Application of an Integrated Plume to Regional Photochemical Model for the Allegheny County Liberty-Clairton $PM_{2.5}$ Attainment Demonstration Modeling

Control # 36

Ralph E. Morris[1], Jaegun Jung[1], Bonyoung Koo[1] and Jason Maranche[2]

1. ENVIRON International Corporation, 773 San Marin Drive, Suite 2115, Novato, CA 94998
2. Allegheny County Health Department, 301 39th Street, Bldg. #17, Pittsburgh, PA 15201

ABSTRACT

The Liberty-Clairton Nonattainment Area (NAA) is approximately 10 miles southeast of the City of Pittsburgh. Based on 2009-2011 observations, for the first time the Liberty-Clairton NAA is attaining the annual 15 µg/m^3 $PM_{2.5}$ National Ambient Air Quality Standard (NAAQS) but still violates the 35 µg/m^3 24-hour $PM_{2.5}$ NAAQS at the Liberty monitoring site. The Allegheny County Health Department (ACHD) is preparing a $PM_{2.5}$ State Implementation Plan (SIP) that demonstrates the Liberty-Clairton NAA will attain the $PM_{2.5}$ NAAQS by 2014. $PM_{2.5}$ in the Liberty-Clairton NAA is influenced by regional transport, including particulate sulfate that is the largest component of the annual $PM_{2.5}$ concentrations. However, $PM_{2.5}$ concentrations at the Liberty monitoring site are also impacted by numerous industrial local sources that are within ~10 km of the monitoring site. Thus, the $PM_{2.5}$ attainment demonstration modeling must account for regional transport of air pollutants from 1000s km away, as well as the impacts of plumes from local sources that are within ~10 km of the Liberty monitoring site.

The Comprehensive Air-quality Model with extensions (CAMx) is a one-atmosphere multi-scale photochemical grid model that includes a subgrid-scale Plume-in-Grid (PiG) chemically reactive Gaussian puff model to treat the near source plume dispersion, dynamics and chemistry within point source plumes. For the Liberty-Clairton NAA $PM_{2.5}$ attainment demonstration modeling, CAMx was configured with a 36 km Continental U.S., 12 km Northeast U.S., 4 km Southwest Pennsylvania (SWPA) and 800 km Liberty-Clairton region domains. Local sources were treated using the PiG module with the PiG puffs sampled using a 100 m receptor array located around the Liberty and Clairton monitoring sites. The Particulate Source Apportionment Technology (PSAT) was used to track the contributions due to the local sources to $PM_{2.5}$ concentrations. CAMx was run for a 2007 base case and 2014 emissions scenario and the CAMx PSAT and PiG results were used to obtain the contributions of local sources. The CAMx 2007 base case results were subjected to a model performance evaluation that revealed good $PM_{2.5}$ model performance that achieved model performance goals by a wide margin. The model was evaluated for $PM_{2.5}$ components with sulfate and ammonium also achieving good model performance and most species achieving the PM performance goals. The model estimated contribution to annual average $PM_{2.5}$ concentrations at Liberty (3.1 µg/m^3) was slightly lower than the contribution obtained by analyzing the excess $PM_{2.5}$ concentrations at Liberty compared to surrounding sites (4.1 µg/m^3), which is due in part to the formulation of the PSAT source apportionment tool that

traces $PM_{2.5}$ back to the sources of the primary precursor (e.g., the ammonium associated with the local source sulfate and nitrate would be attributed to ammonia sources and not the local sources). The results of the new $PM_{2.5}$ modeling methodology that combines near-source plume and regional-scale photochemical grid modeling within a single integrated multiscale model and how it was used to demonstrate $PM_{2.5}$ attainment at the Liberty monitoring site is discussed.

INTRODUCTION

In 1997, the United States Environmental Protection Agency (EPA) for the first time established National Ambient Air Quality Standards (NAAQS) for fine particulate matter (i.e., particulate matter with a diameter of 2.5 micrometers or less, $PM_{2.5}$). The 1997 $PM_{2.5}$ NAAQS had an annual average threshold of 15 $\mu g/m^3$ and a 24-hour average threshold of 65 $\mu g/m^3$. In 2005, the EPA designated the Liberty-Clairton area, a 12 km^2 area completely contained within the borders of the Pittsburgh-Beaver Valley $PM_{2.5}$ nonattainment area (NAA), to be a separate $PM_{2.5}$ NAA due to unique features of the region. The Liberty-Clairton NAA is located approximately 10 miles southeast of the city of Pittsburgh.

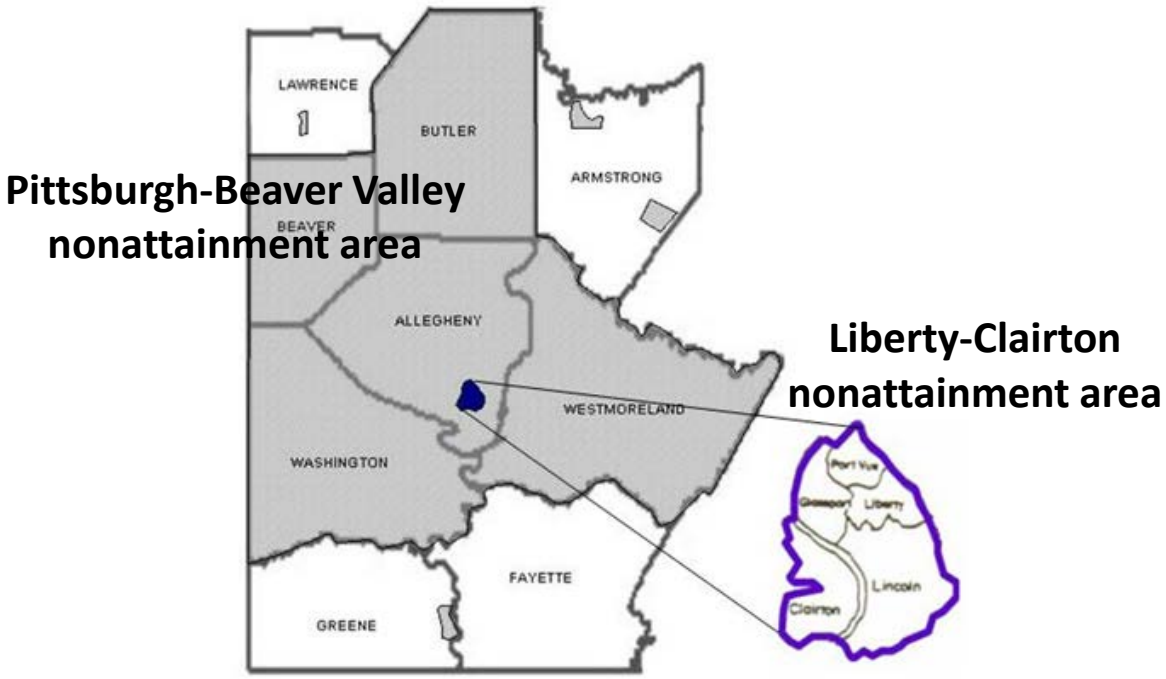
Both the Liberty-Clairton and Pittsburgh-Beaver Valley areas were designated as nonattainment of the 1997 $PM_{2.5}$ NAAQS based on 2001-2003 measured air quality. The Pittsburgh-Beaver Valley NAA prepared a $PM_{2.5}$ SIP that demonstrated the area would achieve the 1997 $PM_{2.5}$ NAAQS by 2010[1]. Whereas, the Liberty-Clairton $PM_{2.5}$ SIP demonstrated that the area would achieve the 1997 $PM_{2.5}$ NAAQS by 2015[2]. However, in fact based on 2009-2011 measured air quality data the Liberty-Clairton actually attained the 1997 $PM_{2.5}$ NAAQS by 2011.

