Appendix F

MDNR/Environ Modeling Protocol

Modeling Protocol

St. Louis Ozone, $PM_{2.5}$ and Air Toxics Modeling Study

Prepared for

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1.0 INTRODUCTION

1.1 Overview

This report constitutes the Air Quality Modeling Protocol for the St. Louis ozone, $PM_{2.5}$ and air toxics modeling study. The Missouri Department of Natural Resources (MDNR) has retained ENVIRON International Corporation and Eastern Research Group, Inc. (ERG) to assist in developing the air quality modeling databases needed to address ozone, $PM_{2.5}$ and air toxics issues in the St. Louis region. This Modeling Protocol describes the overall modeling activities to be performed by the Air Quality Management Plan (AQMP) Technical Workgroup and the ENVIRON/ERG team. The Workgroup consists of staff from the MDNR, Illinois Environmental Protection Agency (IEPA), U.S. EPA Region VII and V, and East-West Gateway Council of Governments (EWGCOG). Collectively, the Workgroup, with technical support from the ENVIRON/ERG team, will be responsible for conducting a comprehensive ozone, $PM_{2.5}$ and air toxics modeling study in support of the next round of ozone and $PM_{2.5}$ State Implementation Plans (SIPs) for the St. Louis area.

A comprehensive Modeling Protocol for an 8-hour ozone and/or $PM_{2.5}$ SIP attainment demonstration study consists of many elements. Its main function is to serve as a means for planning and communicating how a modeled attainment demonstration will be performed *before* it occurs. The protocol guides the technical details of a modeling study and provides a formal framework within which the scientific assumptions, operational details, commitments and expectations of the various participants can be set forth explicitly and means for resolution of potential differences of technical and policy opinion can be worked out openly and within time and budget constraints.

As noted in the U.S. EPA’s current modeling guidance for demonstrating attainment of ozone, $PM_{2.5}$ and regional haze standards, the Modeling Protocol serves several important functions (EPA, 2007):

- Identify the assistance available to the MDNR and IEPA (the lead agencies) to undertake and evaluate the analysis needed to support a defensible attainment demonstration;
- Identify how communication will occur among State, Local and Federal agencies and stakeholders to develop a consensus on various issues;
- Describe the review process applied to key steps in the demonstration; and
- Describe how changes in methods and procedures or in the protocol itself will be agreed upon and communicated with stakeholders and the appropriate U.S. EPA regional office.

Additionally, this modeling study addresses certain air toxics in the St. Louis area to include consideration of these toxics in the control decisions for the relevant criteria pollutants. The Modeling Protocol will also discuss modeling aspects relevant to air toxics.

1.2 Study Background

The previous round of St. Louis SIPs addressed the 1997 8-hour ozone National Ambient Air Quality Standard (NAAQS) that has a threshold of 0.08 ppm (84 ppb) and the annual $PM_{2.5}$

NAAQS with a 15 µg/m^3 threshold and demonstrated attainment in 2010 and 2012, respectively. In March 2008, EPA promulgated a new 8-hour ozone NAAQS that has the same form but lowers the threshold from 0.08 ppm to 0.075 ppm (75 ppb). In January 2010, EPA proposed lowering the ozone NAAQS threshold even more to somewhere in the 0.06-0.07 ppm range and, after a few delays, is expected to promulgate the new lower 8-hour ozone NAAQS by mid-2011. Although the schedule is not finalized, our current (May 2011) understanding is that ozone nonattainment area designations under the 2011 ozone NAAQS would occur no later than summer of 2013. The Section 110(a) SIPs would then be due by July 2014 with the ozone attainment demonstration SIPs due no later than the summer of 2016. The ozone future year that St. Louis needs to demonstrate attainment for will depend on its classification, but moderate nonattainment areas would need to demonstrate attainment no later than 2019. In September 2006, EPA lowered the 24-hour $PM_{2.5}$ NAAQS from 65 to 35 µg/m^3 with the new $PM_{2.5}$ attainment demonstration SIPs due by December 2012.

The St. Louis Community Air Project (CAP) has been performing ambient monitoring of air toxics at several sites in and nearby the downtown St. Louis area. The CAP was a community-based effort to identify and reduce air contaminants in the St. Louis urban area in response to resident's health concerns. The sampling in CAP included volatile organic compounds, semi-volatiles, $PM_{2.5}$ metals, carbonyls and elemental carbon as a surrogate for diesel particulate matter (DPM).

To address the SIP requirements of the new ozone and $PM_{2.5}$ NAAQS and the next steps in the CAP, the MDNR and IEPA have prepared the St. Louis Air Quality Management Plan, which also includes involvement by the East-West Gateway Council of Governments (EWGCOG) Air Quality Advisory Committee. The three government agencies are committed to implementation of the Air Quality Management Plan (referred to as AQMP3[1]) that has the following objectives:

1. Completion of all required Clean Air Act submittals for compliance with the NAAQS in St. Louis preferably using one air quality planning exercise for multiple pollutants under a combined SIP;
2. Inclusion of air toxics exposure as an important metric for consideration of alternative control requirements for all NAAQS;
3. Incorporation of environmental justice and extensive community involvement in the decision-making process including the regulated and environmental communities; and
4. Consideration of other ancillary air quality issues in the development of the SIP including smart growth/transportation, energy issues, and climate change.

