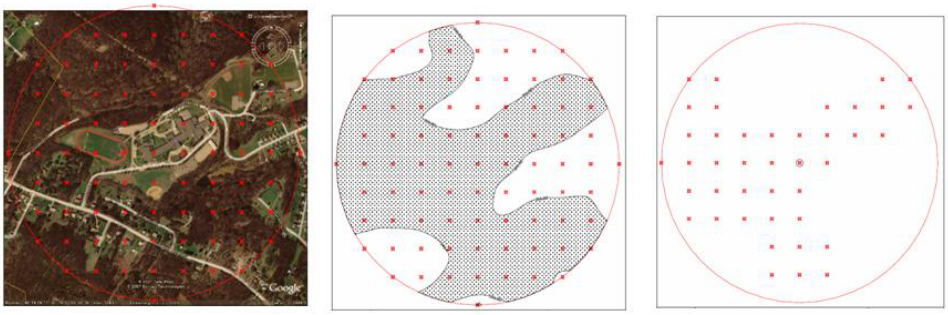
Either a 100-meter or 1-kilometer grid across the area covered by the CMAQ modeling grid number 98, 89 of the MANE-VU modeling will be used to determine an average CALPUFF concentration for each source modeled. Tests will be made of the sensitivity of the model to the choice of grid.

Although the modeling domains are larger in scale to accommodate changing wind patterns, the attainment analysis will only be performed on the 12 km CMAQ grid cell that contain the Liberty-Clairton Area. Final attainment will be based on the nearby receptor impacts located at the FRM sites within the Liberty-Clairton Area on a quarterly (calendar year) basis

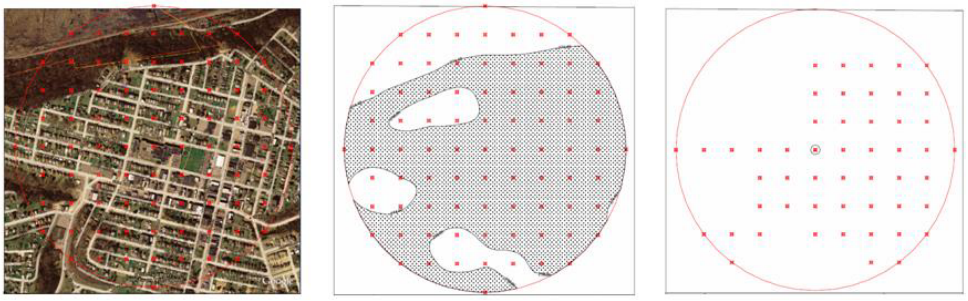
Nearby Receptors

The modeling guidance recommends modeling concentrations at "nearby receptors," receptors close to the 2 PM-2.5 monitors in the Liberty/Clairton area, the Liberty monitor and the Clairton monitor. Nearby receptors have been defined by ACHD as receptors spaced at 100 meter resolution up to a 500 meter radius from the FRM site and located at an elevation no less or greater than 40 feet of the FRM monitor elevation. Once the elevation criterion is not met, receptors at further distances away from the monitor in the same radial direction are excluded.

Liberty Nearby Receptors



Clairton Nearby Receptors



The locations of the Clairton nearby receptors have led to a problem: the receptors located southwest of the monitor are located outside the CMAQ grid cell used in the remaining modeling.

Several options were discussed to deal with this issue:

- Include the next CMAQ grid cell in the analysis, by using the CMAQ concentrations from this grid with the receptors located in that cell. This may lead to some inconsistency.
- Include the next CMAQ grid cell in the analysis, by averaging the CMAQ results of the two grid cells and modeling CALPUFF as a 12 x 24 kilometer grid. This would shift the emphasis off the non-attainment area and into locations further south.
- Do not consider any nearby receptors not located within the CMAQ grid. This may lead to concerns from the excluded areas.
- Locate the CALPUFF modeling grid 0.5 southwest of the CMAQ grid, but use the concentrations provided by the one CMAQ grid cell when combining the results of the two models.

ACHD has chosen the fourth option: make a slight shift to the southwest to the CALPUFF equivalent cell to include the nearby receptors for Clairton (see Figure 4.8.b below). The CALPUFF receptor gird would not include the area represented by the "top" 0.5 km x 12 km of the CMAQ grid cell, and include an area 0.5 km x 12 km area below the identified CMAQ grid cell. This would maintain the mass of a 12 km x 12 km grid, include all the nearby receptors, and maintain consistency of the CMAQ results across the grid. Since there are no major sources affected by such an adjustment, and the average should be similar to that of the exact equivalent CMAQ grid cell area, this shift should not negatively affect the final modeled results.

Figure 4.8.a. Near-Field Domain Aerial Map, with CMAQ Grid Cell Area and Nearby Receptors for Liberty and Clairton