In 2006, EPA lowered the 24-hour $PM_{2.5}$ NAAQS from 65 to 35 $\mu g/m^3$ and retained the 15.0 $\mu g/m^3$ annual threshold. In October 2008 EPA designated the Liberty-Clairton area as an NAA due to a measured violation of the 2006 24-hour $PM_{2.5}$ NAAQS based on 2006-2008 monitoring data with a 24-hour Design Value of 53 $\mu g/m^3$ occurring at the Liberty monitoring site. Thus, the Allegheny County Health Department (ACHD) needs to prepare a $PM_{2.5}$ SIP for the Liberty-Clairton area that demonstrates the area will achieve the 2006 $PM_{2.5}$ NAAQS by 2014. This paper presents the $PM_{2.5}$ attainment demonstration modeling that demonstrates how the Liberty-Clairton NAA will achieve the 2006 $PM_{2.5}$ NAAQS by 2014. Note that in December 2012 EPA lowered the annual $PM_{2.5}$ NAAQS from 15 to 12 $\mu g/m^3$; attainment of the new 12 $\mu g/m^3$ annual $PM_{2.5}$ NAAQS will be addressed in future actions.

CONCEPTUAL MODEL OF THE $PM_{2.5}$ PROBLEM IN THE LIBERTY-CLAIRTON AREA

The Liberty-Clairton nonattainment area (NAA) is made up of complex river valley terrain, approximately 3 miles wide by 5 miles long with a population of approximately 25,000 people. 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. The area is home to numerous industrial sources, including the U.S. Steel Clairton Plant that is the largest coke plant in the United States. There are two Federal Reference Method (FRM) $PM_{2.5}$ monitors in the area (Liberty and Clairton). The Liberty monitoring site exhibits higher $PM_{2.5}$ concentrations than surrounding monitors due to contributions of local sources whose emissions are influenced by the river-valley topography making the Liberty-Clairton NAA quite different than the remainder of the Pittsburg-Beaver Valley NAA. Consequently, the Liberty-Clairton area was designated a separate $PM_{2.5}$ NAA from the Pittsburgh-Beaver Valley NAA. The Liberty-Clairton NAA is completely contained within, but not part of, the Pittsburgh-Beaver Valley NAA as shown in Figure 1.

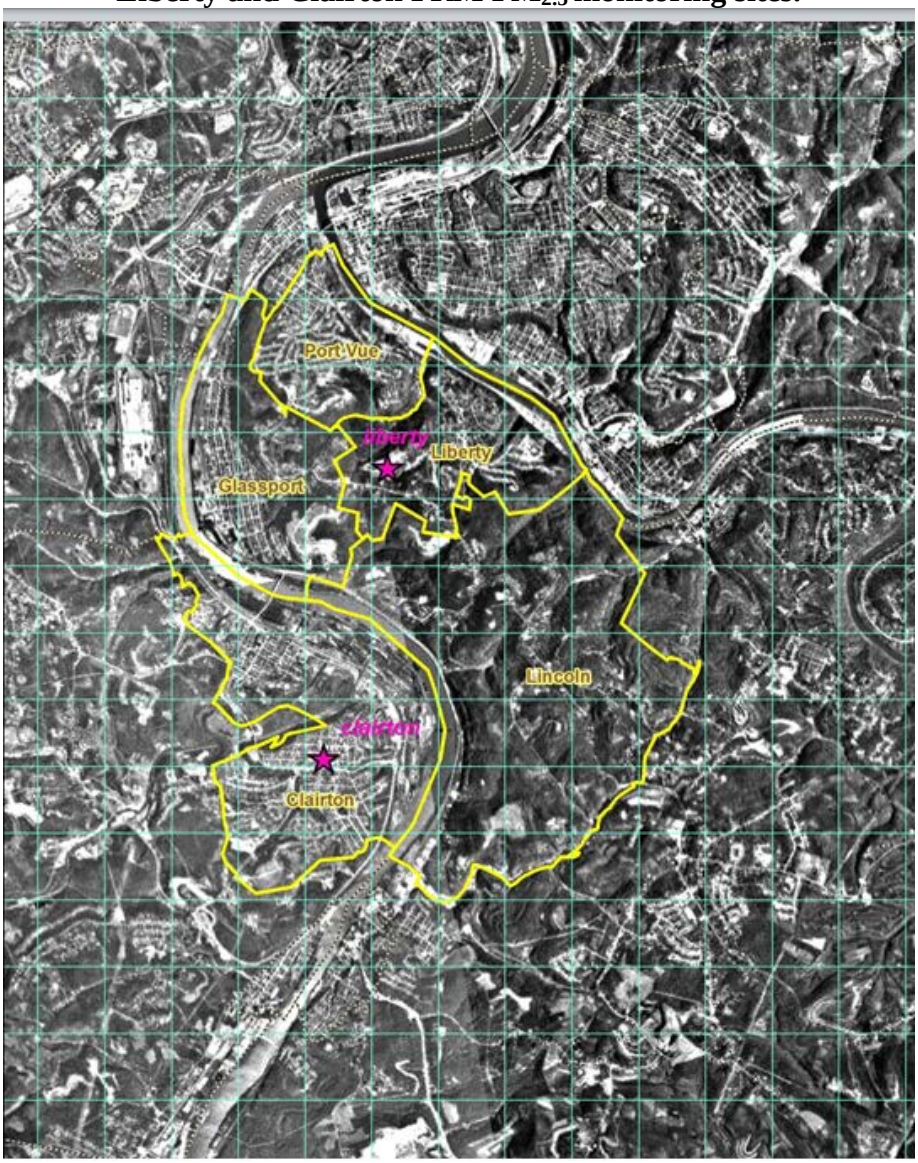
Figure 1: Relationship between the Liberty-Clairton NAA and the Pittsburgh-Beaver Valley NAA (gray area).



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 occur between hilltop and valley floor during clear, low-wind, nighttime conditions (e.g., differences of from 2 to 7°F). Strong nighttime drainage flows can cause differences of up to 180° in wind direction with 3-4 mph downslope flows. Also, strong nighttime inversions can lead to poor dispersion scenarios on several days of the year resulting in high hourly and 24-hour $PM_{2.5}$