An AQMP Technical Workgroup has been formed consisting of state, local and EPA agency personnel who are responsible for planning and management of the AQMP3 including the attainment demonstration modeling for the ozone and $PM_{2.5}$ NAAQS. The Air Quality Advisory Committee (AQAC) consists of state and local agencies, as well as transportation agencies, is a forum for communication and outreach between governments, industrial and environmental stakeholders as well as dealing with conformity and other aspects of the multi-pollutant focus of the AQMP3.

1.3 State Agency Organization and Workgroup

[1] http://www.epa.gov/air/aqmp/pdfs/aug2010/stlouisfinalaqmp.pdf

The States of Missouri and Illinois have determined that the committee structure described below will be 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 emission reduction strategies, and resolving disputes as they arise. The State Air Agencies will meet as appropriate to oversee the progress of this effort. The Missouri Air Conservation Commission has final authority to adopt Missouri's regulations and the final control plan. Similarly, the Illinois Pollution Control Board has the final authority to adopt control requirements in Illinois.

Participants: Air Directors from MDNR and IEPA.

AQMP Technical Workgroup: Responsible for planning and management of the technical work necessary to demonstrate attainment of National Ambient Air Quality Standards in the St. Louis area; including emissions inventory, meteorological, and photochemical modeling. The workgroup is also responsible for data analysis, source apportionment, coordination, and communication of the model results to the Air Quality Advisory Committee, and the State Air Directors. This workgroup will meet on a regular basis to coordinate the development and performance of technical activities. These meetings are open to stakeholders and local agencies having the technical expertise to contribute to work activities**.**

Participants: Staff from MDNR, IEPA, U.S. EPA Region VII and V, and East-West Gateway Council of Governments. Local air pollution control organizations, stakeholders, and academics that can contribute technical capabilities or resources are also invited to participate.

Air Quality Advisory Committee (AQAC): Serves as a forum to communication and outreach between local government, industrial and environmental stakeholders, the Technical Workgroup, and the State Air Directors. The Air Quality Advisory Committee will meet on a regular basis and will endeavor to increase community participation in quality management process. It will also provide assistance in the development of conformity budgets for both States and preparing the resultant conformity demonstrations that are consistent with the relevant SIP (State Implementation Plan). Further, this group will provide for the open discussion of emission control strategies consistent with the AQMP and its multi-pollutant focus.

Participants: MDNR, IEPA, U.S. EPA Regions VII and V, East-West Gateway Council of Governments, Federal Highway Administration, Missouri Department of Transportation, Illinois Department of Transportation, environmental groups, industry stakeholders, and local government agencies.

1.4 Related Regional Modeling Studies

The St. Louis ozone, $PM_{2.5}$ and air toxics modeling study draws from several urban and regional scale emissions, photochemical, PM and visibility modeling efforts performed in the Central

States and across the United States. The procedures used in these previous studies provide a guide to the modeling and QA approach for the St. Louis study.

1.4.1 Related 8-hr Ozone, $PM_{2.5}$ and Regional Haze SIP Studies

8-hour Ozone SIP Modeling Analyses in St. Louis: Meteorological, emissions and photochemical modeling support for the St. Louis 8-hour ozone SIP development was performed by a team led by ENVIRON. The ENVIRON team developed the Modeling Protocol that described the overall modeling activities performed by all the participants in the modeling study (ENVIRON and Alpine, 2005). The MM5 meteorological, SMOKE and EMS emissions, and CMAQ and CAMx photochemical models were used to simulate three 2002 ozone episodes. In addition, ENVIRON performed a number of sensitivity analysis as part of the model performance evaluation. Details of the study results were documented in the Technical Support Document (IEPA, 2007).

St. Louis Annual PM2.5 SIP Modeling: ENVIRON and its subcontracting team provided meteorological, emissions and regional air quality modeling support for the St. Louis annual $PM_{2.5}$ SIP development. Annual simulations for 2002 base year and 2009/2012 future years were conducted (MDNR and ENVIRON, 2009).

Development of 2002 Base Case Modeling Inventory for CENRAP: CENRAP sponsored this study to prepare a 2002 Base Case emissions inventory for the CENRAP states that can be used in emissions and photochemical modeling of the 2002 annual period (Strait, Roe and Vukovich, 2004).

Preliminary PM and Visibility Modeling for CENRAP: Under this study preliminary regional PM and visibility modeling was conducted focused on the CENRAP region using the CMAQ and CAMx models (Pun, Chen and Seigneur, 2004).

VISTAS Phase I Model Sensitivity and Evaluation Study: This study, sponsored by VISTAS, performed extensive model sensitivity testing and evaluation analysis using the CMAQ and CAMx models and three episodes, January 2002; July 1999 and July 2001 (Morris et al., 2004a).

WRAP Section 309 SIP/TIP Modeling Analysis: The WRAP performed a study to generate the necessary modeling data needed to develop Section 309 SIP/TIP for states that opt-in to this program (Tonnesen et al., 2003).

VISTAS Phase II 2002 Annual Modeling: VISTAS performed annual modeling of 2002 using a continental US 36 km domain and eastern US 12 km domain with attendant model evaluation and sensitivity analysis (Morris et al., 2004b).

CENRAP 2002 Annual Modeling: ENVIRON and UCR performed annual emissions and air quality modeling of the 2002 period using SMOKE, CMAQ and CAMx to provide the technical basis for the Regional Haze SIPs due in December 2007[2].