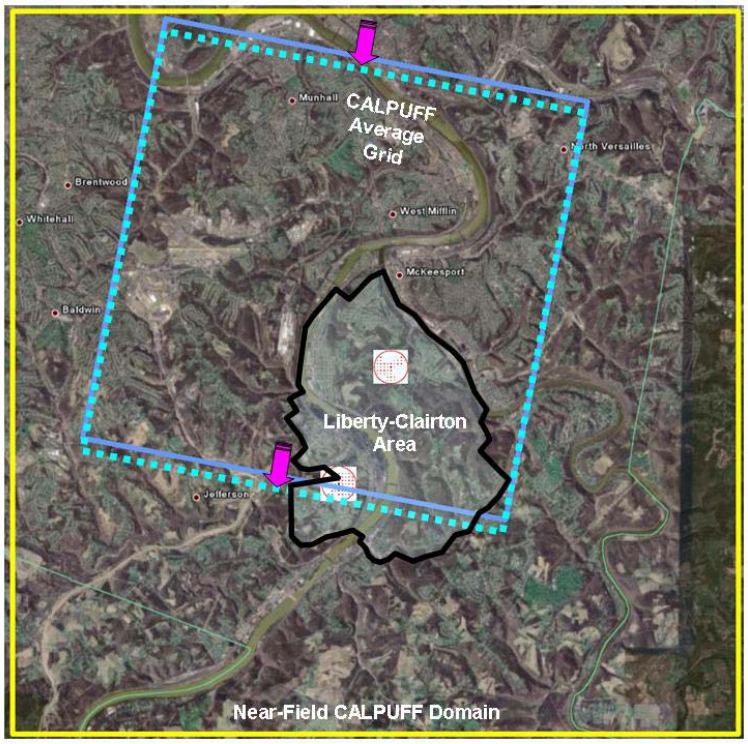


Figure 4.8.b. Near-Field Domain Aerial Map, with CALPUFF Equivalent (Average) Grid Cell Shift and Liberty-Clairton Area and Monitors

4.8 Modeling Tasks

The CALPUFF model will be run for each source, for each quarter, for each of the selected pollutants.

The modeling steps, in brief, are:

a) Select input and results data from MANE-VU CMAQ runs for Liberty-Clairton non-attainment area. Develop software as needed to extract data from the MANE-VU runs.
b) Compare the NEI/MANE-VU PM and VOC emissions inventory against ACHD, PADEP, & WVDEP inventories for Allegheny County sources and select sources from the remainder of the modeling domain. This review will include source parameters.
c) Confirm questionable emission rates and source parameters.
d) Write software, if needed, to combine results from modeling runs of separate groups of sources, specifically to combine CALPUFF and CMAQ results. Results from different CALPUFF runs, i.e., near-field and long-range grids, can be combined using the CALSUM or other postprocessor.
e) Make test runs of individual and groups of sources or small sets of receptors or dates using CALPUFF to check the integrity of input files.
f) Perform test runs for model options as applicable; exclude options not applicable to Liberty-Clairton modeling such as chemical transformation.
g) Set up full modeling runs. If needed, set up separate modeling runs to run simultaneously on separate computers.
h) Combine CALPUFF and CMAQ results, using the process described below.
i) Run the model iteratively to determine the optimum control strategy.
j) Verify the attainment modeling by making a final run using the selected control strategy.
k) Combine CALPUFF results with CMAQ results of the final run.
l) Prepare a technical support document on the final attainment modeling.

5.0 EVALUATION OF RESULTS

This section delineates the procedures for postprocessing modeled results and testing for attainment.

5.1 Combination of CMAQ and CALPUFF

Component-by-Component Analysis

Total concentration of $PM_{2.5}$ can be determined by summing the primary dispersion derived component and the secondary grid model component. The Speciated Modeled Attainment Test (SMAT) will adjust the major species to a total that is more equivalent to an FRM mass concentration on a quarterly basis.

Elsewhere in this document, it is demonstrated that nitrates and sulfates in the Liberty/Clairton are regional, rather than local, in nature. The results of the CMAQ model are sufficient for these components, and CALPUFF will not be run for them. For nitrates, sulfates, and ammonium, the value from CMAQ base and attainment modeling runs will be used. There will be one value each day per 12 x 12-km grid, on a quarterly basis.

CALPUFF modeling will be done for primary filterable and condensible $PM_{2.5}$ emissions. Results will be analyzed and calculated against the same component in CMAQ. For primary filterable, condensable, and other primary $PM_{2.5}$, the value from CMAQ will be combined with CALPUFF modeled values.

CMAQ regional modeling will provide one value per species across the 12 x 12 km grid cell that includes the Liberty-Clairton Area. CALPUFF modeling for the near field domain (long-range domain discussed below), will produce two end-results:

- And array of concentrations in an area equivalent to the area represented by the CMAQ 12 x 12 km cell, from which an average will be calculated. Resolution for this area should be sufficient enough (250 m to 1 km) to realize the maximum and minimum impacts throughout the area. The average from all the receptors from the CALPUFF “equivalent cell” will be used in combination with the CMAQ value to effectively remove any double-counting of average/background concentrations.

- Concentrations at the nearby receptors, at or adjacent to the FRM site locations within the Liberty-Clairton Area, representing community impacts.

The methodology of the CALPUFF procedure is to use CMAQ values as background, remove the equivalent CALPUFF average values from the background (to avoid double-counting), and add the localized CALPUFF impacts at the nonattainment sites.

Based on work done for the Philadelphia air toxics study, the CALPUFF modeling can provide a finer resolution to the terrain within the non-attainment area than the CMAQ model; however, the mass of the CMAQ grid cell should be maintained. For the nearby receptor analysis, ACHD plans to use the equation:

CMAQ + CALPUFF defined sub-grid variability:

$$C_{sub\text{-}Grid} = C_{CMAQ} + C_{CALPUFF} - [C_{CALPUFF}]_{AVG}$$

In this case, the concentration results from the CMAQ attainment run and the concentrations from the CALPUFF attainment runs will be used. The effects of local controls on sources that are not included in the CMAQ modeling would be eradicated from the attainment run if a new, final CALPUFF average were subtracted from each receptor. So, the final attainment calculation would need to be:

$$C_{controlled\_sub\text{-}Grid} = C_{CMAQcontrolled} + C_{CALPUFFcontrolled} - [C_{CALPUFF}]_{AVGuncontrolled}$$

Relative response factors (RRFs) will be applied to elemental and organic carbons base year actual monitor concentrations in order to project future year concentrations. Actual speciation monitor results are not available for Liberty-Clairton in 2002, and averages for 2003-2007 will be extrapolated temporally to represent quarterly averages.