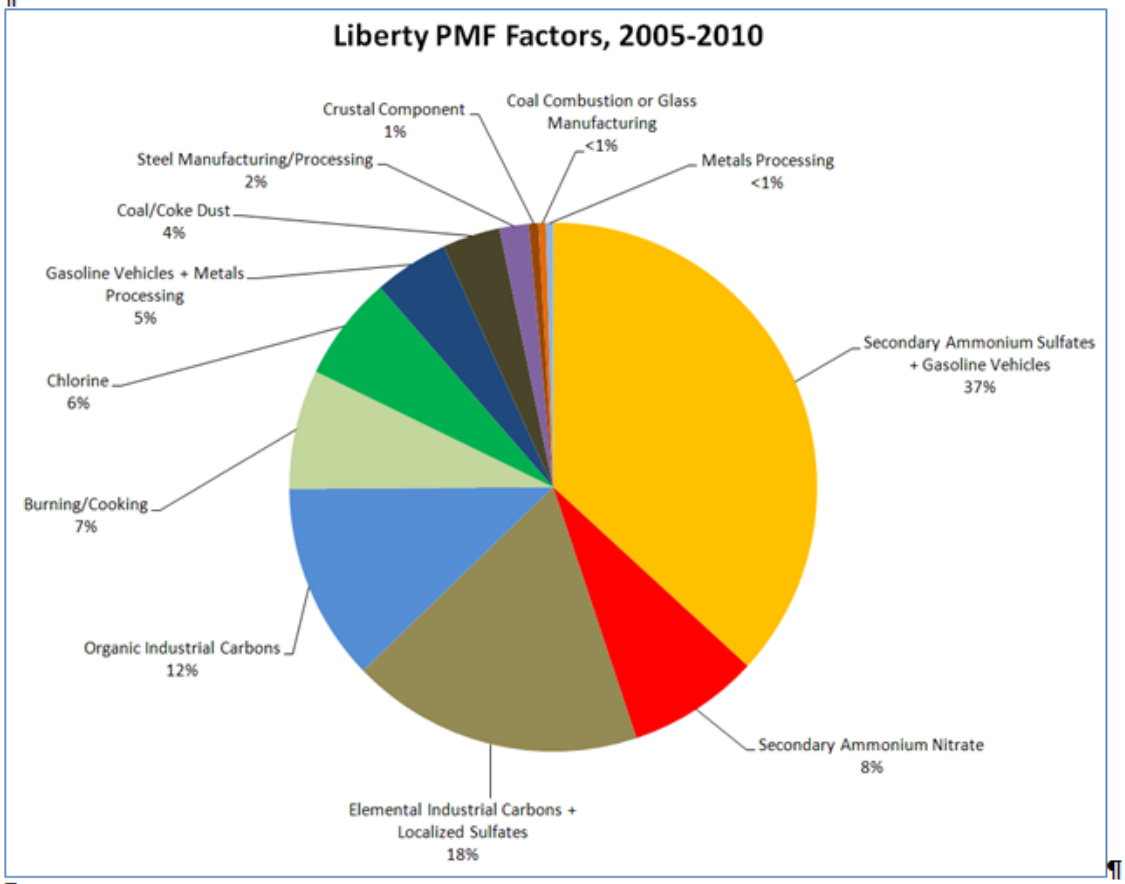
concentrations due to local sources. The Liberty-Clairton NAA is made up of the Boroughs of Lincoln, Liberty, Glassport and Port Vue and the City of Clairton as shown in Figure 2 along with the locations of the Liberty and Clairton FRM $PM_{2.5}$ monitoring sites.

Figure 2: Definition of the Liberty-Clairton NAA (yellow outline) and locations of the Liberty and Clairton FRM $PM_{2.5}$ monitoring sites.



Data analysis has shown that the Liberty-Clairton area is impacted by both regional and localized $PM_{2.5}$ concentrations. ACHD has performed $PM_{2.5}$ source apportionment analysis using the Positive Matrix Factorization (PMF) receptor model and the Liberty Chemical Speciation Network (CSN) speciated $PM_{2.5}$ monitoring data[3,4]. Figure 3 displays the $PM_{2.5}$ source contributions calculated by the PMF receptor model using 2005-2010 observations at the Liberty monitoring site[4]. Secondary sulfate is the largest contributor (36%) that is believed primarily from regional transport. The second largest contributor to $PM_{2.5}$ at Liberty is a PMF category that is believed to be mainly due to local sources and includes industrial carbon, primary sulfate and diesel combustion. Secondary nitrate is the next largest contributor (9%) followed by burning/cooking (7%). There are numerous other categories associated with local industrial sources that also contribute to $PM_{2.5}$ concentrations at Liberty (e.g., coke productions, metals and steel processing, coal/coke dust, etc.).

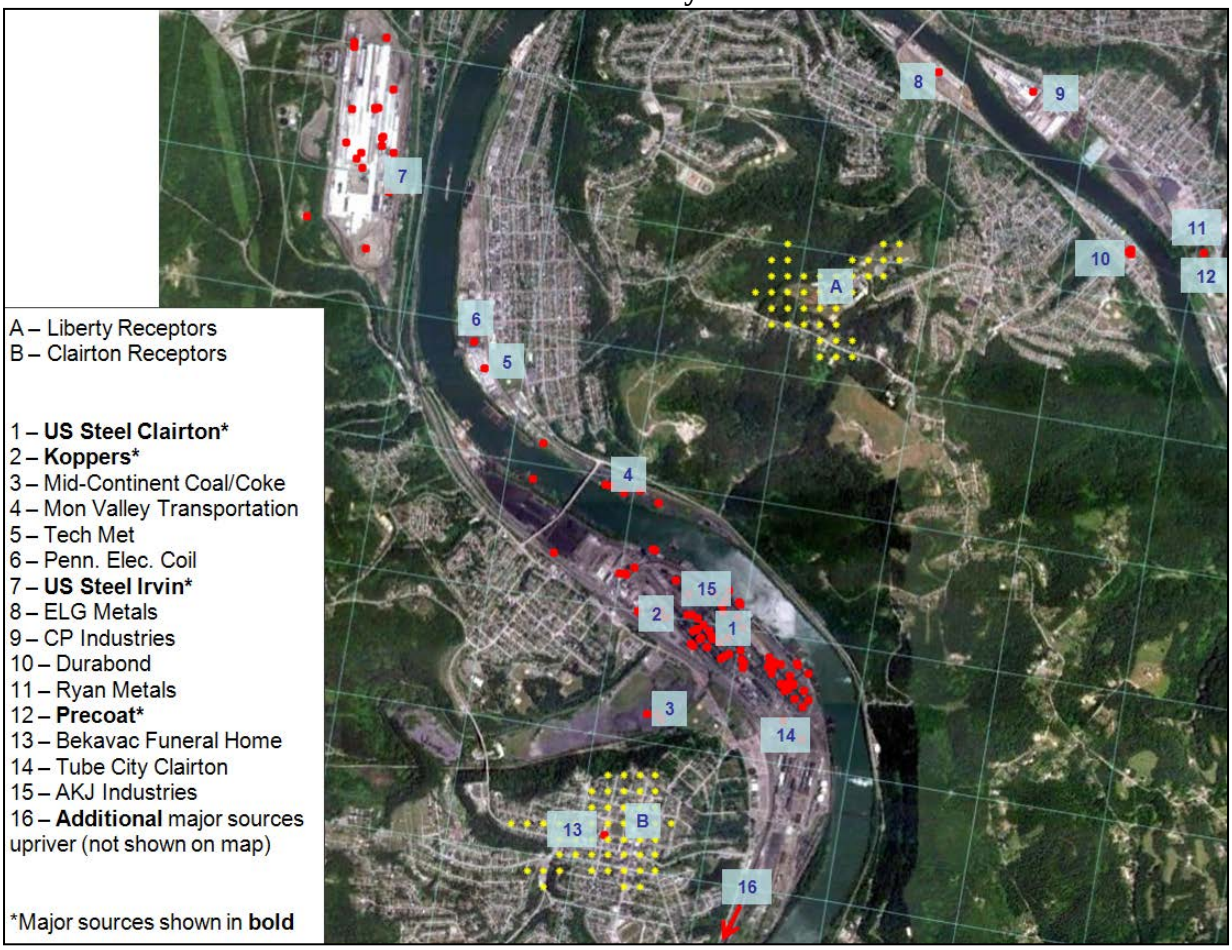
Figure 3: Results of ACHD Positive Matrix Factorization (PMF) receptor modeling PM2.5 source apportionment using the Liberty speciated $PM_{2.5}$ measurements[4].



