1.0 INTRODUCTION

1.1 BACKGROUND

On December 17, 2004, the United States Environmental Protection Agency (EPA) made fine particle ($PM_{2.5}$) nonattainment area determinations. The St. Louis region was declared a $PM_{2.5}$ nonattainment area with a compliance date of 2010 unless a State demonstrates that more time is necessary in which case up to five additional years may be granted. The nonattainment designations triggered the requirement to develop a State Implementation Plans (SIPs) that were due in April 2008. A significant requirement of $PM_{2.5}$ SIPs is an attainment demonstration using, at least in part, modeling analyses to define effective emissions control strategies and confirm that attainment can be achieved after implementation of the strategies by the attainment date.

The St. Louis 8-Hour Ozone and $PM_{2.5}$ Modeling Study was conducted to address the need to demonstrate attainment of the $PM_{2.5}$ National Ambient Air Quality Standard (NAAQS) for the $PM_{2.5}$ SIP, as well as similar needs to demonstrate attainment of the 8-hour ozone NAAQS for the 8-hour ozone SIP that was submitted by the department in June 2007. One of the primary goals of the St. Louis 8-Hour Ozone and $PM_{2.5}$ Modeling Study was to develop photochemical modeling data bases and allied analysis tools necessary to reliably simulate the processes responsible for 8-hour ozone and $PM_{2.5}$ exceedances in the region and to assist the States of Missouri and Illinois in their development of realistic emissions reduction strategies for inclusion in the St. Louis 8-hour ozone and $PM_{2.5}$ SIPs. The St. Louis 8-Hour ozone and $PM_{2.5}$ Modeling Study was conducted in three Phases. The first Phase of the study, which was performed primarily in 2005, focused on the development of photochemical modeling databases for three ozone episodes from 2002 using a 36/12/4 km grid. In 2006, Phase II of the study completed the ozone attainment demonstration modeling for the three 2002 ozone episodes, prepared an air quality Technical Support Document (TSD) for the June 2007 St. Louis 8-hour ozone SIP and began 2002 36/12 km annual modeling to address the $PM_{2.5}$ NAAQS attainment demonstration. Under Phase III of the study, performed in 2007, future-year $PM_{2.5}$ modeling was conducted using a 36/12 km regional 2002 database to project 2009 and 2012 $PM_{2.5}$ Design Values. Although the preliminary regional modeling for 2009 indicated that most $PM_{2.5}$ monitoring sites would achieve the $PM_{2.5}$ NAAQS, one sites still was projected to exceed the $PM_{2.5}$ NAAQS due to the contribution of local sources. Thus, $PM_{2.5}$ attainment in St. Louis will be addressed in two components. The first component is a regional component that is discussed in this TSD which uses the regional 36/12 km modeling database. It is important to note that the monitor projected to be in violation is located in the Illinois portion of the St. Louis area and the "local" PM sources contributing to this projected violation are under the jurisdiction of the Illinois Environmental Protection Agency (IEPA). Therefore, the local component that will examine the contributions of local sources is being conducted by IEPA and will be submitted at a later date.

This Technical Support Document (TSD) describes the regional modeling activities performed by the Missouri Department of Natural Resources (MDNR), Illinois Environmental Protection Agency (IEPA), the St. Louis Modeling and Data Analysis Workgroup (MDAW) and ENVIRON International Corporation to develop the regional component of the $PM_{2.5}$ attainment demonstration for the St. Louis nonattainment area (NAA).

1.2 STATE AGENCY ORGANIZATIONS AND WORK GROUPS

The States of Missouri and Illinois determined the committee structure described below that was used to manage the development and evaluation of control strategies, research, modeling, and other activities:

- **State Air Agencies**: Responsible for providing policy direction and guidance, selecting achievable emissions strategies, and resolving disputes as they arose. The State Air Agencies met as appropriate to oversee the progress of the effort. The Missouri Air Conservation Commission has final authority to adopt Missouri's control plan. Similarly, the Illinois Pollution Control Board has the final authority to adopt control requirements in Illinois.

  Participants: Air Directors from Missouri DNR and Illinois EPA.

- **Modeling and Data Analysis Workgroup (MDAW):** Responsible for the planning and management of the technical work necessary to demonstrate attainment, including emissions, meteorological, and photochemical modeling. The Workgroup was also responsible for contractor selection, data analysis, source apportionment, coordination and communication of model results to AQAC, the Control Strategy Development Workgroup, and the State Agency Air Directors. The Modeling and Data Analysis Workgroup met on a regular basis to coordinate the development and performance of technical activities. Meetings were open to stakeholders and representatives from local agencies having the technical expertise to contribute to work activities.

  Participants: IEPA, MDNR, U.S. EPA Region VII, U.S. EPA Region V, and East-West Gateway. Local organizations, stakeholders, and academics that were able to contribute technical capabilities or resources were also invited to participate.

- **Air Quality Advisory Committee (AQAC):** Served as a forum for communication and outreach between local governmental agencies, stakeholders, the MDAW, Control Strategy Development Workgroup, and the State Agency Air Directors. The AQAC met on a regular basis, and was also responsible for identifying emissions control options for evaluation by the Control Strategy Development Workgroup, for developing conformity budgets, and preparing conformity demonstrations that are consistent with the 8-hour ozone and $PM_{2.5}$ SIPs. The Modeling and Data Analysis Workgroup, the Control Strategy Development Workgroup, and, when possible, the State Agency Air Directors, were present at the meetings to report on activities, and to solicit input on control strategy recommendations.

  Participants: East West Gateway, MDNR, IEPA, U.S. EPA Regions 5 and 7, St. Louis County, St. Louis City, Federal Highway Administration, Missouri Department of Highway and Transportation (MDHT), Illinois Department of Transportation (IDOT), Federal Highway Administration (FHWA), Environmental Groups, Industry, and other local representatives.

- **Control Strategy Development Workgroup (CSDW):** Responsible for the identification and technical evaluation of control strategies needed to demonstrate

attainment of the $PM_{2.5}$ standards, and meet other regulatory requirements; this included preparation of emissions inventories, development of growth and control factors, tracking of control requirements required by the Clean Air Act, identification of other control measures, and evaluation of feasibility and costs. The CSDW was also responsible for coordination and communication of strategies and technical information to AQAC, the MDAW, and the State Agency Air Directors. The CSDW met on a regular basis to coordinate the performance of technical activities. Meetings were open to stakeholders and representatives from local agencies having the technical expertise to contribute to work activities.

Participants: IEPA, MDNR, U.S. EPA Region VII, U.S. EPA Region V, East-West Gateway. Local organizations, stakeholders, and academics that were able to contribute technical capabilities or resources were also invited to participate.