5.2 Attainment Test

Final concentrations for each species will be entered into SMAT analysis, which adjusts the speciated results to more closely match FRM results using the SANDWICH method on a quarterly basis. The SANDWICH method (Sulfate, Adjusted Nitrate, Derived Water, Inferred Carbonaceous mass Hybrid) material balance approach adds water, passive mass, and corrects the organic carbon species.

The EPA Modeling Guidance for $PM_{2.5}$ (and ozone and regional haze) provides the procedures for processing the data by SMAT. Weight of evidence analysis will be needed based on final values for $PM_{2.5}$ for the controlled year.

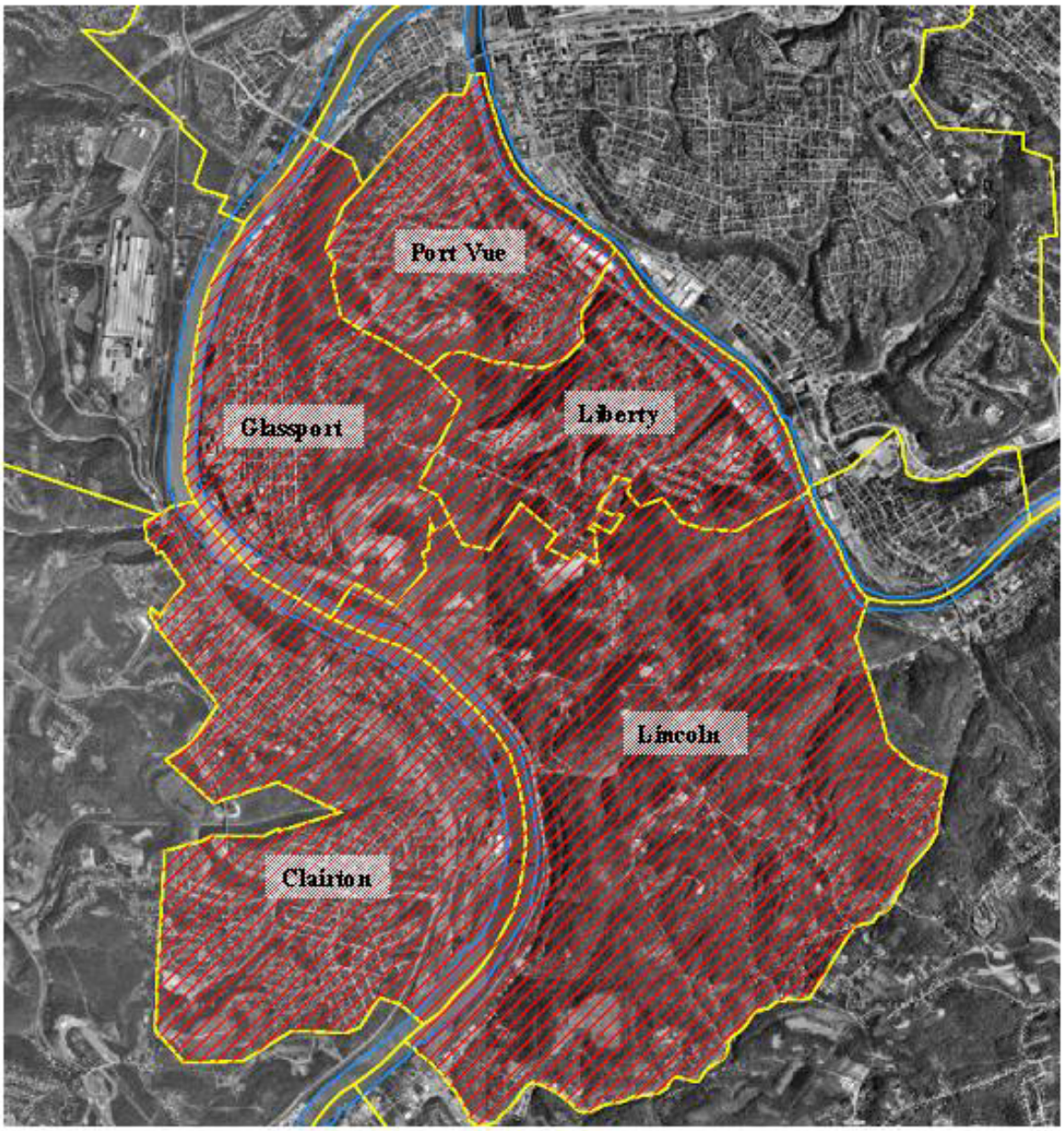
APPENDIX A – Maps of Affected Areas

$PM_{2.5}$ Southwestern PA Designation Areas

Pittsburgh – Beaver Valley Area: includes all of Allegheny, Beaver, Butler, Washington, and Westmoreland Counties, and parts of Armstrong Co. (Washington Twp., Plumcreek Twp., and Elderton Borough), Greene Co. (Monongahela Twp.), and Lawrence Co. (Taylor Twp. south of New Castle)

Liberty – Clairton Area: includes Glassport, Liberty, Lincoln and Port Vue Boroughs, and City of Clairton

Liberty-Clairton Area – Aerial Close-Up (with Municipalities)



Liberty-Clairton Area – Topographic Close-Up

APPENDIX B – Monitored Sites and Data

Two sites have monitored $PM_{2.5}$ (FRM monitors) within in the Liberty-Clairton Area:

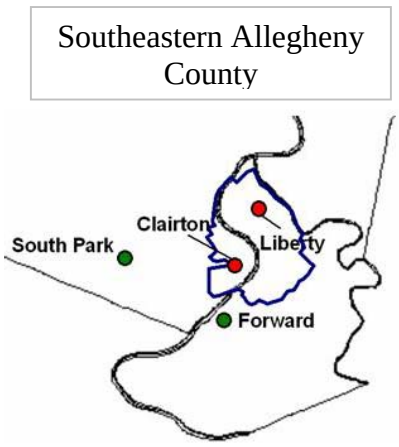
Liberty: Located on a plateau near the center of the Liberty-Clairton Area at an elevation of 1069 ft. (MSL). It has monitored nonattainment for both the annual and the 24-hour standard. It also contains continuous (TEOM) and speciation (STN) monitors. [AQS# 42-003-0064-88101]