[2] http://pah.cert.ucr.edu/aqm/cenrap/index.shtml

Association for Southeastern Integrated Planning PM2.5 SIP Modeling: ENVIRON/Alpine provided the Association for Southeastern Integrated Planning (ASIP) emissions and air quality modeling support for their $PM_{2.5}$ SIP modeling. Annual simulations for 2002 base year and 2009, 2012 and 2018 future year were conducted (Morris et al., 2008).

Birmingham Annual PM2.5 SIP Modeling: ENVIRON/Alpine/ENVAIR provided modeling analyses to support the development of the Alabama SIP for the Birmingham annual $PM_{2.5}$ nonattainment area. Because it has been reported that local sources may be significant contributors of primary PM in the Birmingham area, a sophisticated sub-regional and local-scale modeling strategy was developed and performed (ENVIRON et al., 2009).

VISTAS Regional Haze SIP Modeling: ENVIRON/Alpine/UCR provided emissions and air quality modeling support for the VISTAS Regional Haze SIP development. Annual modeling efforts for 2002 base year and 2018 future year were conducted for the 2018 visibility projection (Morris et al., 2009).

Southeastern Modeling, Analysis, and Planning Project (SEMAP): The SEMAP[3] project is overseen by Metro 4, Inc. and SESARM. SEMAP is the follow-on effort to VISTAS and ASIP and is designed to perform the meteorological, emissions and air quality modeling activities to address the next round of SIPs for the 10 southeastern U.S. SIPs. It has adopted the same 2007 modeling year to be used in the St. Louis AQMP3 modeling so is directly relevant to this study.

Lake Michigan Air Directors (LADCO) Activities: LADCO[4] was formed as a collaborative effort to assist and coordinate meteorological, emissions and air quality activities for the states of Illinois, Indiana, Michigan, Ohio and Wisconsin. Some of the past St. Louis air quality planning activities have been performed by or through LADCO.

1.4.2 Related Federal Air Quality Activities

The federal government has implemented standards and actions to improve air quality across the entire country. These standards have largely involved mobile sources. Federal standards include: the Tier 2 Vehicle Standards, the heavy-duty gasoline and diesel highway vehicle standards, the non-road spark-ignition engines and recreational engine standards, and the large non-road diesel engine rule. The federal government has also implemented regional control strategies for major stationary sources focusing on the eastern U.S. and intends to extend the program to the western U.S. The following is a list of federal regulatory activities that would likely lead to emission reductions in the St. Louis area and will need to be accounted for in the next St. Louis SIPs.

Tier 2 Vehicle Standards: Federal Tier 2 vehicle standards require all passenger vehicles in a manufacturer's fleet, including light-duty trucks and Sports Utility Vehicles, to meet an average standard of 0.07 grams of NOx per mile. Implementation began in 2004, and most vehicles were phased in by 2007. Tier 2 standards also cover passenger

[3] http://www.metro4-sesarm.org/SEMAPAbout.asp
[4] http://www.ladco.org/

vehicles over 8,500 pounds gross vehicle weight rating (the larger pickup trucks and SUVs), which were not covered by the earlier Tier 1 regulations. For these vehicles, the standards were phased in beginning in 2008, with full compliance in 2009. The new standards require vehicles to be 77% to 95% cleaner than those on the road prior to the implementation of the standard. Tier 2 rule also reduces the sulfur content of gasoline to 30 ppm starting in January of 2006. Sulfur occurs naturally in gasoline but interferes with the operation of catalytic converters on vehicles resulting in higher NOx emissions. Lower sulfur gasoline is necessary to achieve Tier 2 vehicle emission standards.

Heavy-duty Gasoline and Diesel Highway Vehicle Standards: New U.S. EPA standards designed to reduce NOx and volatile organic compound (VOC) emissions from heavy-duty gasoline and diesel highway vehicles began to take effect in 2004. A second phase of standards and testing procedures, began in 2007, will reduce particulate matter from heavy-duty highway engines, and will also reduce highway diesel fuel sulfur content to 15 ppm since the sulfur damages emission control devices. The total program is expected to achieve a 90% reduction in PM emissions and a 95% reduction in NOx emissions for these new engines using low sulfur diesel, compared to existing engines using higher-content sulfur diesel.

Non-Road Spark-ignition Engines and Recreational Engines Standards: The new standard, effective in July 2003, regulates NOx, HC and CO for groups of previously unregulated non-road engines. The new standard applies to all new engines sold in the United States and imported after these standards began. It will apply to large spark-ignition engines (forklifts and airport ground service equipment), recreational vehicles (off-highway motorcycles and all-terrain-vehicles), and recreational marine diesel engines. The regulation varies based upon the type of engine or vehicle. Large spark-ignition engines contribute to ozone formation and ambient CO and PM levels in urban areas. Tier 1 of this standard was implemented in 2004 and Tier 2 began in 2007. Like the large spark-ignition engine vehicles, recreation vehicles contribute to ozone formation and ambient CO and PM levels. They can also be a factor in regional haze and other visibility problems in both state and national parks. The standard phase-in for the off-highway motorcycles and all-terrain-vehicles began in model year 2006 and was fully implemented by the end of model year 2007. Recreational marine engines contribute to ozone formation and PM levels, especially in marinas. The standard began phase-in in 2006 with the schedule dependent on the size of the engine. With all of the non-road spark-ignition engines and recreational engines standards fully implemented, an overall 72% reduction in HC, 80% reduction in NOx, and 56% reduction in CO emissions are expected by 2020. These controls will help reduce ambient concentrations of ozone, CO, and fine PM.