1.3 OVERVIEW OF APPROACH

1.3.1 Modeling Protocol

The St. Louis $PM_{2.5}$ Study meteorological, emissions and regional air quality modeling followed the procedures outlined in the Modeling Protocol (ENVIRON and Alpine Geophysics, 2005). The Modeling Protocol addressed attainment demonstration modeling for both the 8-hour ozone and $PM_{2.5}$ standards and describes the overall modeling activities performed by the MDNR, IEPA, EPA Region 7, Ameren and the MDAW as well as the modeling contractor. Its main function was to serve as a means for planning and communicating how the modeled attainment demonstrations would be performed. The protocol guided the technical details of the modeling study and provided a formal framework within which the scientific assumptions, operational details, commitments and expectations of the various participants were communicated explicitly. The modeling protocol also set forth means for resolution of potential differences of technical and policy opinion to be worked out openly and within prescribed time and budget constraints.

1.3.2 Model Selection

The model selection methodology for the St. Louis $PM_{2.5}$ modeling rigorously adhered to EPA's guidance for regulatory modeling in support of ozone and fine particulate attainment demonstrations (EPA, 1991; 1999; 2005; 2006; 2007). Unlike previous modeling guidance, the agency now recommends that models be selected for SIP studies on a 'case-by-case' basis with appropriate consideration being given to the candidate model's

- Technical formulation, capabilities and features,
- Pertinent peer-review and performance evaluation history,
- Public availability, and
- Demonstrated success in similar regulatory applications.

Detailed discussion of the selection process for each model component may be found in the Modeling Protocol (ENVIRON and Alpine Geophysics, 2005). Here follows a brief summary of each of the model components and a description of how it fits into the St. Louis $PM_{2.5}$ modeling.

- **MM5:** The Mesoscale Meteorological Model (MM5) was developed by the National Center for Atmospheric Research and Pennsylvania State University and is a nonhydrostatic, prognostic meteorological model routinely used for urban- and regional-scale photochemical, fine particulate, and regional haze regulatory modeling studies (Dudhia, 1993; Seaman, 2000). Developed in the 1970s, the MM5 modeling system maintains its status as a state-of-the-science model through enhancements provided by a broad user community worldwide (Stauffer and Seaman, 1990; Xiu and Pleim, 2000; Byun et al., 2005a,b). MM5 is used nearly exclusively for regulatory air quality applications in the U.S. In recent years, the modeling system has been successfully applied in continental-scale annual simulations. MM5 is being replaced by the Weather Research Forecasting model, which is just beginning to be used for air quality studies.

- **SMOKE**: The Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system is an emissions modeling system that generates hourly gridded speciated emission inputs of mobile, nonroad, area, point, fire and biogenic emission sources for photochemical grid models (Coats, 1995; Houyoux et al., 2000). As with most 'emissions models', 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, modern tool for converting emissions inventory data into the formatted emission files required by an air quality simulation model. For mobile sources, SMOKE actually simulates emissions rates based on input mobile-source activity data, emission factors and outputs from transportation travel-demand models.

- **CMAQ:** EPA's Models-3/Community Multiscale Air Quality (CMAQ) modeling system is also 'One-Atmosphere' photochemical grid model capable of addressing ozone, particulate matter (PM), visibility and acid deposition at regional scale for periods up to one year (Byun and Ching, 1999). The CMAQ modeling system was designed to approach air quality as a whole by including state-of-the-science capabilities for modeling multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation. CMAQ was also designed to have multi-scale capabilities so that separate models were not needed for urban and regional scale air quality modeling. The CMAQ modeling system contains three types of modeling components: a meteorological module for the description of atmospheric states and motions, an emission models for man-made and natural emissions that are injected into the atmosphere, and a chemistry-transport modeling system for simulation of the chemical transformation and fate.

- **CAMx:** The Comprehensive Air Quality Model with Extensions (CAMx) modeling system is a state-of-science 'One-Atmosphere' photochemical grid model capable of addressing ozone, particulate matter (PM), visibility and acid deposition at regional scale for periods up to one year (ENVIRON, 2006). The Comprehensive Air quality Model with extensions is a publicly available open-source computer modeling system for the integrated assessment of gaseous and particulate air pollution. Built on today's understanding that air quality issues are complex, interrelated, and reach beyond the urban scale, CAMx is designed to simulate air quality over many geographic scales; treat a wide variety of inert and chemically active pollutants including ozone, inorganic and organic $PM_{2.5}$ and PM_{10}, and mercury and toxics;

provide source-receptor, sensitivity, and process analyses; and be computationally efficient and easy to use. The U.S. EPA has approved the use of CAMx for numerous ozone and PM SIPs throughout the U.S, and has used this model to evaluate regional mitigation strategies.

The MM5 meteorological model was applied to generate the meteorological fields used with the SMOKE emissions and CMAQ/CAMx air quality models. The MM5 meteorological modeling was conducted in a similar fashion as was done for the CENRAP visibility modeling (Johnson, 2007) and the St. Louis ozone modeling. The following table illustrates the physics options selected for the 36/12km MM5 analyses. The configure.user file for the MM5 analyses and an example MM5.deck file are included in TSD Appendix D to provide additional documentation.

Physics Option	Selection	Configure.user file
Moisture	Mixed Phase (Reisner 1)	IMPHYS = 5,5 (MPHYSTBL=0)
Cumulus Parameterization	Kain-Fritsch 2	ICUPA = 8,8
Planetary Boundary Layer	Pleim-Xiu	IBLTYP=7,7
Radiation	RRTM	FRAD=4,4
Land Surface Model	Pleim-Xiu	ISOIL=3
Shallow Convection	No	ISHALLO=0,0
Nudging	Surface=Yes Analysis=Yes	FDDAGD=1

Emissions were generated by processing the Central Regional Air Partnership (CENRAP) base emissions (Strait, Roe and Vuckovich, 2004; Reid et al., 2004a,b) along with emissions from the Midwest Regional Planning Organization (MRP01 and Visibility Improvements States and Tribes of the Southeast (VISTAS) using the SMOKE emissions modeling system. Both EPA's Models-3 Community Multiscale Air Quality (CMAQ; Byun and Ching, 1999) modeling system and the Comprehensive Air-quality Model with extensions (CAMx; ENVIRON, 2006) air quality models were applied to the 2002 annual period on a 36/12 km grid to make future-year $PM_{2.5}$ projections in the St. Louis NAA. The application of the CMAQ/CAMx air quality models benefited from the extensive testing and evaluation conducted by CENRAP (Morris et al., 2005c; 2007), VISTAS (ENVIRON et al., 2003b,c,d; Morris et al., 2004a,b,c; 2005a,b; 2007), MRPO (Baker, 2004) and St. Louis 8-hour ozone modeling. The CMAQ/CAMx model application followed the relevant guidance documents (EPA, 1991; 1999; 2001; 2003a,b; 2005; 2006; 2007a).