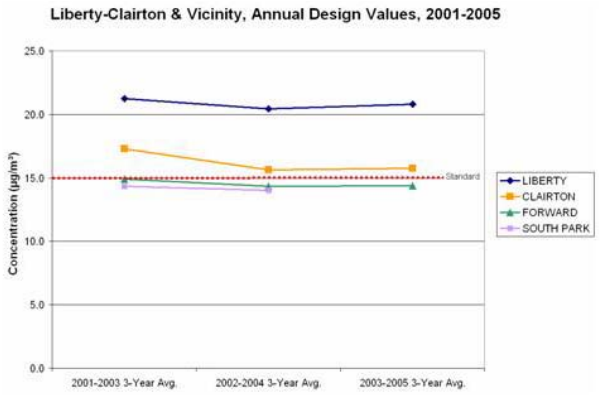
Clairton: Located within the Monongahela River valley in the western portion of the area at an elevation of 953 ft. (MSL). It has monitored nonattainment for the annual standard only. [AQS# 42-003-3007-88101]

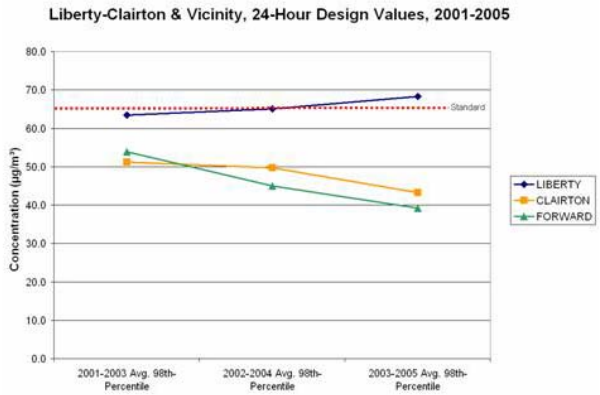
Two additional sites have monitored $PM_{2.5}$ (FRM monitors) within the vicinity of the Liberty-Clairton Area:

Forward: Located on a plateau to the south of the Liberty-Clairton Area at an elevation of 1170 ft. (MSL). It has monitored attainment of both standards. It was relocated from the South Park site in Feb. 2003 and was discontinued in Dec. 2005. AQS# 42-003-0133-88101

South Park: Located on a plateau to the west of the area at an elevation of 1221 ft. (MSL). It monitored attainment for both standards. It was discontinued and moved to the Forward site in Feb. 2003. AQS# 42-003-0131-88101