The FRM $PM_{2.5}$ monitor at Liberty is located atop a school at relatively higher elevation near the north-center of the Liberty-Clairton area to the northeast of the Monongahela River. The FRM monitor at Clairton is located atop a school at relatively lower elevation in the western portion of the area west of the Monongahela River. In the Liberty-Clairton area there are numerous

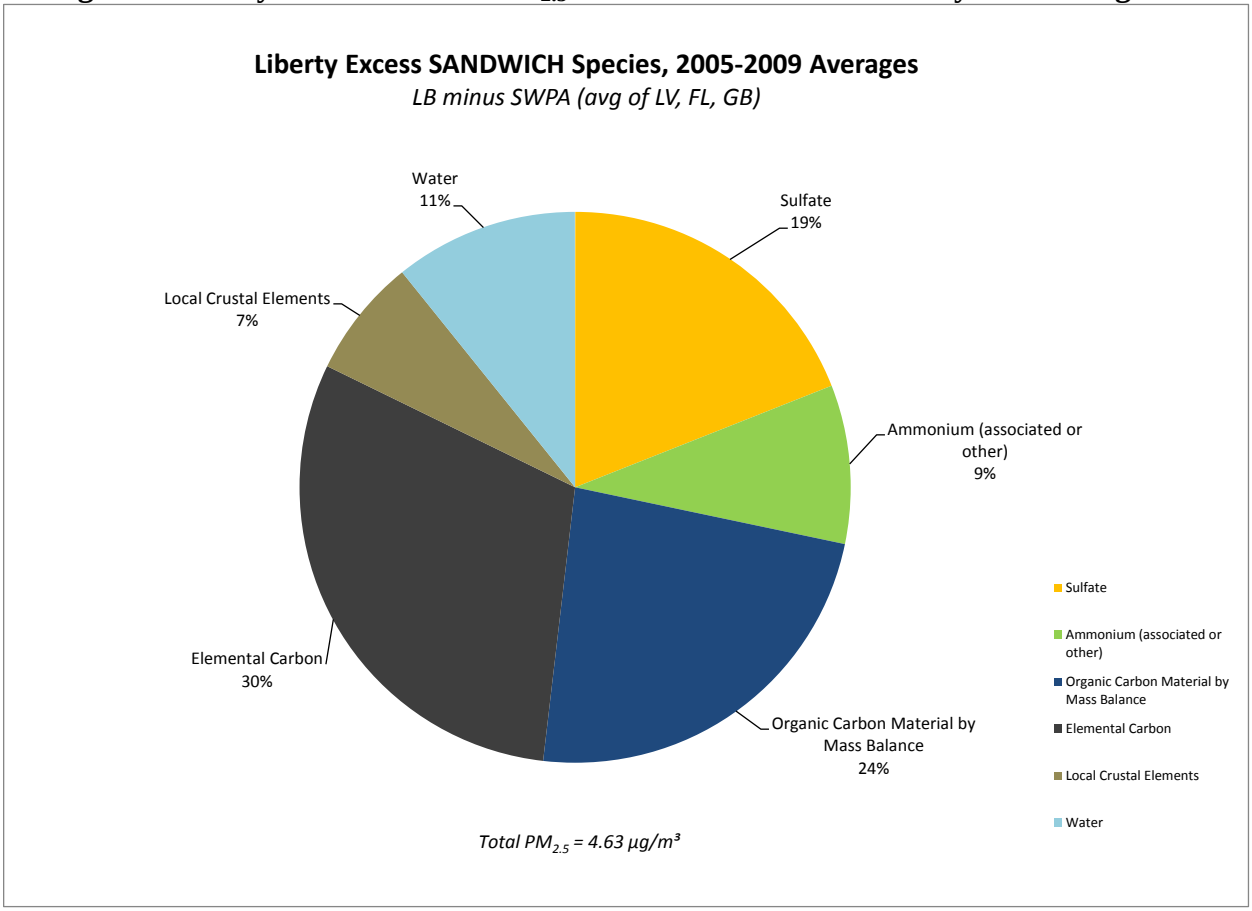
industrial sources with many located adjacent to the Monongahela River. Figure 4 displays the locations of the Liberty and Clairton FRM monitoring sites, the 100 m receptor network around the monitors used in the modeling and industrial sources in the region. Figure 4 highlights 5 high emitting local industrial facilities including US Steel Clairton and Koppers that are located to the southwest of Liberty so are aligned with the predominate wind direction from the southwest so that emissions from these sources are advected toward the Liberty monitor. Recent observations from 2008-2010 shows that the Clairton monitor is in attainment of the 2006 $PM_{2.5}$ NAAQS, while Liberty monitor is in violation of both the annual standard of 15 µg/m³ and the 24-hour standard of 35 µg/m³ based on 2008-2010 observations. Other FRM monitors located near the Liberty-Clairton area have monitored attainment of both standards.

Figure 4: Locations of the Liberty (A) and Clairton (B) FRM $PM_{2.5}$ monitoring sites and local sources in the Liberty-Clairton area.



ACHD analyzed the results from the Liberty $PM_{2.5}$ speciation monitor and found that organic and elemental carbon, ammonium, sulfate, particle bound water (PBW) and some trace elements are higher at the Liberty monitoring site than at other nearby monitoring sites with an annual average $PM_{2.5}$ concentration of approximately 4.6 µg/m³ attributed to local sources as shown in Figure 5 (4.1 µg/m³ local source contribution without PBW).

Figure 5: Analysis of the excess $PM_{2.5}$ concentrations at the Liberty monitoring site[4].



LIBERTY-CLAIRTON $PM_{2.5}$ MODELING APPROACH

The 2007 year was selected for the Liberty-Clairton $PM_{2.5}$ attainment demonstration modeling because it was the most appropriate year for modeling during the 2006-2008 three-year period used to designate the Liberty-Clairton as a $PM_{2.5}$ NAA. Three types of models were used in the Liberty-Clairton attainment demonstration modeling: meteorological, emissions and air quality models.

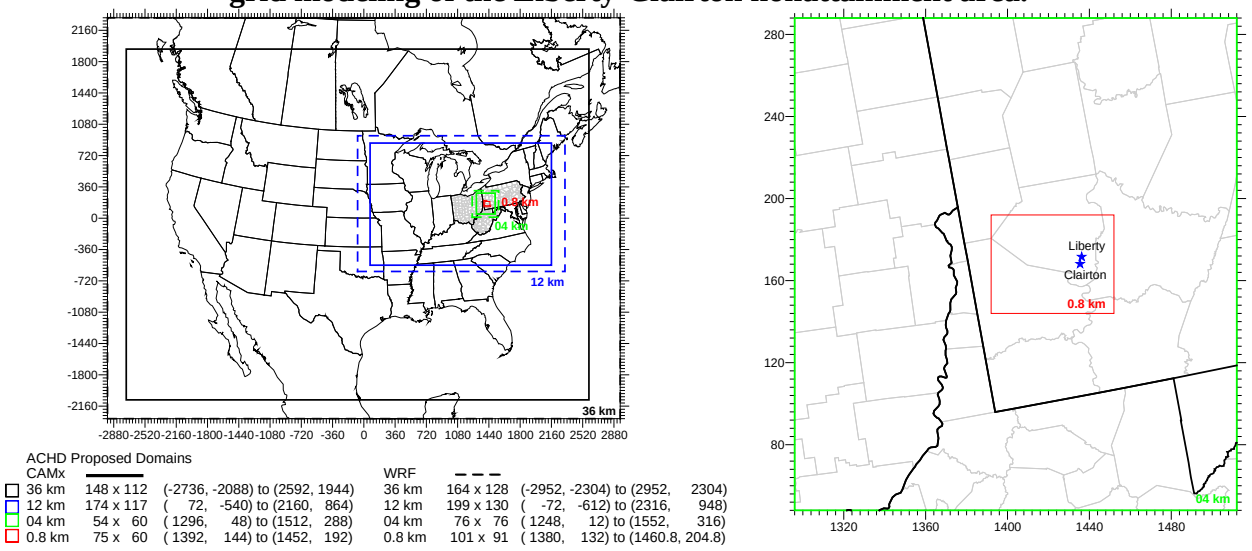
- The Weather Research and Forecasting (WRF[5]) meteorological model was selected to generate the 2007 three dimensional winds, temperature and other meteorological variables needed for air quality and emissions modeling.
- Emissions modeling was performed using the Sparse Matrix Operator Kernel Emissions (SMOKE[6]) modeling system. For on-road mobile sources the Motor Vehicle Emissions Simulator (MOVES[7]) model was used. Biogenic emissions were generated using the Biogenic Emissions Inventory System (BEIS[8]).
- The Comprehensive Air-quality Model with extensions (CAMx[9]) Photochemical Grid Model (PGM) was selected for the Liberty-Clairton attainment demonstration modeling