1.3.3 Modeling Domains

The St. Louis regional $PM_{2.5}$ modeling was conducted on a 36/12 km modeling domain as depicted in Figure 1-1. Two different 12 km domains were evaluated, with the final model simulations based on the larger 12 km domain shown in Figure 1-1. The RPO Lambert Conformal Projection (LCP) grid system was adopted that is defined by the following parameters:

- Alpha = 33.0
- Beta = 45.0
- Gamma = -97.0
- Xcent = -97.0

- Ycent = 40.0

The 36 km grid (Domain 1) consisted of an array of 68 x 68 grid cells with an origin at (-792.0, -1656.0). The larger 12 km domain had an origin at (-264.0, -1272.0) with 128 by 149 12 km grid cells.

For the CMAQ simulations, one-way grid nesting was used between the St. Louis 36 km and 12 km regional-scale modeling domains (i.e., CMAQ was first run on the 36 km grid and the three-dimensional hourly instantaneous concentrations were then processed into boundary conditions for the 12 km CMAQ simulation). Whereas for the CAMx St. Louis 36/12 km simulations, two-way interactive grid nesting was used (i.e., concentrations are allowed to pass back and forth between the 36 km and 12 km domains during the simulations). For both the CMAQ and CAMx St. Louis 36/12 km regional-scale modeling, the boundary conditions (BCs) along the lateral edges of the 36 km domain were defined using output from the VISTAS continental U.S. 36 km CMAQ simulation of the 2002 annual period for the 2002, 2009 and 2018 Base G emission scenarios (Morris et al., 2007). The VISTAS 2002 and 2009 CMAQ results were used to define BCs for the 2002 and 2009 St. Louis simulations, whereas the BCs for the St. Louis 2012 simulations were obtained by interpolating between the 2009 and 2012 VISTAS results.

The CMAQ/CAMx St. Louis regional 36/12 km air quality modeling domain is nested within the MM5 domain. The selection of the MM5 domain is described in "Meteorological Model Performance Evaluation of an Annual 2002 MM5 (Version 3.6.3) Simulation" by Johnson, M. 2007 which is attached as Appendix F. Figure 1-1 displays the nested 36/12/4 km domains established by the MDNR for photochemical modeling and emissions modeling of the three summer 2002 8-hour ozone episodes. Both MM5 and CMAQ/CAMx employed the Regional Planning Organization (RPO) unified grid definition for the 36 km continental domain for the ozone modeling. The RPO unified grid consists of a Lambert-Conformal map projection using the projection parameters listed in Table 1-1.

The MM5 36 km grid includes 164 cells in the east-west direction by 128 cells in the north-south direction. The CMAQ/CAMx 36 km grid includes 148 cells in the east-west direction and 112 cells in the north-south direction. Because the MM5 model is also nested within the Eta model, there is a possibility of boundary effects near the MM5 boundary that occur as the Eta meteorological variables are simulated by MM5 and are forced into dynamic balance with MM5's meteorological fields. Thus, a larger MM5 domain was selected to provide a buffer of 6 grid cells around each boundary of the CMAQ/CAMx 36 km domain. This was designed to eliminate any errors in the meteorology from boundary effects in the MM5 simulation at the interface of the MM5 and Eta models. The buffer region used here complies with the EPA suggestion of a buffer of at least 3-6 grid cells at each boundary (EPA, 2006).

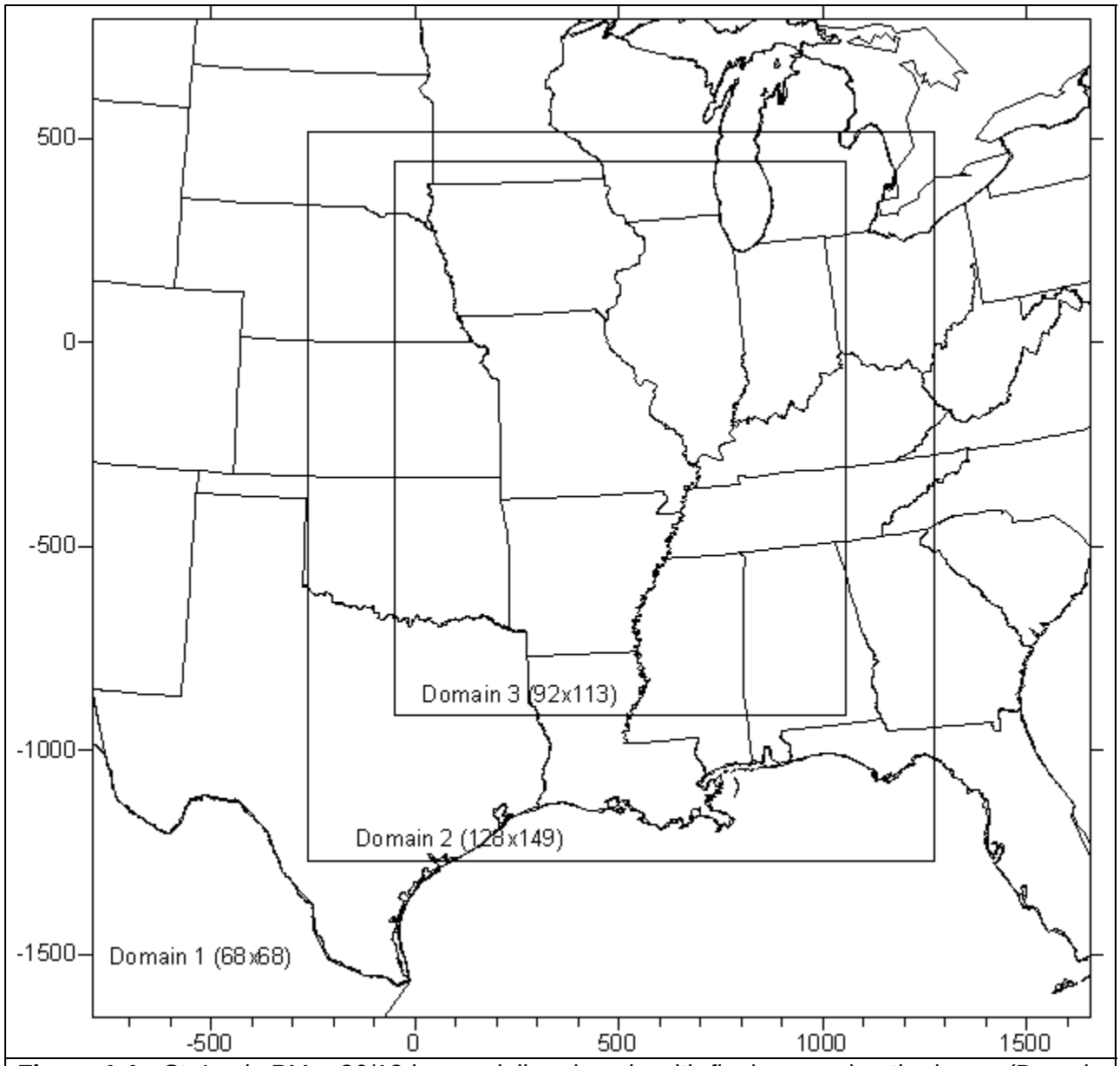

Figure 1-1. St. Louis $PM_{2.5}$ 36/12 km modeling domain with final runs using the larger (Domain 2) of the two 12 km domains.