Large Non-Road Diesel Engine Rule: The U.S. EPA promulgated in May 2004 new rules for large non-road diesel engines, such as those used in construction, agricultural, and industrial equipment, to be phased in between 2008 and 2014. The non-road diesel rules also reduce the allowable sulfur in non-road diesel fuel by over 99%. Non-road diesel fuel currently averages about 3,400 ppm sulfur. The new rules limited non-road diesel sulfur content to 500 ppm in late 2006 and 15 ppm in 2010. The combined engine and fuel rules reduce NOx and PM emissions from large non-road diesel engines by over 90%, compared to current non-road engines using higher-content sulfur diesel.

Cross State Air Pollution Rule (CSAPR) and Clean Air Interstate Rule (CAIR): In 2005, the U.S. EPA promulgated the "Rule to Reduce Interstate Transport of Fine Particulate Matter and Ozone", referred to as the Clean Air Interstate Rule (CAIR). This rule established the requirement for States to adopt rules limiting the emissions of NOx and SO_2 and a model for the states to use in developing their own state rules. The purpose of the CAIR is to reduce interstate transport of precursors of fine particulate and ozone. It provides annual state caps for NOx and SO_2 for large fossil-fuel-fired electric generating units. This program includes a cap and trade program if a state chooses to participate. Due to court challenges of CAIR in 2008, the U.S. EPA has made changes to the CAIR program and re-issued a regional control plan for the eastern U.S. similar to CAIR as the Cross State Air Pollution Rule (CSAPR)[5] in July 2011. However, the court upheld the control provisions of the 2005 CAIR that will remain in place until the U.S. EPA implements CSAPR. Additionally, the Transport Rule revisions to the CAIR program are expected to be as stringent as the existing program.

VOC MACT: Maximum Achievable Control Technology (MACT) standards are standards set by the U.S. EPA for chemicals known to cause cancer or other serious health effects. Many of the chemical substances regulated as VOCs are also listed as HAPs. Therefore, many of the MACT control requirements effectively reduce emissions of VOCs as well.

Federal Reformulated Gasoline: Federal reformulated gasoline allows for a maximum of 1 percent benzene by volume. Preliminary VOC and air toxics standards took effect with phase I of the rule in 1995. Phase II took effect in 2000. Phase II required 25 to 29 percent VOC emission reductions and 20 to 22 percent air toxics reductions.

Federal Non-Road Spark-Ignition Engines and Equipment: U.S. EPA issued final emission standards for spark-ignition engines used in marine vessels, including outboard engines, personal watercraft, and sterndrive/inboard engines in their proposed rule, "Control of Emissions from Non-road Spark-Ignition Engines and Equipment," in 2008. The engines and vehicles covered by this account for about 25 percent of mobile source hydrocarbon emissions and 30 percent of mobile source carbon monoxide emissions. These new more stringent standards for outboard and personal watercraft engines start with the 2010 model year. The standards set specific levels of HC + NOx and CO emissions for different types of marine vessels.

Locomotive Engines and Marine Compression-Ignition Engines Final Rule: Locomotives and marine diesel engines are important contributors to the nation's air pollution, as they emit large amounts of direct PM and NOx. To dramatically reduce emissions from these engines, U.S. EPA issued the rule, "Control of Emissions of Air Pollution from Locomotive Engines and Marine Compression-Ignition Engines Less than 30 Liters per Cylinder." It set new exhaust emission standards on all types of locomotive engines and on all types of marine diesel engines below 30 liters per cylinder displacement.

Low-Sulfur Fuels: Associated with the Tier 2 on-road vehicle fleet standards is a requirement to reduce sulfur levels in gasoline nationwide. Refiners had to meet a

[5] http://www.epa.gov/airtransport/

corporate average gasoline sulfur standards beginning in 2004. The cap was further reduced in 2006, and most refineries were required to produce gasoline averaging no more than 30 ppm sulfur.

Clean Air Visibility Rule (CAVR): The Clean Air Visibility Rule (CAVR) requires specific sources that are shown to reasonably contribute to visibility impairment at a Class I area to install Best Available Retrofit Technology (BART). The BART requirements apply to sources built between 1962 and 1977 that have the potential to emit 250 tons per year (TPY) of a visibility impairing pollutants (SO_2, NOx, PM and/or VOC) and are one of 26 specific source categories. EPA has published guidelines for the BART component of the CAVR (EPA, 2005b).

1.4.3 State-Specific Emission Control Measures

Both Missouri and Illinois incorporated "on-the-books" emission controls in their SIPs for the St. Louis 8-hour ozone nonattainment area. These controls reflect state's rulemaking efforts and other controls related to enforcement actions as well as the federal activities described above. The following list shows state-specific control measures in the St. Louis area, as identified in AQMP3:

Missouri
- Open Burning Restrictions
- Control of Emissions from Aerospace Manufacture and Rework Facilities
- Control of Emissions from Rotogravure and Flexographic Printing Facilities
- Control of Emissions from Bakery Ovens
- Control of Emissions from Lithographic Printing
- Control of Emissions from Traffic Coatings
- Control of Emissions from Aluminum Foil Rolling
- Control of Emissions from Wood Furniture Manufacturing Operations
- Control of Emissions from Solvent Cleanup Operations
- Control of Emissions from Volatile Organic Liquid Storage
- Control of Emissions from Batch Process Operations
- Control of Petroleum Liquid Storage, Loading, and Transfer (Stage I)
- Stage II Vapor Recovery (Automobile refueling control)
- NOx RACT controls - Missouri