A preliminary 36/12/4/0.8 km domain structure was selected for the WRF and SMOKE/CAMx modeling as shown in Figures 6 and 7. The four domains use a Lambert Conic Conformal (LCC) projection. The LCC grid projection has a pole of projection of 40 degrees North, -97 degrees East and standard parallels of 33 and 45 degrees, the so-called RPO projection. The four domains are defined as given in Figure 6 and are as follows:

- A 36 km continental U.S. (CONUS) domain that is defined to be the standard RPO domain that is routinely used in many photochemical modeling studies.
- A 12 km NEUS domain that includes all of the states in the Midwestern and Northeastern U.S. that the Cross State Air Pollution Rule (CSAPR[10]) identified as contributing significantly to $PM_{2.5}$ nonattainment at Liberty. The CAMx revised 2007 base case simulation for the 36 km CONUS 12 km NEUS domains was performed using two-way grid nesting with the results post-processed to generate Boundary Conditions (BCs) for the 4 km SWPA domain.
- A 4 km domain that covers southwestern Pennsylvania (SWPA) and adjacent areas in West Virginia and Ohio.
- A nested grid of 0.8 km (800 m) for the area within and surrounding the Liberty-Clairton area. The 4 km and 0.8 km domains are run linked together using two-way grid nesting.

The WRF domains are defined to be slightly larger than the CAMx/SMOKE domains to eliminate any boundary artifacts in the WRF simulations from influencing the CAMx meteorological inputs.

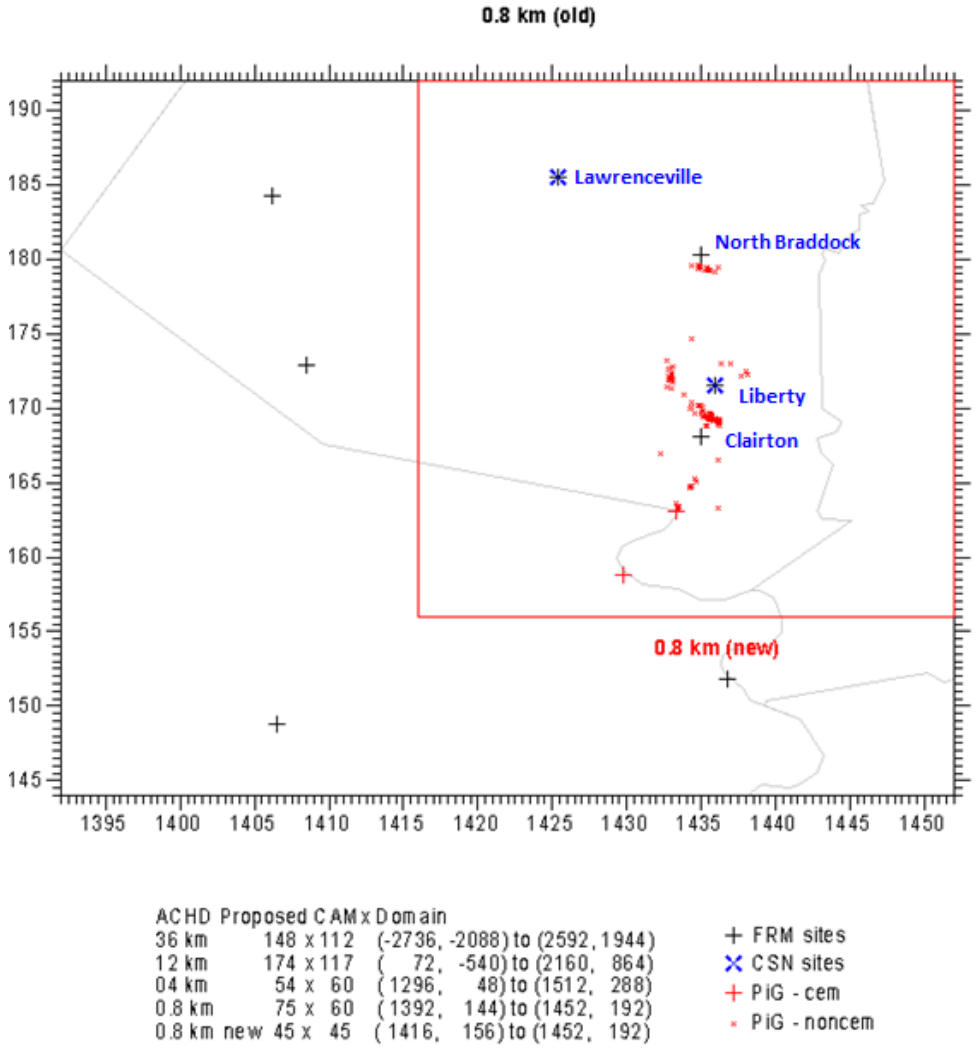
Figure 6: Definitions of the original 36/12/4/0.8 km (left) and 4/0.8 km (right) domain structure for the WRF meteorological (dotted lines) and CAMx (solid lines) photochemical grid modeling of the Liberty-Clairton nonattainment area.



Initial tests of CAMx using the 4/0.8 km two-way grid nesting configuration found the model run times for the 2007 calendar year simulation would be excessively long. To reduce the run time, the 0.8 km domain proposed in the Modeling Protocol[11] was reduced by approximately a factor of 2. Figure 7 displays the original proposed 75 x 60 0.8 km domain and the final 45 x 45 0.8

km domain used in the CAMx modeling. Also shown in Figure 7 are the locations of the Liberty, Clairton and two other Federal Reference Method (FRM) $PM_{2.5}$ monitoring sites (blue symbols) and the local sources (red symbols) showing large electrical generating units with continuous emissions monitoring (CEM) devices and other non-CEM industrial sources. The new 0.8 km domain still completely contains the Liberty-Clairton NAA and all monitoring sites and local sources of interest so the smaller 0.8 km domain does not in any way compromise the purpose for using the 0.8 km fine grid domain.

Figure 7: Comparison of the original proposed and final (red domain) 0.8 km modeling domains used in the Liberty-Clairton $PM_{2.5}$ attainment demonstration modeling. Also shown are the FRM $PM_{2.5}$ monitoring sites (blue symbols) and locations of the local sources (red symbols) treated by the Plume-in-Grid module.



2007 BASE CASE MODELING

CAMx modeling inputs were developed for the 2007 year and the 36/12/4/0.8 km modeling domains and a CAMx 2007 base case simulation performed that was subjected to a model performance evaluation.

2007 Base Case Input Development

Meteorological inputs for the 36/12/4/0.8 km domains and 2007 were generated using the WRF prognostic meteorological model[5]. The WRF meteorological model was evaluated by comparison the predicted surface wind speed, wind direction, temperature and water vapor mixing ratio with observations across the four modeling domains. The WRF precipitation fields were also compared against analysis fields based on observations from the Climate Prediction Center (CPC). The WRF model performance evaluation indicated that it was performing as good as or better than past meteorological model applications performed in support of attainment demonstration modeling studies in the past[12]. The WRF meteorological model output was processed using the WRFCAMx processor to generate meteorological inputs for the CAMx model.