1.3.4 Vertical Structure of Modeling Domain

The CMAQ/CAMx model vertical structure is primarily defined by the vertical grid used in the MM5 modeling. The MM5 model employed a terrain-following coordinate system defined by pressure, and had 34 vertical layers that extend from the surface upward to 100 mb. CAMx and CMAQ were applied with exactly the same vertical layer structure. A layer averaging scheme was adopted for CMAQ/CAMx to reduce the computational burden of the CMAQ and CAMx simulations. The effects of layer averaging were evaluated by western Regional Air Partnership (WRAP) and VISTAS and were found to have a relatively minor effect on the model performance metrics when both the 34 layer (no layer averaging) and 19 layer (layers averaged) CMAQ model simulations were compared to ambient monitoring data (Morris et al., 2004a). For the St. Louis Ozone modeling, 16 vertical layers were used. Table 1-1 details the mapping

from the 34 vertical layers used by MM5 to the 16 vertical layers used by CMAQ and CAMx in the St. Louis Study.

Table 1-1: Vertical layer definition for MM5 simulations (left most columns), and approach for reducing CMAQ/CAMx layers by collapsing multiple MM5 layers (right columns).

MM5					CMAQ/CAMx			
Layer	Sigma	Pres (mb)	Height (m)	Depth (m)	Layer	Pres (mb)	Height (m)	Depth (m)
34 (top)	**0.000**	**100**	**18123**	**2856**	**16**	**100**	**18123**	**7987**
33	0.050	145	15267	2097				
32	0.100	190	13170	1659				
31	0.150	235	11510	1374				
30	**0.200**	**280**	**10136**	**1173**	**15**	**280**	**10136**	**3106**
39	0.250	325	8963	1024				
28	0.300	370	7938	909				
27	**0.350**	**415**	**7030**	**817**	**14**	**415**	**7030**	**2866**
26	0.400	460	6213	742				
25	0.450	505	5471	680				
24	0.500	550	4791	627				
23	**0.550**	**595**	**4163**	**582**	**13**	**595**	**4163**	**1635**
22	0.600	640	3581	543				
21	0.650	685	3038	509				
20	**0.700**	**730**	**2528**	**386**	**12**	**730**	**2528**	**664**
19	0.740	766	2142	278				
18	**0.770**	**793**	**1864**	**269**	**11**	**793**	**1864**	**443**
17	0.800	820	1596	174				
16	**0.820**	**838**	**1421**	**171**	**10**	**838**	**1421**	**338**
15	0.840	856	1251	167				
14	**0.860**	**874**	**1083**	**164**	**9**	**874**	**1083**	**324**
13	0.880	892	920	161				
12	**0.900**	**910**	**759**	**79**	**8**	**910**	**759**	**158**
11	0.910	919	680	78				
10	**0.920**	**928**	**601**	**78**	**7**	**928**	**601**	**155**
9	0.930	937	524	77				
8	**0.940**	**946**	**447**	**76**	**6**	**946**	**447**	**152**
7	0.950	955	371	75				
6	**0.960**	**964**	**295**	**75**	**5**	**964**	**295**	**149**
5	0.970	973	220	74				
4	**0.980**	**982**	**146**	**37**	**4**	**982**	**146**	**37**
3	**0.985**	**987**	**109**	**37**	**3**	**987**	**109**	**37**
2	**0.990**	**991**	**73**	**36**	**2**	**991**	**73**	**36**
1	**0.995**	**996**	**36**	**36**	**1**	**996**	**36**	**36**
0 (ground)	**1.000**	**1000**	**0**	**0**	**0**	**0**	**0**	**0**

1.3.4.1 Air Quality Data

Data from ambient monitoring networks for both gas and aerosol species were used in the model performance evaluation. However, in the model performance evaluation presented in this TSD, we focused on the evaluation of modeled surface layer $PM_{2.5}$ mass and species concentrations within the 12km regional-scale domain (Figure 1-1) and the St. Louis NAA. Three monitoring networks were operating in the St. Louis NAA during the 2002 modeling period:

- $PM_{2.5}$ mass was collected at 12 Federal Reference Method (FRM) monitoring sites in the St. Louis NAA as depicted in Figure 1-2.
- Speciated $PM_{2.5}$ concentrations were measured at 4 Speciated Trends Network (STN) monitoring site, as well as at the East St. Louis locations as part of the St. Louis Super Site (StL-SS) as shown in Figure 1-3.