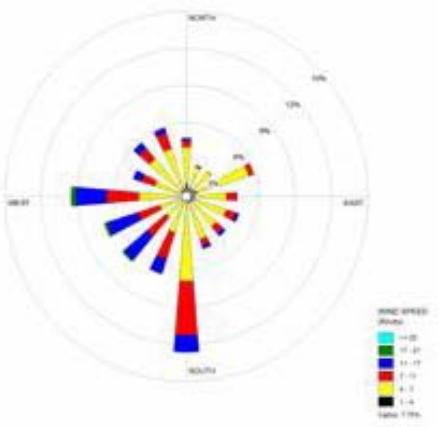




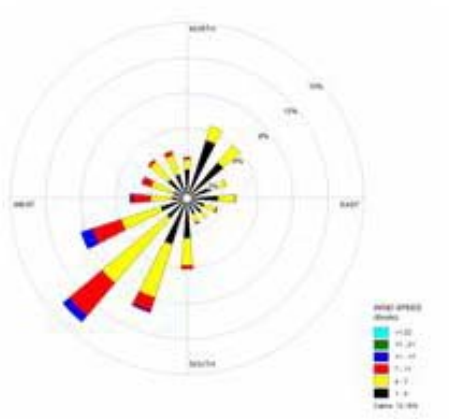


APPENDIX C – Meteorological Sites with Wind Roses

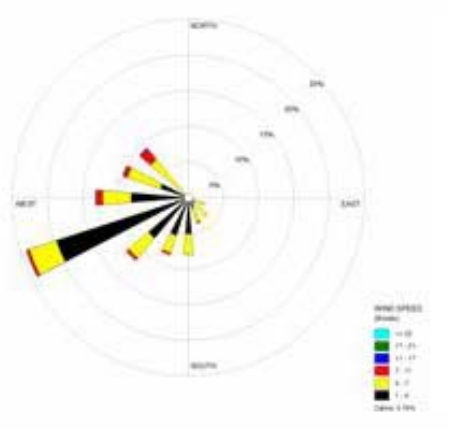
Allegheny County Airport



Liberty



Clairton

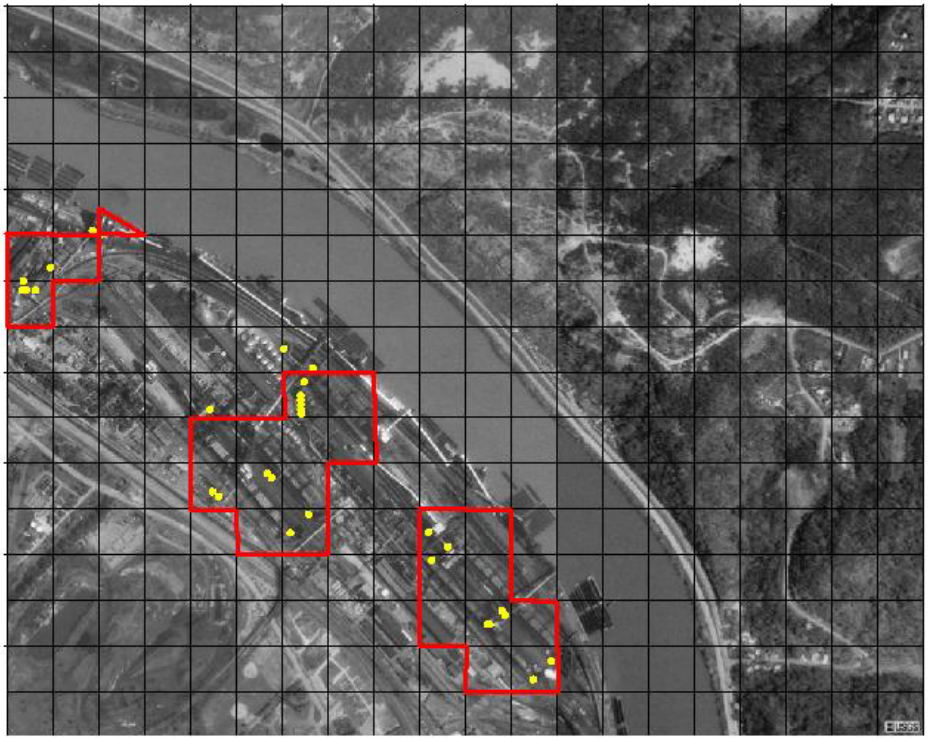


APPENDIX D – Surface Characteristics and Heat Flux Areas

Annual Average CALMET Default Surface Characteristics with Adjusted Anthropogenic Heat Flux

Land Use Type	Description	Albedo	Bowen Ratio	Soil Heat Flux	Anthropogenic Heat Flux	Leaf Area
11	RESIDENTIAL	0.19	1.20	0.19	5.00	1.68
13	INDUSTRIAL	0.18	1.50	0.25	30.00	0.00
15	INDUSTRIAL AND COMMERCIAL COMPLEXES	0.18	1.50	0.25	5572.73	0.00
21	CROPLAND AND PASTURE	0.15	1.00	0.15	0.00	3.00
41	DECIDUOUS FOREST LAND	0.10	1.00	0.15	0.00	7.00
42	EVERGREEN FOREST	0.10	1.00	0.15	0.00	7.00
43	MIXED FORESTLAND	0.10	1.00	0.15	0.00	7.00
52	LAKES (RIVERS)	0.10	0.00	1.00	0.00	0.00
75	STRIP MINES, QUARRIES, AND GRAVEL PITS	0.30	1.00	0.15	0.00	0.05
76	TRANSITIONAL AREAS	0.22	1.25	0.20	0.00	0.35