Illinois
- Consent Decree – Dynegy Midwest Generation (Consent Decree entered May 27, 2005 by U.S. District Court for the Southern District of Illinois)
- Consent Decree---ConocoPhillips (Consent Decree filed January 27, 2005 by U.S. District Court for the Southern District in Texas)
- Control of Emissions from Consumer and Commercial Products
- Control of Emissions from Architectural and Industrial Maintenance (AIM) Coatings
- Control of Emissions from Rotogravure and Flexographic Printing Facilities
- Control of Emissions from Lithographic Printing
- Control of Emissions from Pavement Painting Operations
- Control of Emissions from Wood Furniture Manufacturing Operations
- Control of Emissions from Solvent Cleanup Operations

- Control of Emissions from Volatile Organic Liquid Storage
- Control of Emissions from Batch Process Operations
- Control of Petroleum Liquid Storage, Loading, and Transfer (Stage I)

1.5 Overview of Modeling Approach

The St. Louis ozone, $PM_{2.5}$ and air toxics modeling study includes emissions, meteorological, ozone and fine particulate simulations using a nested 36/12/4/1.333 km grid with the 4 km domain focused on the state of Missouri and southwestern Illinois and the 1.333 km domain focused on the St. Louis urban area. After detailed performance testing of these simulations by the AQMP Technical Workgroup, CMAQ and/or CAMx modeling systems will then be exercised with a variety of emissions control scenarios aimed at enabling the State Agencies (MDNR and IEPA) to assess the effects of future year emission control strategies on ozone, $PM_{2.5}$ and other air quality issues including toxics exposure. More specifically, the St. Louis modeling effort will focus on the use of the SMOKE and MOVES emissions, WRF meteorological, and CMAQ and CAMx air quality modeling systems for simulating ozone over the 36/12/4 km domains and PM and air toxics over the 4/1.333 km domains.

Although the modeling system will be set up to simulate ozone, $PM_{2.5}$ and air toxics, the St. Louis area is currently in nonattainment of just the ozone NAAQS. Consequently, the primary focus for setting up the modeling system will be for demonstrating attainment of the ozone NAAQS. But the modeling system will also be capable of simulating $PM_{2.5}$ and air toxics and the co-benefits of reducing $PM_{2.5}$ and air toxics of the ozone attainment control strategy will also be evaluated.

1.5.1 Ozone and $PM_{2.5}$ Episode Selection

This section presents the rationale behind the selection of the ozone modeling episodes and 2007 calendar year for PM modeling to address attainment demonstration of the 8-hour ozone and PM standards in the St. Louis area.

1.5.1.1 EPA Guidance for Episode Selection

EPA’s current guidance on 8-hour ozone/$PM_{2.5}$/Regional Haze modeling (EPA, 2007) identifies specific criteria to consider when selecting one or more episodes for use in demonstrating attainment of the 8-hour ozone and $PM_{2.5}$ NAAQS, and demonstrating reasonable progress in attaining the regional haze goals. This guidance builds off the 1-hour ozone modeling guidance (EPA, 1991) in selecting multiple episodes representing diverse meteorological conditions that result in ozone exceedances in the region under study:

- A variety of meteorological conditions should be covered, this includes the types of meteorological conditions that produce 8-hour ozone exceedances in the St. Louis area;
- To the extent possible, the modeling data base should include days for which extensive data bases (i.e. beyond routine aerometric and emissions monitoring) are available;
- Sufficient days should be available such that relative response factors (RRFs) can be based on several (i.e., $\geq$ 10) days with at least 5 days being the absolute minimum; and

- If possible and appropriate, modeling for an entire ozone season is recommended.

For annual $PM_{2.5}$ modeling, the EPA guidance goes further by suggesting that the preferred approach is to model a full, *representative* year (EPA, 2007). Similar recommendations are made for regional haze modeling. For annual $PM_{2.5}$ modeling, component-specific RRFs are based on quarterly averages. EPA has developed a Speciated Modeled Attainment Test (SMAT) that contains specific procedures for combining Federal Reference Method (FRM) $PM_{2.5}$ measurements with speciated $PM_{2.5}$ observations (Timin, 2007; EPA, 2007). The SMAT procedures include provisions for applying speciated data from the EPA Chemical Speciation Network (CSN) and Interagency Monitoring of Protected Visual Environments (IMPROVE) networks to the FRM $PM_{2.5}$ mass measurements that account for measurement artifacts and spatial distribution of monitors.

EPA also lists several "other considerations" to bear in mind when choosing potential 8-hour ozone and PM/regional haze 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 areas as possible.

1.5.1.2 Selection of the Ozone and PM Episodes for the St. Louis Area

The 2007 calendar year was selected for the St. Louis ozone and $PM_{2.5}$ SIP and air toxics modeling. 2007 was selected because it is the most recent year with elevated ozone and $PM_{2.5}$ concentrations. Details on the episode selection are provided in Chapter 3.