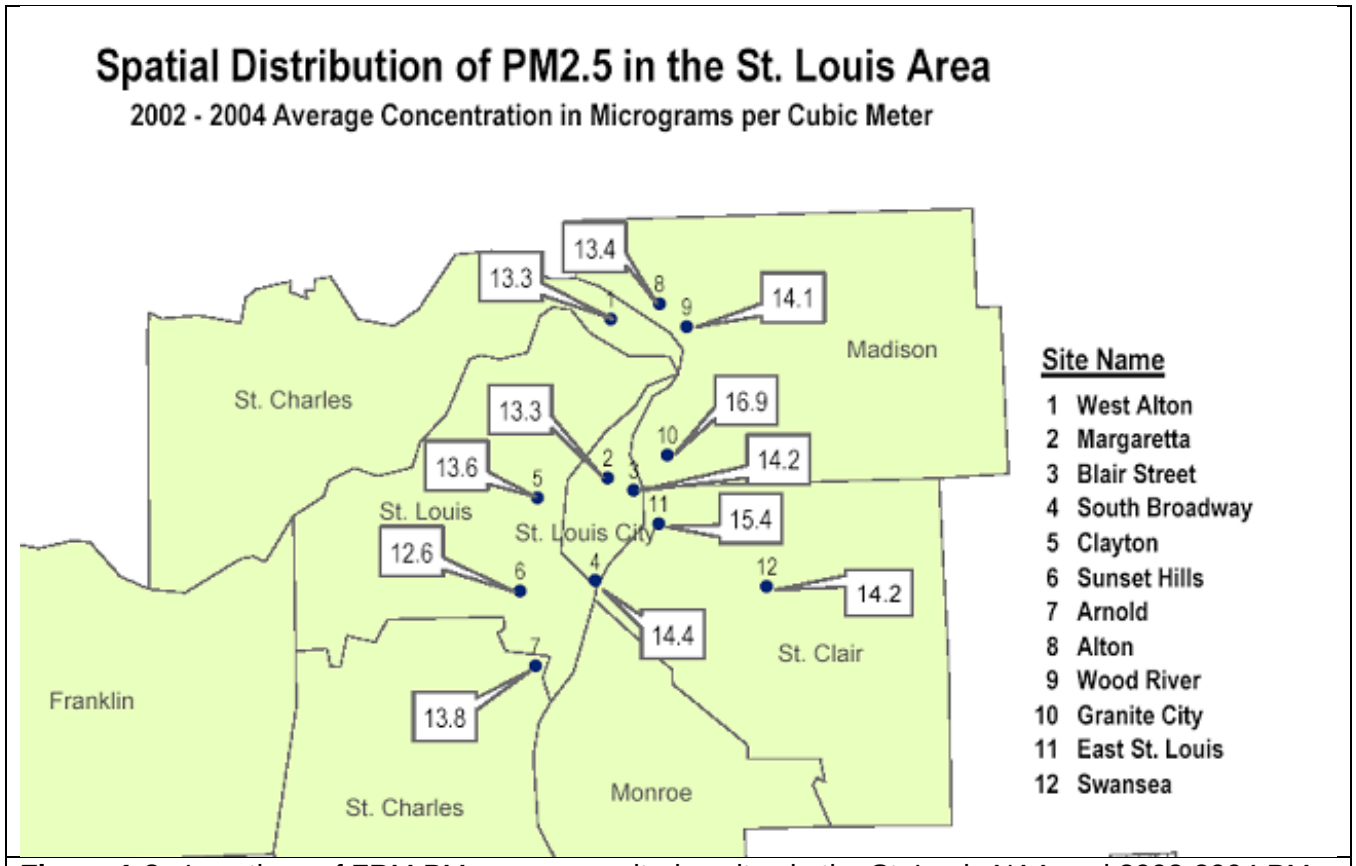

Figure 1-2. Locations of FRM $PM_{2.5}$ mass monitoring sites in the St. Louis NAA and 2002-2004 $PM_{2.5}$ Design Values ($\mu g/m^3$).

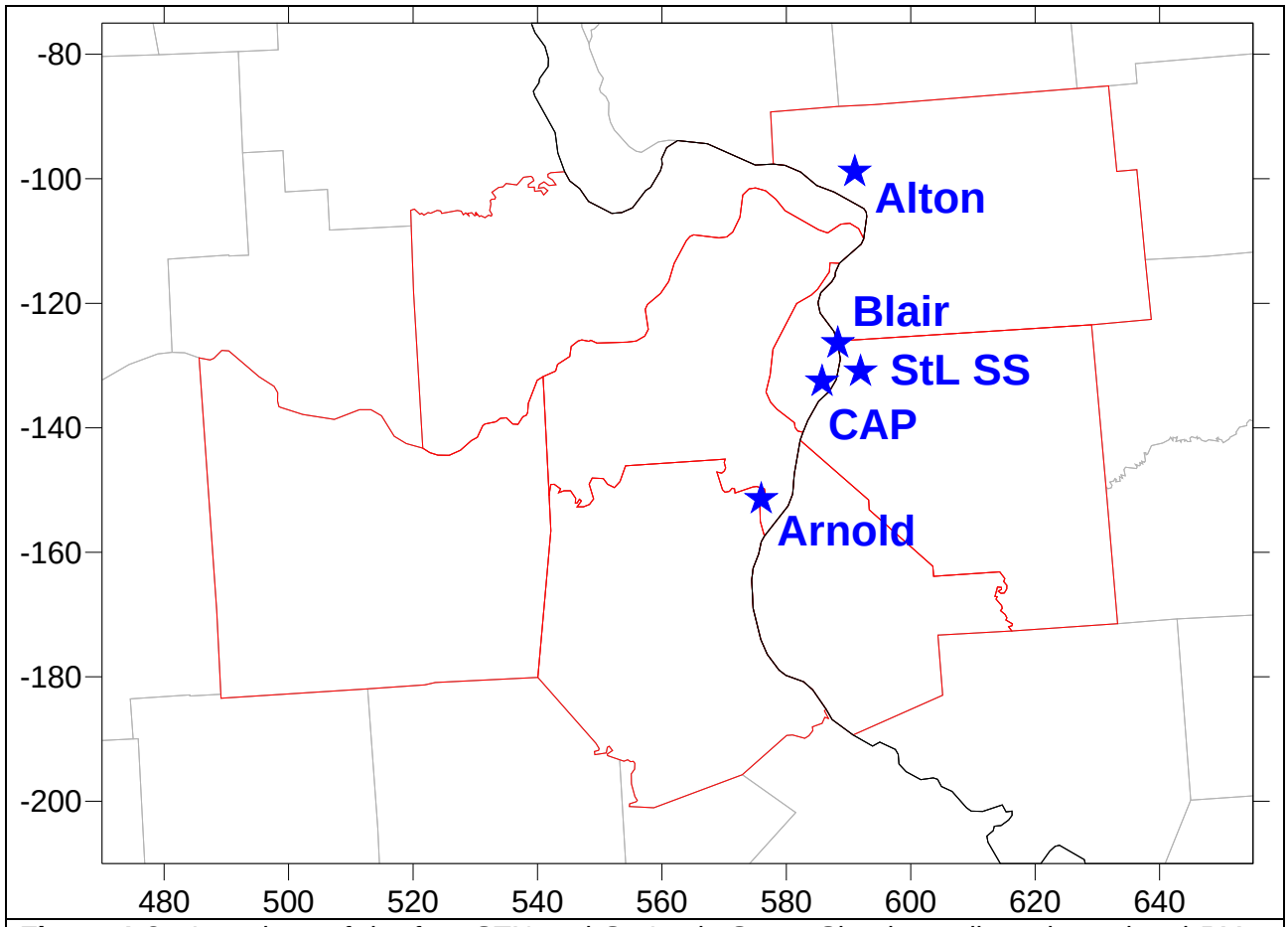

Figure 1-3. Locations of the four STN and St. Louis Super Site that collected speciated $PM_{2.5}$ measurements.

1.3.4.2 Ozone Column Data

Additional data used in the air quality modeling include the Total Ozone Mapping Spectrometer (TOMS) data. TOMS data are available for 24-hour average time periods, and are obtained from http://toms.gsfc.nasa.gov/eptoms/ep.html. The TOMS data are used in the CMAQ (JPROC) and CAMx (TUV) radiation models to calculate photolysis rates. The TOMS data were completely missing for the period of 3 August through 12 August, 2002, as well as on 10 June, 2002. In addition, 2 August and 18-19 November, 2002 had partially missing data.

The CAMx TUV processor allows for the use of monthly average data, so that option was used and the missing data ignored. The CMAQ JPROC processor does not allow for the use of monthly average data so the data from 1 August was used for 2 August through 7 August, and the data from 13 August was used for 8 August through 12 August. Data from 9 June was used for 10 June. Data from 17 November was used for 18 November, and data from 20 November was used for 19 November.