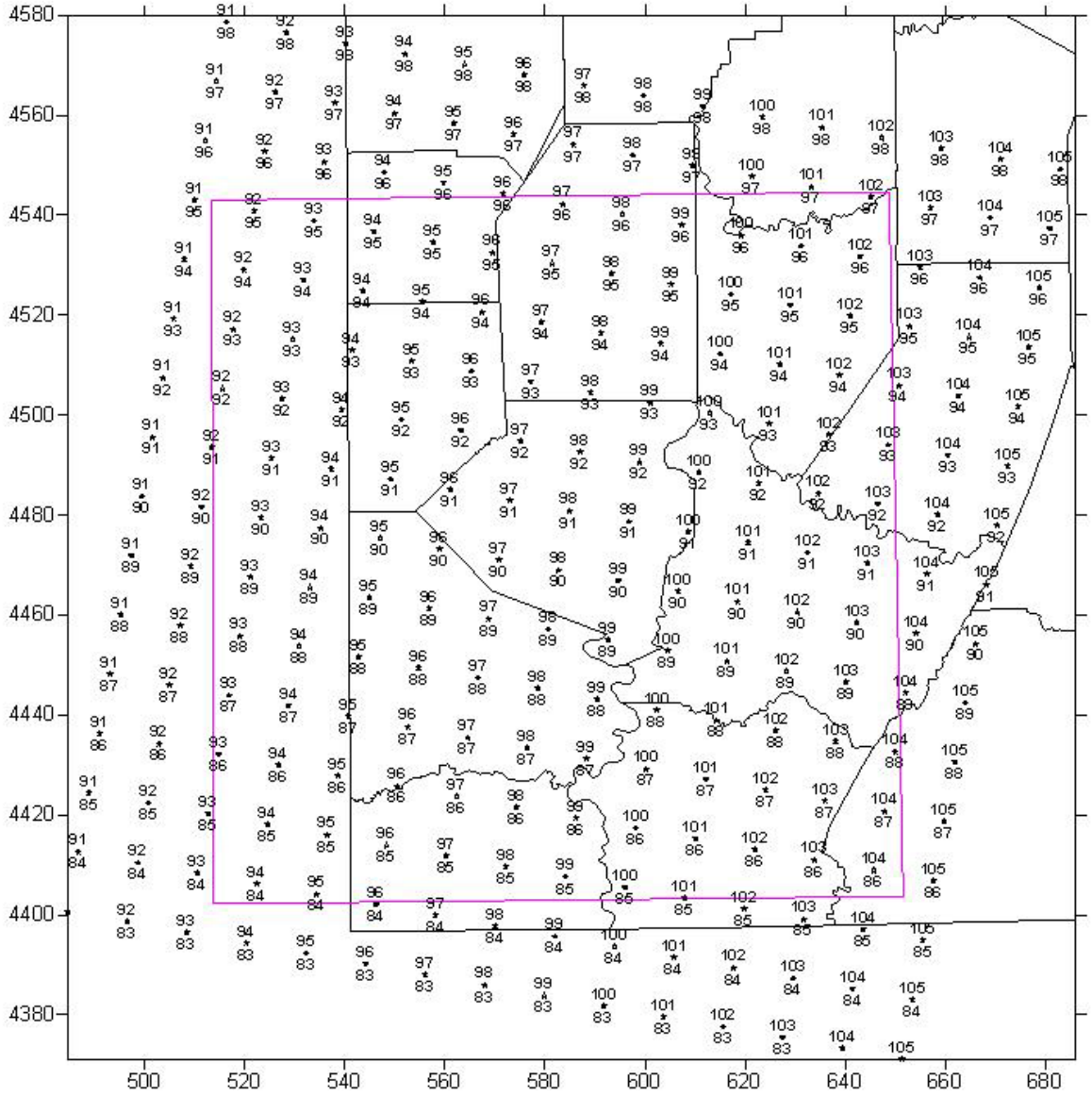
Adjusted Anthropogenic Heat Flux Areas



Near-field grid cells in red contain high anthropogenic heat flux based on combustion sources (shown in yellow)

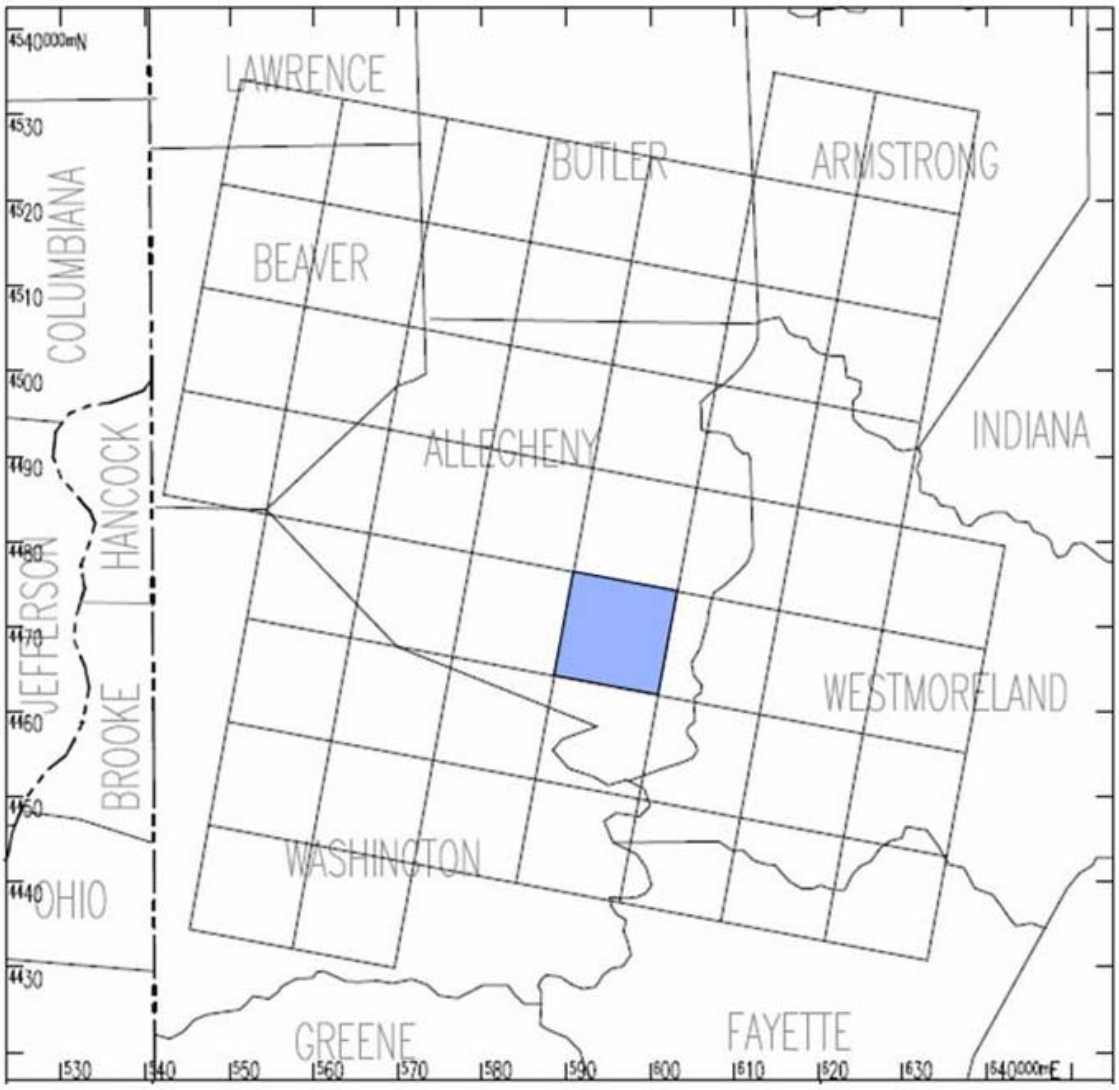
APPENDIX E – MANE-VU Grid Cells and Configuration

MM5 Grid Center Points and MM5 Coverage



Grid points at 12 km spacing

CMAQ Grid Cells with SW PA Counties



Grid cell containing Liberty-Clairton shown in blue

MANE-VU Regional Modeling System Grid Configurations

OTC MM5/SMOKE/CMAQ modeling system for 2002 annual simulation is applied with a Lambert Conformal Conic projection with parallels at 33N and 45N. A spherical earth radius of 6370km is used in these programs.

MM5 Setup

MM5 was run with two-way nesting at 36 and 12km horizontal grid spacing and with 29 vertical layers. The top is at 50 mb.