1.5.2 Model Selection

The WRF prognostic meteorological model was selected for the St. Louis modeling study. Emissions modeling will be performed using the SMOKE emissions model. The MOVES model will be used for on-road mobile sources. Two "one-atmosphere" air quality models will be applied initially, CMAQ and CAMx. Details on the rationale for model selection are provided in Chapter 2. Both CMAQ and CAMx will be applied for the initial run and model performance evaluation (MPE) will be conducted for both. Based on the MPE and other factors, a better performing one will be selected for the final attainment demonstration and the other model will be utilized for the weight-of-evidence analysis as described in Section 1.5.9.

1.5.3 Conceptual Model

The conceptual model is designed to provide an explanation of events that transpired to cause high pollutant levels during these modeling time periods. Typically, it includes a discussion of meteorology, emissions, and transported pollutants and their precursors into the metropolitan area. For example, previous study has shown that there are several types of synoptic weather patterns associate with high ozone in the St. Louis region. Most of the local surface weather patterns are calm or light winds in the morning hours and continued calm or a "push" to the suburban areas in the afternoon resulting in high 8-hour concentrations. The development of the

Conceptual Model for ozone, $PM_{2.5}$ and air toxics is an important component of the SIP development as it drives the design of the modeling system needed to demonstrate attainment of the ozone and $PM_{2.5}$ NAAQS and simulate air toxics in the St. Louis region.

1.5.4 Emissions Input Preparation and QA/QC

Quality Assurance (QA) and Quality Control (QC) of the emissions datasets are some of the most critical steps in performing air quality modeling studies. Because emissions processing is tedious, time consuming and involves complex manipulation of many different types of large data sets, rigorous QA measures are a necessity to prevent errors in emissions processing from occurring. The St. Louis modeling study will perform a multistep emissions QA/QC approach. This includes the initial emissions QA/QC by the ENVIRON/ERG team on all existing emissions inventories collected from various sources, as well as QA/QC by the AQMP Technical Workgroup and the ENVIRON/ERG team as the dataset is processed and made available for modeling. This multistep process with separate groups involved in the QA/QC of the emissions is designed to detect and correct errors prior to the air quality model simulations.

QA/QC performed as part of the emissions processing includes:

EPA Input Screening Error Checking Algorithms: Although the SMOKE emissions model is the primary tool used for emissions processing, some additional input error checking algorithms like those used with the EMS and EPS emission models may be considered to screen the data and identify potential emission input errors. Additionally, EPA has issued a revised stack QA and augmentation procedures memorandum that will be used to identify and augment any outlying stacks.

SMOKE Warning Messages: SMOKE provides various cautionary or warning messages during the emissions processing. The SMOKE output will be reviewed for these messages. An archive of the log files will be maintained so that the warning messages can be reviewed at a later date if necessary.

SMOKE Emissions Summaries: QA functions built into the SMOKE processing system will be used to provide summaries of processed emissions as daily totals according to species, source category and county and state boundaries. These summaries will then be compared with summary data prepared for the pre-processed emissions, e.g., state and county totals for emissions from the augmented emissions data.

MOVES QA/QC: The MOVES model to be used for generating the on-road mobile source emissions also has extensive QA/QC and error messaging system that will be used to QA this portion of the inventory.

After the CMAQ-ready emission inputs have been prepared, additional emissions QA/QC will be performed as appropriate, such as:

Spatial Summary: Sum the emissions for all 24 hours to prepare plots showing the spatial distribution of daily total emissions using the Package for Analysis and Visualization for Environmental (PAVE)[6] data. In our base case simulations these plots

[6] http://www.cmascenter.org

will be presented as tons per day. Typically emission categories are processed using 5 streams of modeling: biogenic, on-road mobile, non-road mobile, other low-level anthropogenic and point sources (fires are also analyzed separately when available). If possible, separate spatial QA plots will be generated for low-level and elevated point sources. The objective of this step is to identify errors in the spatial distribution of emissions.

Short Term Temporal Summary: The total domain emissions for each hour will be accumulated and time series plots prepared by source category that display the diurnal variation in total hourly emissions. The objective of this step is to identify errors in temporal profiles.

Long Term Temporal Summary: The total domain emissions for each day will be accumulated and displayed as time series plots that show the daily total emissions across the domain as a function of time. The objective of this step is to identify particular days for which emissions appear to be inconsistent with other days for no reason (e.g., not a weekend) and compare against the general trend.

Control Strategy Spatial Displays: Spatial summary plots of the daily total emissions differences between a future year scenarios and base case emissions scenarios will be generated. These plots can be used to immediately identify a problem in a control strategy. For example, if a state's NOx emissions control strategy is being analyzed and there are changes in emissions for other pollutants or for NOx outside of the St. Louis area, problems in emissions processing can be identified prior to the air quality model simulation.

The emissions QA/QC displays will be made available to study participants for review.

1.5.5 Meteorology Input Preparation and QA/QC

Iowa Department of Natural Resources (IDNR) performed the 36/12 km WRF modeling and ENVIRON has conducted evaluation of the meteorological fields to assure that it has been transferred correctly, to obtain an assessment of the quality of the data, and to determine whether the results are suitable to be used for initial and boundary conditions for the 4/1.333 km WRF simulation.

ENVIRON will perform the following QA/QC of the 4/1.333 km WRF meteorological fields developed for the St. Louis study:

- Initial examination of the WRF data to assure that it has been executed correctly;
- Evaluation of the WRF data using the METSTAT program and the surface meteorological network;
- Evaluation of upper-air WRF meteorological estimates by comparison to upper-air observations and satellite images;
- Evaluation of WRF precipitation estimates against observations from the Advanced Hydrologic Prediction Service (AHPS)[7];

[7] http://water.weather.gov/ahps/

- Generation of the CMAQ-ready meteorological inputs using the MCIP processor and CAMx-ready inputs with the WRFCAMx processor, and review of summary statistics generated by those programs; and
- Backup and archiving of critical model input/output data.