1.3.4.3. Initial and Boundary Conditions Data

A 10-day spin up period was used to limit the influences of initial concentrations (IC) on the model estimates. Boundary conditions (BCs) along the lateral edges of the St. Louis 36 km domain (see Figure 1-1) were based on the VISTAS/ASIP CMAQ simulations of the 2002

annual period and the Inter-RPO 36 km continental U.S. domain (Morris et al., 2007a; 2008a). VISTAS performed CMAQ simulations for the 2002 current and 2009 and 2018 future years. The St. Louis $PM_{2.5}$ simulations of the 2002 and 2009 years used BCs based on the VISTAS/ASIP CMAQ results for the same years, whereas for the 2012 modeling the BCs were interpolated from the 2009 and 2018 CMAQ results.

1.3.5 Episode Selection

The calendar year 2002 was selected for the St. Louis $PM_{2.5}$ modeling. EPA recommends that the selection of a modeling period for annual $PM_{2.5}$ modeling be based on the following four criteria (EPA, 2007a):

1. Choose time periods from each quarter which reflect a variety of meteorological conditions that represent average concentrations for that quarter and year,
2. Model time periods in which observed concentrations are close to the appropriate baseline design value,
3. Model time periods fort which extensive air quality/meteorological data bases exist, and
4. Model a sufficient number of days so that the modeled attainment test applied at each monitor violating the NAAQS is based on multiple days.

.

EPA also lists several 'other considerations' to bear in mind when choosing potential PM episodes including: choose periods which have already been modeled, choose periods which are drawn from the years upon which the current design values are based, include weekend days among those chosen, and choose modeling periods that meet as many episode selection criteria as possible in the maximum number of nonattainment or Class I areas as possible.

The St. Louis $PM_{2.5}$ study team elected to model a complete single Calendar Year (CY) to assure that sufficient days are present to represent each quarter of the Year, which follows EPA recommendations (page 149, EPA, 2007a). The 2002 calendar year was selected by the St. Louis $PM_{2.5}$ modeling study for annual $PM_{2.5}$ modeling for the following reasons:

- Based on available information, 2002 appears to be a fairly typical year in terms of meteorology,
- 2003 and 2004 appeared to be colder and wetter than typical in the eastern US,
- The enhanced IMPROVE and IMPROVE Protocol and Supersite PM monitoring data were fully operational by 2002 with much less IMPROVE monitoring data available during 2000-2001,
- The STN speciated $PM_{2.5}$ and FRM $PM_{2.5}$ mass monitors were fully operational in 2002, and
- 2002 was being modeled by CENRAP, VISTAS and other RPOs.
- 2002 was the base year used for the 8-hour ozone analysis in St. Louis.

1.3.6 Emissions Input Preparation and QA/QC

The primary function of the emissions modeling software is to speciate emission inventory data, allocate it in space and time, and place it into formatted files that can be directly input into the chemical transport model. An important part of this process is the quality control checks integral to the emissions modeling software that generate warning or error messages on suspect or

incorrect records because of data that is missing, "out-of-bounds", duplicative, lacking matching cross-reference data, or is otherwise deficient. Numerous software programs, external to the main emissions modeling software, have been written by IEPA staff and other EMS users to generate data summaries, graphical depictions of emissions data, and other data probing or analysis techniques to assure the highest quality emission inputs are being used for photochemical modeling. These programs were relied upon extensively in the processing of inventories.

Illinois and Missouri, both separately and jointly, conducted quality assurance checks on their respective state inventories. Additionally, ENVIRON, the consultant, retained to provide assistance with the St. Louis modeling, constituted a third independent entity to assess the inputs and outputs to the emissions model. For emissions outside of the States of Missouri and Illinois, the latest inventories from the CENRAP, VISTAS and MRPO Regional Planning Organizations (RPOs) were utilized.

The process of producing a model validation inventory is iterative, with data corrections or improvements invariably leading to a succession of more refined modeling inventories. The Midwest RPO modeling effort has gone from "Base A" to "Base K" inventories. The St. Louis validation modeling commenced with "Basecase 1" and concluded with "Basecase 5b", and the latter reflects processing of Midwest RPO inventory updates through the "Base K" inventory, and the CENRAP and VISTAS Base G inventories.

1.3.7 Meteorological Input Preparation and QA/QC

Meteorological data were generated using the MM5 prognostic meteorological model. MM5 runs for the 2002 annual period were performed at 5½ day increments on the 36/12 km domains that overlapped by 12 hours. A 12 hour spin up period was used for each 5½ day increment. The MM5 parameterization and module settings are essentially the same as those used by the Iowa Department of Natural Resources for their 2002 annual MM5 simulation on the 36 km continental US domain. Details on the configuration may be found in "Meteorological Model Performance Evaluation of an Annual 2002 MM5 (Version 3.6.3) Simulation" by Johnson, M. 2007 which is attached as Appendix F.

The MDAW Modeling Hubs processed the MM5 data using the MCIP and MM5CAMx processors to generate meteorological inputs for the CMAQ and CAMx models, respectively. MDAW modeling hub participants performed the 36 km annual and 12 km MM5 modeling and conducted their own QA/QC and evaluation of the meteorological fields. In addition, the ENVIRON Team also performed some QA/QC of the meteorological data to assure that it was transferred correctly, to obtain an assessment of the quality of the data, and to assist in the interpretation of the air quality modeling results.

The MDNR/MDAW and Team meteorological gatekeepers performed the following tasks:

- Analyses of the MM5 data to assure that it had been transferred correctly,
- Evaluation of the MM5 data using METSTAT and the surface meteorological network,

- Evaluation of upper-air MM5 meteorological estimates by comparing them to upper-air observations and satellite images,

- Comparison of the MDAW modeling hub's 2002 36 km MM5 simulation with those generated by WRAP and VISTAS, and

- Generation of the CMAQ-ready meteorological inputs using the MCIP2.3 processor and CAMx-ready inputs with the MM5CAMx processor.

1.3.8 Air Quality Model Input Preparation and QA/QC

Key aspects of QA for the CMAQ and CAMx input and output data included the following:

- Verification that correct configuration and science options were used in compiling and running each module in the CMAQ and CAMx modeling systems, where these included (for CMAQ) the MCIP, JPROC, ICON, BCON and the CCTM;

- Verification that the correct configuration and science options were used in running each model in the CAMx modeling system where these included MM5CAMx, TUV, land use, CAMx, and the CMAQ-to-CAMx emissions and IC/BC processors;

- Verification that correct input data sets were used when running each model;

- Evaluation of CMAQ and CAMx results to verify that model output was reasonable and consistent with general expectations;

- Processing of ambient monitoring data for use in the model performance evaluation;

- Evaluation of the CMAQ and CAMx results against concurrent observations and each other; and

- Backup and archiving of critical model input data.