For 36km domain, the center is at 97W and 40N. There are 149 grids (dot-points) in east-west direction and 129 grids (dot-points) in north-south direction. The south-west corner is at (-2664km, -2304km) and the north-east corner is at (2664km, 2304km)

For 12km domain, there are 175 grids in east-west direction and 175 grids in north-south direction. The south-west corner is at (252km, -900km) and the north-east corner is at (2340km, 1188km)

The 30 sigma-levels for the 29 vertical layers are:
1.0000, 0.9974, 0.9940, 0.9890, 0.9820, 0.9720, 0.9590, 0.9430, 0.9230, 0.8990, 0.8710, 0.8390, 0.8030, 0.7630, 0.7180, 0.6680, 0.6180, 0.5680, 0.5180, 0.4680, 0.4180, 0.3680, 0.3180, 0.2680, 0.2180, 0.1680, 0.1230, 0.0800, 0.0400, 0.0000

CMAQ Setup

CMAQ 36km modeling domain has 145 cells in east-west direction and 102 cells in north-south direction. The south-west corner is at (-2628km, -1728km) and the north-east corner is at (2592km, 1944km)

CMAQ 12km modeling domain has 172 cells in east-west directions and 172 cells in north-south direction. The south-west corner is at (264km, -888km) and the north-east corner is at (2328km, 1176km)

There are 22 vertical layers for CMAQ. The sigma-levels for these 22 layers are:

1.0000, 0.9974, 0.9940, 0.9890, 0.9820, 0.9720, 0.9590, 0.9430, 0.9230, 0.8990, 0.8710, 0.8390, 0.8030, 0.7630, 0.7180, 0.6680, 0.5680, 0.4680, 0.3680, 0.2680, 0.1680, 0.0800, 0.0000

SMOKE Setup

SMOKE modeling domains are same as CMAQ, except that the emissions are limited to the lower 16 CMAQ layers.

APPENDIX F – Facilities Potentially Affecting Liberty-Clairton

Below are facilities potentially affecting the Liberty-Clairton PM2.5 Nonattainment Area, lying within the nonattainment area or adjacent municipalities, according to the ACHD permit tracking list. Emissions data are based on NEI 2002 emissions inventory (actuals).

Major/Minor/Synthetic Minor Sources w/$PM_{2.5}$ > 1 TPY
Clairton Slag, *W. Elizabeth*.....10.46 tpy
CP Industries, *McKeesport*.....1.05 tpy
Eastman Chemical, *W. Elizabeth*.....13.04 tpy
Guardian, *W. Elizabeth*.....21.89 tpy
Marsh Asphalt, *Dravosburg*.....4.66 tpy
Mid-Continent Coal, *Clairton*.....4.10 tpy
Koppers, *Clairton*.....6.71 tpy
US Steel Clairton, *Clairton*.....319.04 tpy
US Steel Irvin, *W. Mifflin*.....26.41 tpy

Major/Minor/Synthetic Minor Sources w/$PM_{2.5}$ < 1 but Other Criteria > 1 TPY
GE International, *W. Mifflin*
GM, *W. Mifflin*
Kinder Morgan, *Dravosburg*
Liberty Pultrusions, *W. Mifflin*
Marathon Ashland, *W. Elizabeth*
Nash, *Elizabeth*
Precoat, *McKeesport*
Sanyo Chemical, *W. Elizabeth*

Major/Minor/Synthetic Minor Sources w/All Criteria < 1 TPY
PA Electric Coil, *Glassport*

Minor Sources w/No Emissions Inventory
AKJ Industries, *Clairton*
Elizabeth Carbide, *McKeesport*
Harbison Walker, *W. Mifflin*
MonValley Transportation Center, *Glassport*
Penn Rilton, *W. Elizabeth*
Ryan Metal, *McKeesport*
Tech Met, *Glassport*
TYK Refractories, *Clairton*

PA DEP Sources
Reliant Energy – Elrama, *Union Twp.*
Allegheny Energy – Mitchell, *Union Twp.*

APPENDIX G - Sample CMAQ Output

Data below is shown for year 2002 (base year), by hourly major species in µg/m³. The species A25 is primary un-speciated $PM_{2.5}$.