1.5.6 Air Quality Modeling Input Preparation and QA/QC

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

- Verification that correct configuration and science options are used in compiling and running each module in the CMAQ modeling system, where these include MCIP, JPROC, ICON, BCON, and CCTM.
- Verification that correct configuration and science options are used in compiling and running each module in the CAMx modeling system, where these include WRFCAMx, TUV, CAMx, and the CMAQ2CAMx emissions and IC/BC processors.
- Verification that correct input datasets are used when running each model.
- Evaluation of CMAQ and CAMx results to verify that model output is 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.
- Backup and archiving of critical model input data.

The most critical element for CMAQ and CAMx simulations is 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 is 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 we have employed a system of naming conventions using environment variables in the compile and run scripts that guarantee that correct inputs and science options are used. Similar procedures are used in CAMx modeling using file and directory naming conventions. A redundant naming system is employed 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 are located. This is accomplished by using the environment variables in the scripts to specify the names and locations of key input files.

A second key QA procedure is to never "recycle" run scripts, i.e., the modeling team always preserves the original runs scripts and directory structure that were used in performing a model simulation.

The modeling team will also perform a post-processing QA of the CMAQ and CAMx output files similar to that described for the emissions processing. Animated graphic files will be generated using PAVE that can be viewed to search for unexpected patterns in the CMAQ and CAMx output files. In the case of model sensitivity studies, the animated graphic files will be prepared as difference plots for the sensitivity case minus the base case. Often, viewing the animations can discover errors in the emissions inputs. Finally, daily maximum 8-hour ozone and 24-hour average PM plots will be produced for each day of the CMAQ and CAMx simulations. This will provide a summary that can be useful for quickly comparing various model simulations.

The Model Performance Evaluation (MPE) is a multi-step process using several different techniques:

> **ENVIRON Analysis Tools:** ENVIRON has developed ozone performance statistical techniques, "Soccer Plots", time series plots, spatial maps and other summary plots that displays model performance across networks, episodes, species, models and sensitivity tests and compare them against performance goals. These tools can interface with Excel® to generate scatter plots and time series plots. It can also interface with SURFER® to generate spatial maps of model performance. ENVIRON has also developed software to generate 8-hour performance metrics and displays as recommended in EPA's preliminary draft 8-hour ozone modeling guidance (EPA, 1999) that analyze predicted and observed daily maximum 8-hour ozone concentrations near each monitor.
>
> **UCR Analysis Tools:** The University of California at Riverside (UCR) has developed analysis tools that are used extensively in the CENRAP, VISTAS, and WRAP regional haze studies. Graphics are automatically generated using GNUPLOT that generates: (a) tabular statistical measures; (b) time series plots; and (c) scatter plots by all sites and all days, all days for one site, and all sites for one day.
>
> **Atmospheric Model Evaluation Tool (AMET):** AMET was developed by U.S. EPA to aid in the evaluation of meteorological and air quality simulations. AMET utilizes an open source relational database program and an open source statistical program to store and analyze model predictions against observations. AMET is currently script based, and includes numerous scripts for performing common analysis such as scatter plots, box plots, spatial and time series plots, and output of many different statistics.

The evaluation of the CAMx and CMAQ base case simulations will use the appropriate analysis tools listed above to take advantage of their different descriptive and complementary nature. The use of multiple model evaluation tools is also a useful QA/QC procedure to assure that errors are not introduced in the model evaluation process. Statistical performance measures for ozone, ozone precursors, and products species will be calculated to the extent allowed by the St. Louis ambient monitoring network database. For the $PM_{2.5}$ and air toxics simulations, the evaluations will be performed for all resolved gas-phase and particulate species for which data from the various monitoring networks are available.

1.5.7 Proposed Model Performance Goals

The issue of model performance goals for 8-hr ozone and PM species is an area of ongoing research and debate. For 1-hour ozone modeling, EPA has established performance goals for unpaired peak performance, mean normalized bias (MNB) and mean normalized gross error (MNGE) of <±20%, <±15% and <35%, respectively (EPA, 1991). The EPA 8-hour ozone modeling guidance stresses performing corroborative and confirmatory analysis to assure that the model is working correctly (EPA, 2007). EPA's draft 8-hour ozone modeling guidance included comparisons of predicted and observed daily maximum ozone concentrations near the monitor with a <±20% performance goal (EPA, 1999), however this goal was dropped from the final guidance (EPA, 2007). EPA modeling guidance notes that PM models may not be able to achieve goals similar to those of ozone, and that better performance should be achieved for those

PM components that make up the major fraction of total PM mass than those that are minor contributors. Measuring PM species is not as precise as ozone monitoring. In fact, the differences in measurement techniques for some species likely exceed the more stringent performance goals, such as those for ozone. For example, recent comparisons of the PM species measurements using the IMPROVE and STN measurement technologies found differences of approximately $\pm$20% (SO_4) to $\pm$50% (EC) (Solomon et al., 2004).