The most critical element for CMAQ and CAMx simulations was the QA/QC of the meteorological and emissions input files, which is discussed above. The major QA issue specifically associated with the air quality model simulations was verification that the correct science options were specified in the model itself and that the correct input files were used when running the model. For CMAQ modeling, the modeling hubs employed a system of naming conventions using environment variables in the compile and run scripts that guaranteed that correct inputs and science options were used. Similar procedures were used in CAMx modeling using file and directory naming conventions. The Team employed a redundant naming system so that the names of key science options or inputs are included in the name of the CMAQ and CAMx executable program, in the name of the CMAQ and CAMx output files, and in the name of the directory in which the files were located. This was accomplished by using the environment variables in the scripts to specify the names and locations of key input files.

A second key QA procedure was to avoid "recycling" run scripts, i.e., the Team always preserved the original run scripts and directory structures that were used in performing a model simulation.

The MDAW modeling hubs and the Team also performed a post-processing QA of the CMAQ and CAMx output files similar to that described for the emissions processing. Animated graphic files were generated using PAVE, and were viewed to search for unexpected patterns in the CMAQ and CAMx output files. In the case of model sensitivity studies, the animated graphic files were prepared as difference plots for the sensitivity case minus the base case. This was done to screen for errors in the emissions inputs.

1.3.9 Conceptual Model

Using the enhanced measurements from the St. Louis Super Site, along with the routine STN and FRM monitors, Turner and co-workers (2007a,b,c,d) have developed a Conceptual Model on the sources and causes of elevated $PM_{2.5}$ concentrations in the St. Louis NAA. Regional transport of sulfate, nitrate, ammonium and organic carbon mass (OCM) are major contributors to the St. Louis $PM_{2.5}$ problem. The sulfate contribution is primarily transported from outside of the St. Louis NAA, with approximately 20% of the nitrate believed to be local in origin. Regional transport of OCM from outside the area is primarily believed to be secondary organic aerosols (SOA) with biogenic VOCs (e.g., isoprene and terpene) being the primary contributors.

Local sources are believed to be major contributors to $PM_{2.5}$ at the St. Louis FRM site that currently violates the annual $PM_{2.5}$ standard (Granite City, IL). The U.S. Steel facility, in particular, is identified as contributing to $PM_{2.5}$ nonattainment at this monitor. Chapter 2 provides the details of the Conceptual Model for $PM_{2.5}$ in the St. Louis area.

1.3.10 Base Case Modeling and Model Performance Evaluation

The St. Louis $PM_{2.5}$ Study performed annual modeling of the 2002 calendar year using a 36/12 km grid with several iterations of the 2002 base case emission scenarios. The final 2002 base case emissions scenario was Base 5b. In Chapter 4 of this TSD we present the model performance evaluation of the CMAQ and CAMx models for the 2002 Base 5b emissions scenario with additional model evaluation plots presented in Appendix A. The focus of this model evaluation was on the operational evaluation of $PM_{2.5}$ mass and $PM_{2.5}$ species model performance. The model was evaluated on the regional-scale using PM measurements for all PM monitors within Missouri/Illinois and nearby states. The model was also evaluated focusing on PM measurements within the St. Louis NAA.

The main implications of the major findings in the St. Louis PM model performance evaluation were as follows:

- <u>Good Sulfate Performance:</u> The CMAQ and CAMx performance for sulfate was generally good. There was a tendency for underpredicting the observed summer sulfate levels on the regions-scale. However, in St. Louis the sulfate performance was consistently good with low bias and error. This is an important result given the large contribution of sulfate to annual $PM_{2.5}$ levels in St. Louis and the fact that most of the benefits in $PM_{2.5}$ reductions between the current (2002) and future (2009 and 2012) years are due to reductions in sulfate.

- <u>Nitrate Underprediction Bias</u>: NO_3 is routinely underpredicted during the summer and adjacent months throughout the St. Louis 12 km modeling region. This underprediction

is due to modeled NO_3 concentrations near zero, when observed values are low, but above zero (typically < 1 μg/m^3). However, NO_3 is generally a very minor contributor to total $PM_{2.5}$ mass at FRM monitors in the St. Louis nonattainment region. Thus, the NO_3 performance issues are not a large concern in the $PM_{2.5}$ projections.

- OCM Underprediction Bias: The OCM under-prediction bias is a cause for concern since it is a major component of the $PM_{2.5}$ mass at St. Louis FRM monitoring sites with maximum contributions to the 2012 $PM_{2.5}$ Design Values of ~8 μg/m^3, minimum values of ~3 μg/m^3 and a mean value of ~4 μg/m^3. The reasons for the underestimation of OCM are unclear, but the fact that the underpredictions are higher in the urban than rural areas suggest that there may be missing anthropogenic emission sources, or possibly the urban OCM emissions are over diluted across the 12 km grid resolution used in the St. Louis modeling. The changes in projected OCM concentrations between the current and projected $PM_{2.5}$ Design Values are mostly less than 2% (i.e., $0.98 < RRF_{OCM} < 1.02$). Thus, the changes in OCM between the current and future year are having a minor influence on the projected $PM_{2.5}$ Design Values.

- Elemental Carbon (EC) Performance Issues: For the most part, both models performed well for EC at the urban sites and the slight overprediction does not affect the relative changes in the model response to anthropogenic EC emissions changes. Therefore, any EC performance issues were not a cause for concern.

- SOIL Performance Issues: The model performance for the SOIL species (aluminum, iron, titanium, calcium, and silicon) is quite poor. This SOIL component of the 2012 projected $PM_{2.5}$ Design Value ranges from 0.7 to 1.1 μg/m^3. The RRFs for SOIL indicate that it is mostly increasing, with summer (Q3) SOIL RRFs typically ranging from 1.1 to 1.2, which is relatively insignificant compared to SO4 contributions. Therefore, the SOIL performance issues will not significantly affect the projected 2012 $PM_{2.5}$ Design Values.

1.3.11 Future-Year Modeling and Modeled Attainment Demonstration

Future-year $PM_{2.5}$ modeling was performed with CMAQ and CAMx for 2009 originally. However, the 2009 future design value at Granite City site was 15.53 μg/m^3; which is just at the highest value allowed for a weight of evidence (WOE) attainment demonstration. Further, given late publication of the implementation rule by EPA, there was not sufficient time to identify and implement "local" control measures in 2009. Also, the first phase of the Illinois multi-pollutant utility rule will require significant emission reductions by 2012. The St. Louis modeling group concluded that it was impractical for the St. Louis NAA to attain the annual NAAQS by 2010 and requested that the attainment year be extended to 2012. The 2002 emissions were projected to 2009 and 2012 assuming growth and currently on-the-book (OTB) controls. Regional growth and control factors developed by EPA for the Clean Air Interstate Rule (CAIR) and by the various RPOs were used, and were enhanced with information specific to the St. Louis area. The control factors reflect federally promulgated Maximum Achievable Control Technology (MACT) standards, New Source Performance Standards, implementation of the NOx SIP Call, CAIR, Reasonably Available Control Technology (RACT), and court settlements (consent decrees) reached with refineries and ethanol producers.