2002 DATE/HOUR	PM2.5	SO4	NO3	NH4	EC	OM	A25
2002010100	14.8025	1.3307	4.7542	1.8792	0.9320	3.1156	2.7910
2002010101	15.3689	1.3787	5.2984	2.0551	0.8850	2.9497	2.8019
2002010102	16.6705	1.4380	5.7607	2.2116	1.0383	3.2216	3.0002
2002010103	17.4495	1.4135	6.0682	2.2917	1.1672	3.3952	3.1137
2002010104	18.2931	1.3158	6.2770	2.3157	1.4417	3.7457	3.1972
2002010105	19.1490	1.2872	6.5669	2.3892	1.5920	4.0079	3.3058
2002010106	20.2648	1.3094	6.8786	2.4880	1.7428	4.3646	3.4815
2002010107	21.6470	1.3800	7.1915	2.6053	1.9126	4.8193	3.7383
2002010108	23.0140	1.4724	7.4489	2.7147	2.0777	5.2884	4.0118
2002010109	23.9955	1.5170	7.5192	2.7518	2.2311	5.7673	4.2090
2002010110	22.7164	1.4829	7.3748	2.6971	1.9189	5.1758	4.0669
2002010111	19.0075	1.5060	6.7729	2.5310	1.2314	3.7132	3.2531
2002010112	16.8398	1.5920	6.0480	2.3528	1.0356	3.1239	2.6875
2002010113	14.7394	1.4883	5.1577	2.0554	0.9184	2.8217	2.2979
2002010114	14.7165	1.7929	4.5507	1.9933	0.9118	2.9348	2.5330
2002010115	18.3694	2.4379	4.7795	2.3016	1.4067	4.0730	3.3708
2002010116	25.1637	3.0168	5.2343	2.6509	2.6888	6.7227	4.8501
2002010117	26.7666	3.0794	5.4420	2.7346	2.9395	7.3119	5.2592
2002010118	27.4995	2.8928	5.7316	2.7487	3.0251	7.5641	5.5372
2002010119	27.5892	2.5784	6.2197	2.7725	2.9400	7.4624	5.6162
2002010120	27.6079	2.4022	6.9326	2.9134	2.6696	7.0359	5.6543
2002010121	28.0412	2.4297	7.7505	3.1610	2.3317	6.5527	5.8156
2002010122	28.5227	2.4908	8.4058	3.3742	2.1049	6.2427	5.9043
2002010123	28.4715	2.4801	9.0439	3.5554	1.8190	5.8264	5.7467
2002010200	28.5442	2.4498	9.6462	3.7187	1.6405	5.5451	5.5440
2002010201	28.5095	2.3856	10.1459	3.8397	1.5482	5.2945	5.2956
2002010202	27.9996	2.2779	10.5305	3.9106	1.4436	4.9544	4.8827
2002010203	27.1029	2.0935	10.8094	3.9222	1.3915	4.5832	4.3030
2002010204	26.5643	1.8992	11.0418	3.9170	1.4700	4.4141	3.8223
2002010205	26.6821	1.7940	11.2865	3.9487	1.5957	4.4630	3.5942
2002010206	27.7236	1.7927	11.5551	4.0265	1.7779	4.7855	3.7858
2002010207	29.2867	1.8215	11.8191	4.1141	1.9983	5.2701	4.2636
2002010208	31.0866	1.8323	11.9975	4.1701	2.3076	5.9724	4.8067
2002010209	32.1544	1.8350	11.9859	4.1678	2.5024	6.4990	5.1644
2002010210	32.4919	1.8761	11.7850	4.1249	2.5866	6.7837	5.3357
2002010211	30.5268	1.9863	11.4494	4.0688	1.9995	6.0451	4.9777

Data below is shown for year 2009 (projected controlled year), by hourly major species in µg/m³. The species A25 is primary un-speciated $PM_{2.5}$.

2009 DATE/HOUR	PM2.5	SO4	NO3	NH4	EC	OM	A25
2009010100	14.8876	1.3012	4.5373	1.8052	0.8266	2.9902	3.4270
2009010101	15.5982	1.3455	5.1189	1.9906	0.7798	2.9132	3.4501
2009010102	16.9447	1.4077	5.6291	2.1620	0.9286	3.1959	3.6215
2009010103	17.9199	1.3966	6.0175	2.2707	1.0499	3.4234	3.7618
2009010104	19.1311	1.3606	6.3414	2.3512	1.3040	3.8370	3.9368
2009010105	20.1977	1.3785	6.7085	2.4645	1.4501	4.1066	4.0895
2009010106	21.4533	1.4089	7.1108	2.5927	1.6039	4.4602	4.2768
2009010107	22.9384	1.4749	7.4603	2.7189	1.7765	4.9358	4.5720
2009010108	24.1541	1.5480	7.6171	2.7919	1.9399	5.4106	4.8466
2009010109	24.7023	1.5710	7.4795	2.7605	2.0888	5.8086	4.9940
2009010110	23.1497	1.5152	7.1775	2.6520	1.7875	5.2040	4.8135
2009010111	19.8690	1.5492	6.5987	2.4967	1.1423	3.8143	4.2679
2009010112	17.7946	1.5684	5.9031	2.3019	0.9705	3.3074	3.7432
2009010113	15.1120	1.3903	5.0817	1.9967	0.8669	2.8797	2.8967
2009010114	14.8956	1.5468	4.7077	1.9468	0.8624	2.9512	2.8806
2009010115	18.6337	2.2076	4.8671	2.2408	1.3461	4.1493	3.8228
2009010116	25.2866	2.8490	5.1714	2.5697	2.5839	6.7801	5.3325
2009010117	26.5864	2.9371	5.3500	2.6546	2.8013	7.3009	5.5427
2009010118	26.8451	2.7775	5.5809	2.6618	2.8683	7.4350	5.5216
2009010119	26.6377	2.5079	6.0007	2.6825	2.7749	7.2544	5.4172
2009010120	26.4796	2.3599	6.6394	2.8124	2.4986	6.8063	5.3630
2009010121	26.8580	2.4039	7.5016	3.0792	2.1531	6.3244	5.3959
2009010122	27.4114	2.4839	8.2222	3.3184	1.9236	6.0151	5.4483
2009010123	27.4115	2.4911	8.8209	3.4949	1.6514	5.6011	5.3521
2009010200	27.5247	2.4746	9.3355	3.6381	1.4889	5.3409	5.2467
2009010201	27.6184	2.4298	9.7513	3.7419	1.4061	5.1489	5.1404
2009010202	27.4627	2.3327	10.1203	3.8126	1.3089	4.8818	5.0064
2009010203	27.1154	2.1354	10.4421	3.8320	1.2688	4.6171	4.8201
2009010204	26.9430	1.8966	10.7264	3.8250	1.3460	4.5387	4.6102
2009010205	27.2242	1.7482	10.9961	3.8477	1.4665	4.6382	4.5274
2009010206	28.1514	1.7195	11.1761	3.8893	1.6420	4.9743	4.7503
2009010207	29.5240	1.7458	11.2989	3.9348	1.8551	5.4591	5.2302
2009010208	31.1821	1.7829	11.3681	3.9689	2.1481	6.1377	5.7762
2009010209	32.1814	1.8262	11.2908	3.9628	2.3377	6.6178	6.1461
2009010210	32.4737	1.8990	11.1115	3.9380	2.4279	6.8134	6.2838
2009010211	30.4246	2.0083	10.8156	3.8931	1.8801	5.8411	5.9864