The emissions databases used for the 2007 base year were provided by a variety of sources. The emissions data for the 0.8 km fine grid was developed and provided for modeling by ACHD. Emissions data for areas outside of the 0.8 km grid were provided by MARAMA, SEMAP, LADCO, and EPA. The emissions data were then processed with SMOKE to provide the hourly, gridded, speciated files required by CAMx. State emissions databases were provided by the following groups:

- MARAMA – Connecticut, Delaware, the District of Columbia, Maine, Maryland, Massachusetts , New Hampshire, New Jersey, New York, Pennsylvania, Rhode Island, Vermont, and Virginia.
- SEMAP/SESARM – Alabama, Florida, Georgia, Kentucky, Mississippi, North Carolina, South Carolina, Tennessee and West Virginia.
- Midwest RPO (LADCO) States – Illinois, Indiana, Michigan, Ohio and Wisconsin.
- EPA 2008 NEIv1.5 was used for all other states
- ACHD and TransSystems|Pechan provided emissions inventories for the local sources.
- Boundary Conditions (BCs) for the 36 km CONUS domain were generated by processing output from the Model for OZone And Related chemical Tracers (MOZART) global chemistry model[13]. More details on the CAMx 2007 base case modeling inputs can be found in the CAMx 2007 base case and model performance evaluation report[14].

CAMx Model Performance Evaluation

An updated version of the CAMx Version 5.4 (released in October 2011[9]) was used for the 2007 base case modeling. The update consisted of a correction to the CAMx in-line Tropospheric Ultraviolet and Visible (TUV) photolysis rate adjustment that attenuates photolysis rates based on the model estimated particulate matter concentrations. CAMx was first run for the 36/12 km

domains using Boundary Conditions (BCs) for the 36 km CONUS domain based on the MOZART global chemistry model. The CAMx 36/12 km model output was post-processed to generate BCs for the 4 km SWPA domain. CAMx was then exercised for the 2007 base case using two-way grid nesting with the 4/0.8 km modeling domains. Local sources were treated using the subgrid-scale Plume-in-Grid (PiG) module. The PiG module treats the early chemistry and dispersion of point source plumes using a Gaussian puff model. When the size of the PiG puff is commensurate with the size of the 0.8 km grid cell the mass from the puff is released to the photochemical grid model. The local sources were also tagged to be treated by the Particulate Source Apportionment Technology (PSAT) that tracked the contributions of the local sources to all particulate matter species except secondary organic aerosol (SOA) (i.e., treats sulfate, nitrate, ammonium and primary PM). SOA due to local sources was not tracked using the PSAT source apportionment tool due to the extremely small amount of SOA precursors from the local sources and the more extensive computational requirements of the SOA treatment in PSAT. The CAMx PiG puffs were sampled at 100 m receptors surrounding the Liberty and Clairton monitoring sites (see Figure 4). The total concentrations in each CAMx 0.8 km grid cell were obtained by averaging the live puffs sampling across all the receptors in a grid cell with the CAMx grid model estimate (0.8k_puffs). The CAMx concentration estimates without the local source contributions are obtained by subtracting the PSAT local source contribution from the CAMx grid model estimate (without live puff receptor contributions) (0.8k_nolocal). The local source $PM_{2.5}$ contribution can then be obtained by taking the difference between the 0.8k_puffs and 0.8k_nolocal concentration estimates.

The CAMx 36/12/4/0.8 km modeling results were compared against measured ambient concentrations as part of a model performance evaluation. CAMx was evaluated for total $PM_{2.5}$ mass, speciated $PM_{2.5}$ (e.g., sulfate, nitrate, ammonium, EC, OA and other $PM_{2.5}$), ozone and $PM_{2.5}$ precursor and product species (e.g., NO_X, SO_2, HNO_3 and wet sulfate, nitrate and ammonium deposition). Details of the CAMx 2007 base case model performance evaluation is presented in the CAMx base case and model performance evaluation report[14], with a summary for total $PM_{2.5}$ mass model performance given below.

Total $PM_{2.5}$ mass is evaluated using observed data from the FRM, CSN and IMPROVE networks and at the Liberty TEOM monitoring site. Table 1 displays the annual fractional bias and error performance statistics across the FRM network in the 12, 4 and 0.8 km domains using the 24-hour total $PM_{2.5}$ mass measurements and compares them with the PM Performance Goals and Criteria[15,16,17] developed by the Regional Planning Organizations (RPOs) to support the development of visibility SIPs. CAMx is exhibiting very low fractional bias (FB) for FRM $PM_{2.5}$ with FB values of +10.5%, +4.6%, and +4.1% for the 12 , 4 and 0.8 km domains, respectively, that not only achieves the PM Performance Goal for bias ($\leq \pm 30\%$) but also achieves the more stringent ozone Performance Goal ($\leq \pm 15\%$) for bias[18]. The FRM $PM_{2.5}$ fractional error is between 35% and 40% across the three domains, which achieves the PM Performance Goal by a fair margin ($\leq 50\%$), although it is slightly above the more stringent ozone Performance Goal ($\leq 35\%$). Similar good annual $PM_{2.5}$ model performance statistics are seen across the CSN and IMPROVE monitoring network with FB (-10% to +4%) and FE (38% to 43%) that achieves the PM Performance Goals by a wide margin (Table 2).

Table 1. Comparisons of annual FRM $PM_{2.5}$ fractional bias and error performance statistics with the PM Performance Goals and Criteria for the 12, 4 and 0.8 km domains and the CAMx revised 2007 base case simulation.