The St. Louis future-year modeling used the 2002 MM5 meteorological conditions. That is, the meteorological conditions for the 2009 and 2012 future-years are assumed to be the same as 2002. This allowed for the comparison of the changes in $PM_{2.5}$ concentrations in the study area from the current (2002) to future-years due to changes in emissions. This means that the effects of climate change, land use variations and climatic variations were not accounted for in the future-year meteorological inputs. Boundary conditions along the lateral edges of the St. Louis 36 km domain (Figure 1-1) were based on VISTAS/ASIP CMAQ 36 km simulations for 2002, 2009 and 2018 emissions scenarios. The St. Louis BCs for the 2002 and 2009 simulations were based on the corresponding ASIP 2002/2009 CMAQ simulations, whereas the BCs for the St. Louis 2012 simulations were interpolated from the VISTAS/ASIP 2009 and 2018 CMAQ simulations

The St. Louis modeling results were used to project future-year $PM_{2.5}$ Design Values. The procedures for performing the $PM_{2.5}$ Design Value projections are outlined in EPA's modeling guidance (EPA, 2007a) and are discussed in chapter 5. These procedures involve the use of the model in a relative sense to scale the observed current year $PM_{2.5}$ Design Value based on the relative changes in the modeled $PM_{2.5}$ species concentration between the current-year (2002) and future-years (2009 and 2012) using the Speciated Modeled Attainment test (SMAT). Per the guidance, the current year "design value" is the average of the three design values that contain the base year (2000-02, 2001-03, and 2002-04). The EPA has developed a Modeled Attainment Test Software (MATS) that codifies the SMAT procedures that was used with the CMAQ 2002/2012 Base 5b12 modeling results to projected 2012 $PM_{2.5}$ Design Values that are shown in Table 1-2. The CMAQ 2012 $PM_{2.5}$ Design Values for the Base 5b12 emissions scenario are all projected to be below the annual $PM_{2.5}$ NAAQS, with the exception of the Granite City FRM monitor that is (15.28 $\mu g/m^3$) above the annual $PM_{2.5}$ NAAQS (15.0 $\mu g/m^3$). Thus, the modeled attainment demonstration projects that the maximum modeled $PM_{2.5}$ Design Value in 2012 is well within the range (14.5-15.5 $\mu g/m^3$) where additional analysis can be used to perform a Weight of Evidence (WOE) attainment demonstration, which is discussed next.

Table 1-2. Projected 2009 & 2012 $PM_{2.5}$ Design Values using 2009 Base 5a & 2012 Base 5b12 12 km CMAQ modeling results.

FRM Site ID	Site Name		Excel	MATS v1.3.1
		(2002)* $PM_{2.5}$ DVC Observed	(2009) $PM_{2.5}$ DVF CMAQ Base 5a	(2012) $PM_{2.5}$ DVF CMAQ Base 5b12
17_119_0023	Washington Ave.	N/A	N/A	N/A
17_119_1007	Granite City	17.27	15.53	15.28
17_119_2009	Alton	14.58	12.99	12.29
17_119_3007	Wood River	14.70	13.09	12.51
17_157_0001	Tilden City	12.41	10.94	10.31
17_163_0010	East St. Louis	16.19	14.54	14.13
17_163_4001	Swansea	14.68	13.10	12.58
29_099_0012	Arnold	14.43	12.91	12.27
29_183_1002	West Alton	14.08	12.54	11.93
29_189_0004	Sunset Hills	12.52	11.36	10.76
29_189_2003	Clayton	14.02	12.70	12.02
29_189_5001	Ferguson	13.77	12.16	11.93
29_510_0007	S. Broadway	14.55	13.29	12.70
29_510_0085	Blair St.	14.93	13.42	13.12
29_510_0086	Margaretta	13.93	12.59	12.07
29_510_0087	2nd & Mound	15.16	13.62	13.10

* Average of the three design values containing 2002 (2000-02, 2001-03, and 2002-04)

1.3.12 Weight of Evidence (WOE) Attainment Demonstration

Guidance from EPA states that if there are future-year $PM_{2.5}$ Design Values between 14.5-15.5 $\mu g/m^3$ at one or more FRM sites, then "a weight of evidence demonstration should be conducted to determine if aggregate supplemental analyses support the modeled attainment test" (EPA 2007a). In fact, EPA suggests that a weight of evidence (WOE) always be performed to corroborate the modeled attainment demonstration test. In a WOE determination, results from several types of air quality analyses are considered and the results reviewed for consistency with the conclusion of the modeled attainment test regarding the likelihood that the proposed control strategy will result in a NAA meeting the NAAQS. The credibility of each type of analysis used in the WOE determination must be assessed and finally, a conclusion reached regarding the likelihood of attainment.

For the St. Louis regional 36/12 km modeling, a WOE attainment demonstration is used because the maximum projected 2012 $PM_{2.5}$ Design Value at any Granite City at 15.28 $\mu g/m^3$, is 0.24 $\mu g/m^3$ above the threshold needed for a modeled attainment demonstration (<15.05 $\mu g/m^3$), and well within the WOE range (14.5-15.5 $\mu g/m^3$). Chapter 6 provides some additional analyses to support a WOE attainment demonstration. However, the main facts supporting the WOE attainment demonstration are as follows:

- The 2012 projected $PM_{2.5}$ Design Value at Granite City (15.28 $\mu g/m^3$) is just (0.24 $\mu g/m^3$) above the level needed to for a modeled attainment demonstration,
- The Chemical Mass Balance Source Apportionment results (see Chapter 6) for the Granite City Area and Urban Excess showed that local Granite City sources are the dominant influence on air quality impacts to the VFW (24-hour only) and also the Granite City fire station sites,
- The Conceptual Model for $PM_{2.5}$ in the St. Louis area has identified local sources as contributing a significant fraction, 2 - 3 $\mu g/m^3$, of the annual $PM_{2.5}$ concentrations at the Granite City FRM monitor (see Chapter 2), and
- As the local sources contributing to $PM_{2.5}$ at Granite City monitor are on the Illinois side of St. Louis, the IEPA is performing local-scale analysis using a hybrid of the CMAQ results presented here and AERMOD to identify the level of additional control on local sources needed to attain the annual $PM_{2.5}$ NAAQS.

The department feels confident that the IEPA will achieve the necessary level of emissions reduction from their local sources and therefore achieve attainment of the annual $PM_{2.5}$ NAAQS in the St. Louis NAA by 2012. At this time, the IEPA is actively pursuing a regulation to limit emissions from direct PM emission sources at the culpable local sources.

1.3.12 Additional Analyses

Chapter 6 of this TSD contains additional modeling analysis to the 2012 Base 5b $PM_{2.5}$ Design Value projections using the MATS tool and CMAQ modeling results. These additional modeling analyses include:

- $PM_{2.5}$ projections using alternative projection tools, and

- Projections for the 2009 and 2012 future-years and for different future-years control scenarios.