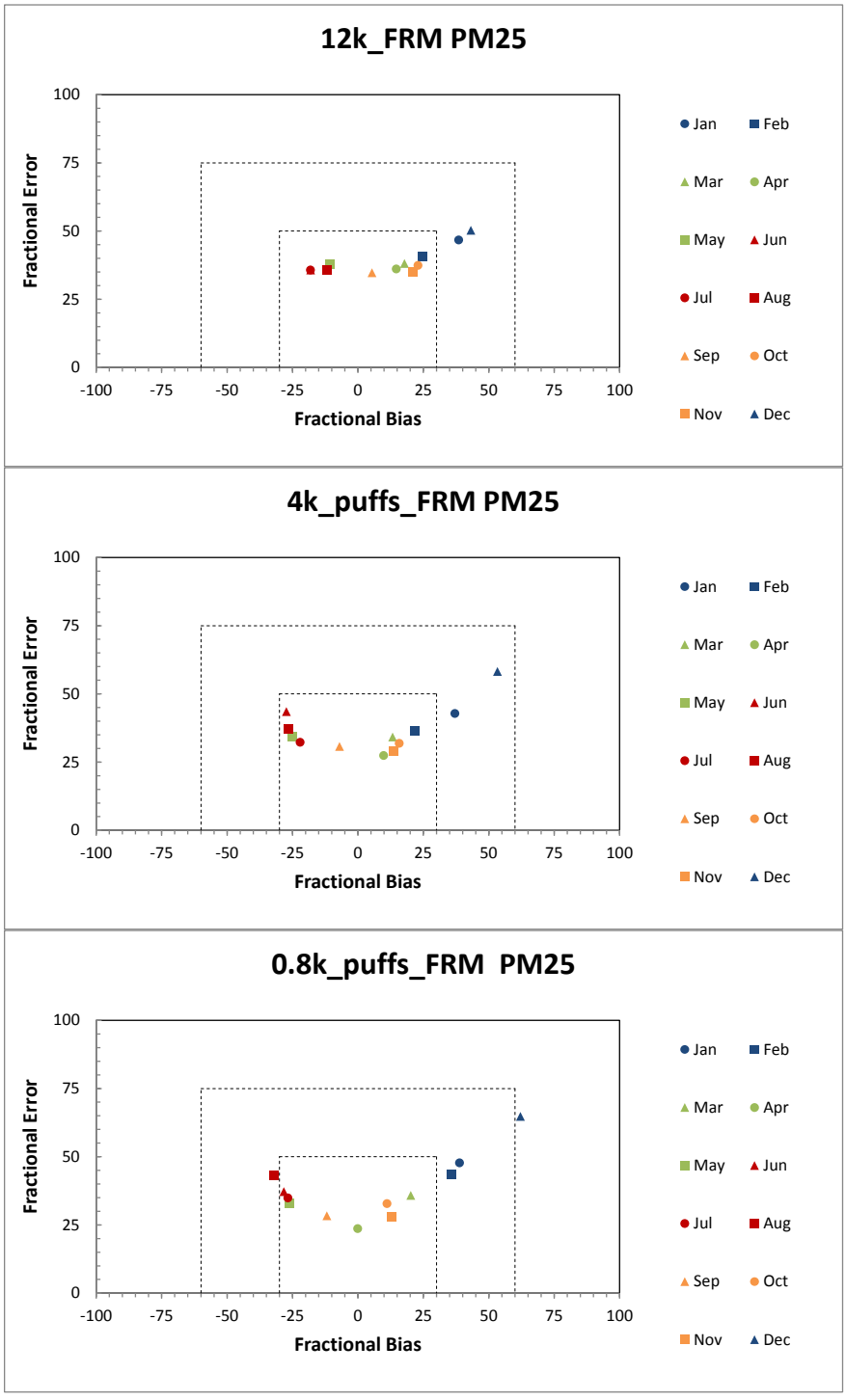
Domain	Number Sites	Fractional Bias	Fractional Error
Performance Goal		≤±30%	≤50%
Performance Criteria		≤±60%	≤75%
12 km Domain	536	+10.5%	38.5%
4 km Domain	30	+4.6%	36.2%
0.8 km Domain	4	+4.1%	37.8%

Table 2. Comparisons of annual CSN and IMPROVE $PM_{2.5}$ fractional bias and error performance statistics for the CAMx revised 2007 base case simulation with the PM Performance Goals and Criteria for the 12, 4 and 0.8 km domains.

Domain	Number Sites	Fractional Bias	Fractional Error
Performance Goal		≤±30%	≤50%
Performance Criteria		≤±60%	≤75%
CSN			
12 km Domain	110	+3.2%	38.7%
4 km Domain	8	-9.5%	39.1%
0.8 km Domain	2	-8.9%	40.0%
IMPROVE			
12 km Domains	40	+4.1%	43.2%
4 km Domain	3	+3.1%	38.3%

Soccer plots, which display monthly fractional bias (FB) versus fractional error (FE) performance metrics along with the PM Performance Goals and Criteria, for the FRM network in the 12, 4 and 0.8 km domains are shown in Figure 8. The CAMx $PM_{2.5}$ monthly modeling performance across the FRM sites in the 12, 4 and 0.8 km domains achieves the PM Performance Criteria for all months and domains except for December within the 0.8 km domain whose error just barely exceeds the 75% Performance Criteria. Across the 12 km domain, the FRM $PM_{2.5}$ monthly performance exhibits a slight summer underestimation and winter overestimation bias with 10 out of the 12 months achieving the PM Performance Goals; the two months that the CAMx 12 km FRM performance fails to achieve the PM performance goal are December and January that exhibit an overestimation bias such that they fall between the PM Performance Goals and Criteria. Similar performance across the FRM monitors is seen for the CAMx 4 km modeling results with all months achieving the PM Performance Criteria and 10 of 12 months achieving the PM Performance Goal with again January and December being the two months whose performance statistics fall between the PM Performance Goals and Criteria. The CAMx FRM $PM_{2.5}$ performance degrades a little bit across the 0.8 km domain with 8 out of 12 months achieving the PM Performance Goals. The summer underestimation bias increases in the 0.8 km domain modeling so that one month (August) falls just outside of the PM Performance Goal and the winter overestimation bias increases so that the three winter months falling outside of the PM Performance Goal with the overestimation bias for December being so large that it falls just outside of the PM Performance Criterion for Fractional Bias.

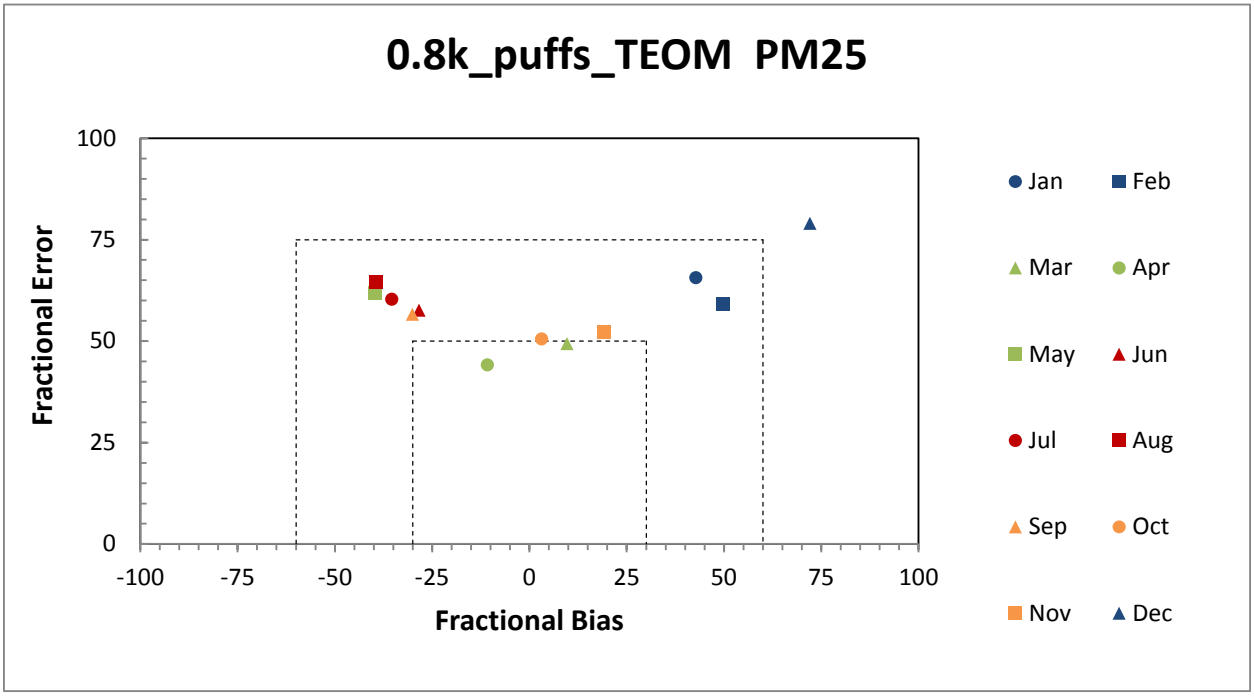
Figure 7: Soccer Plots comparing FRM $PM_{2.5}$ monthly FB and FE with the PM Performance Goals and Criteria for the 12 km (top), 4 km (middle) and 0.8 km (bottom) domains.



$PM_{2.5}$ is measured at the Liberty monitoring site using the FRM, CSN and TEOM measurement technology. The CAMx 0.8k_puffs annual performance for 24-hour $PM_{2.5}$ concentrations achieves the PM Performance Goals using the FRM and CSN monitors. The CAMx annual bias (FB) performance for hourly $PM_{2.5}$ using TEOM is near zero and achieves the PM Performance Goal. However, the TEOM hourly $PM_{2.5}$ annual error (FE) exceeds the PM Performance Goal, although the TEOM FE at Liberty it does achieve the PM Performance Criterion. It should be pointed out that the PM Performance Goals and Criteria were developed for 24-hour $PM_{2.5}$ concentrations and one would expect higher error when examining hourly $PM_{2.5}$ concentrations.

Figure 8 displays a soccer plot of monthly FB and FE using the TEOM hourly $PM_{2.5}$ data at Liberty. The Liberty monitoring site $PM_{2.5}$ exhibits the same summer underestimation and winter overestimation bias as seen across all sites in the three modeling domains (Figure 7). The Liberty TEOM $PM_{2.5}$ FB/FE meets the PM Performance Criteria for all months but December, which fails to achieve the PM Performance Criteria due to a too high overestimation bias and too high of an error. The FB for the transition months of March, April, October and November achieves the PM Performance Goal with the FE right at the PM Performance Goal. The warmer months of May through September have an FB underestimation that falls between the PM Performance Goal and Criterion. Whereas the cooler months of December, January and February have an FB overestimation that fails to achieve the PM Performance Goal.

Figure 8. Monthly soccer plot for TEOM hourly $PM_{2.5}$ concentrations at the Liberty monitor using the CAMx 0.8 km revised 2007 base case modeling results.



The ACHD performed an analysis to estimate the excess $PM_{2.5}$ concentrations at Liberty compared to surround monitoring sites and found that Liberty was on average 4.1 $\mu g/m^3$ higher than the surrounding sites (without accounting for particle bound water, PBW), which they attributed to local sources[4]. The CAMx annual average $PM_{2.5}$ concentrations due to local sources in 2007 was obtained by the sampling of the local sources PiG live puffs at receptors near Liberty and the local source PSAT contributions at Liberty and found CAMx estimated 3.1 $\mu g/m^3$ $PM_{2.5}$ contribution due to local sources at Liberty (also not accounting for PBW); which is ~24% lower than the ACHD estimate based on analysis of observations. Note that we expect the CAMx local source contribution to be lower than observed because the CAMx PSAT source apportionment tool traces the $PM_{2.5}$ components back to their primary precursor so that $PM_{2.5}$ components that are associated with the local source emissions but not emitted by them will not be attributed to the local sources (e.g., the ammonium component of the local source ammonium sulfate and ammonium nitrate contributions). Thus, the CAMx 0.8 km modeling results with PiG and PSAT is providing a reasonable estimate of the contributions of local sources to annual average $PM_{2.5}$ concentrations at Liberty, albeit with an underestimation bias.

2014 MODELING AND FUTURE-YEAR $PM_{2.5}$ PROJECTIONS

CAMx was exercised for a 2014 base case emissions scenario using the same model configuration as the 2007 base case (i.e., use of 36/12 km and 4/0.8 km two-way grid nests and treating local sources using the PiG module and PSAT tool). The 2014 remedy emissions scenario from the Cross State Air Pollution Rule (CSAPR[10]) was the basis for the 2014 base case emissions scenario with local source updates provided by ACHD. In addition to the CAMx model configuration, several inputs to CAMx were held constant between the 2007 and 2014 base case simulations: MOZART 2007 BCs for the 36 km CONUS domain; WRF 2007 meteorological conditions; biogenic emissions from SMOKE-BEIS; sea salt emissions; and emissions from fires (wildfires, prescribed burns and agricultural burning).

The CAMx 2007 and 2014 base case modeling results were used to make 2014 $PM_{2.5}$ Design Values (DV) projections at the Liberty monitoring site three ways:

- Total Species Approach: Use of the CAMx grid model 2007 and 2014 concentration estimates for the grid cell containing the Liberty monitoring site plus the CAMx PiG live puff concentrations at the receptor located at the Liberty monitoring site to make 2014 $PM_{2.5}$ DV projections at Liberty using spreadsheets;
- Regional/Local Species Approach: Use of the CAMx grid model 2007 and 2014 concentration estimates for the grid cell containing the Liberty monitoring site with the PSAT local source contributions removed to projected the regional component of the DV and the 2007 and 2014 CAMx PiG plus PSAT estimates at the Liberty monitoring site to project the local component of the DV at Liberty and combining the regional and local components of the projected 2014 DVs; and
- MATS Approach: Use of the CAMx grid plus average live PiG puff receptor (0.8k_puffs and 4k_puffs) modeling results to project $PM_{2.5}$ DVs at all FRM monitoring sites using the Modeled Attainment Test Software (MATS[19]) version 2.5.1.

All three methods used the EPA recommended[20] Speciated Modeled Attainment Test (SMAT) to project observed current year $PM_{2.5}$ DV to 2014 using the relative changes in the CAMx modeling results between 2007 and 2014. The observed $PM_{2.5}$ DVs based on the FRM observations were speciated using the SANDWICH[21] (sulfate, adjusted nitrate, derived water, inferred carbonaceous material balance approach) observed $PM_{2.5}$ speciation data. The first two modeled attainment demonstration methods above were performed for the Liberty and Clairton sites using the FRM DVs at the two sites and the Liberty CSN $PM_{2.5}$ speciation data. The third approach applied MATS to all FRM monitoring sites in the 0.8 km and 4 km modeling domains using default MATS options and data, except for removal of Liberty CSN data for two quarters when there were data capture issues and capping the Liberty Sea Salt concentrations at 0.1 $\mu g/m^3$ to remove anomalous values. MATS was also used to perform an unmonitored area analysis (UAA) for annual $PM_{2.5}$ DVs; note that MATS does not contain a capability to perform a UAA for 24-hour $PM_{2.5}$ DVs.

Using the three methods, the projected 2014 24-hour $PM_{2.5}$ DV at Liberty were in the 31-35 $\mu g/m^3$ range that is right below the 2006 24-hour $PM_{2.5}$ NAAQS (36 $\mu g/m^3$ or higher) so demonstrated attainment of the $PM_{2.5}$ NAAQS. The projected 2014 24-hour $PM_{2.5}$ DVs at all other monitoring sites, as well as projected 2014 annual $PM_{2.5}$ DVs, were all even further below the NAAQS than seen at Liberty. Details on the 2014 $PM_{2.5}$ DV projections are provided in the Liberty-Clairton PM2.5 SIP Air Quality Technical Support Document (AQTSD[22]).

SUMMARY

$PM_{2.5}$ attainment demonstrations modeling was conducted using a hybrid grid/plume modeling approach based on the CAMx photochemical grid model that was able to simulate the contributions due to: (1) local sources using a Plume-in-Grid (PiG) module and high (0.8 km) resolution grid; (2) urban sources in and around Pittsburgh using a 4 km grid; (3) regional eastern U.S. sources using a 12 km grid resolution; (4) continental U.S. sources using a 36 km grid resolution; and (5) international sources using output from a global chemistry model. The multiscale hybrid CAMx integrated grid/plume modeling approach was applied for a 2007 base case and reproduced the observed $PM_{2.5}$ concentrations to within PM model performance goals and criteria. The results from the CAMx 2014 and 2007 simulations were used to project 2014 future $PM_{2.5}$ Design Values that were below the 2006 $PM_{2.5}$ NAAQS thereby demonstrating attainment of the $PM_{2.5}$ NAAQS.

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KEY WORDS

Particulate Matter

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CAMx