For the St. Louis PM modeling, we will utilize several levels of model performance goals and criteria that have been used for other PM modeling studies (SCAQMD, 1997, 2003; ENVIRON, 1998; Boylan and Russell, 2006). However, we are not suggesting that specific performance goals be generally adopted and used as pass/fail tests. Rather, we are just using them to frame and put the PM model performance into context and to facilitate model performance intercomparison across episodes, species, models and sensitivity tests.

As noted in EPA's modeling guidance, less abundant PM species should have less stringent performance goals. Accordingly, we are also using performance goals that are a continuous function of average observed concentrations proposed by Dr. James Boylan at the Georgia Department of Natural Resources that have the following features:

- Asymptotically approaching proposed performance goals or criteria when the mean of the observed concentrations are greater than 2.5µg/m^3;
- Approaching 200% error and $\pm$200% bias when the mean of the observed concentrations are extremely small.

Dr. Boylan uses bias/error goals and criteria of ±30%/50% and ±60%/75% and plots bias and error as a function of average observed concentrations. As the mean observed concentration approaches zero the bias performance goal and criteria flare out to ±200% creating a horn shape, hence the name "Bugle Plots".

1.5.8 Diagnostic and Sensitivity Studies

Rarely does a modeling team find that the first simulation satisfactorily meets all (or even most) model performance expectations. Indeed, our experience has been that initial simulations that "look very good", usually do so as the result of compensating errors. The norm is to engage in a logical, documented process of model performance improvement wherein a variety of diagnostic probing tools and sensitivity testing methods are used to identify, analyze, and then attempt to remove the causes of inadequate model performance. This is invariably the most technically challenging and time consuming phase of a modeling study. We anticipate that both the 36/12/4 km ozone and 4/1.333 km $PM_{2.5}$ and air toxics simulations will present some performance challenges that may necessitate focused diagnostic and sensitivity testing in order for them to be resolved. Below we identify the types of diagnostic and sensitivity testing methods that might be employed in diagnosing inadequate model performance and devising appropriate methods for improving the model response.

1.5.8.1 Traditional Sensitivity Testing

Model sensitivity experiments are useful in three distinct phases or "levels" of an air quality modeling study and all will be used as appropriate in the St. Louis modeling study. These levels are:

<u>Level I</u>: Model algorithm evaluation and configuration testing;
<u>Level II</u>: Model performance testing, uncertainty analysis and compensatory error diagnosis; and
<u>Level III</u>: Investigation of model output response (e.g., ozone, aerosol, deposition) to changes in precursors as part of emissions control scenario analyses.

Most of the Level I sensitivity tests with CMAQ and/or CAMx have already been completed by the model developers and the RPOs. However, given the open community nature of the CMAQ and CAMx models, the frequent science updates to the models and supporting databases and the immaturity of fine PM modeling, it is possible that some additional configuration sensitivity testing will be necessary.

Potential Level II sensitivity analyses might be helpful in accomplishing the following tasks:

- To reveal internal inconsistencies in the model;
- To provide a basis for compensatory error analysis;
- To reveal the parameters (or inputs) that dominate (or do not dominate) the model's operation;
- To reveal propagation of errors through the model; and
- To provide guidance for model refinement and data collection programs.

At this time, it is not possible to identify one or more Level II sensitivity runs that might be needed to establish a reliable CMAQ and/or CAMx base case. The merits of performing Level II sensitivity testing will depend upon whether performance problems are encountered in the operational evaluation. Also, the number of tests possible, should performance difficulties arise, will be limited by resources and schedule. Thus, at this juncture, one cannot be overly prescriptive on the number and emphasis of sensitivity runs that may ultimately be desirable. However, from past experience with CMAQ, CAMx and other models, it is possible to identify examples of sensitivity runs could be useful in model performance improvement exercises with the CMAQ/CAMx modeling databases. These include:

- Alternative meteorological realizations of the modeling period;
- Alternative vertical mixing and minimum vertical diffusion coefficient;
- Alternative and/or modified biogenic emissions estimates;
- Modified on-road motor vehicle emissions;
- Modified air quality model vertical grid structure;
- Modified boundary conditions;
- Modified fire emissions;
- Modified EGU emissions;
- Modified ammonia emission estimates;
- Modified aerosol/N_2O_5/HNO_3 chemistry; and
- Modified NH_3 and HNO_3 deposition velocities.

If necessary, Process Analysis extraction outputs can be included in these Level II diagnostic sensitivity simulations in order to provide insight into why the model responds in a particular way to each input modification. Again, the number, complexity, and importance of these types of traditional sensitivity simulations can only be determined once the initial CMAQ/CAMx base case simulations are executed.

Level III sensitivity analyses have two main purposes. First, they facilitate the emissions control scenario identification and evaluation processes. Today, four complimentary sensitivity "Probing Tools" can be used in regional photochemical models depending upon the platform being used. These methods include: (a) traditional or "brute force" testing, (b) the decoupled direct method (DDM), (c) Ozone Source Apportionment Technology (OSAT) and Particulate Source Apportionment Technology (PSAT), and (d) Process Analysis (PA). Each method has its strong points and they will be employed where needed and as resources are available. The second purpose of Level III sensitivity analyses is to help quantify the estimated reliability of the air quality model in simulating the atmosphere's response to significant emissions changes.

Based on experience in other regional studies, examples of Level III sensitivity runs for St. Louis ozone, $PM_{2.5}$ and air toxics modeling might include:

- Ozone, sulfate, nitrate, ammonium and other aerosol sensitivities to SO_2, VOC, NOx, NH_3 and other emissions;
- Ozone, sulfate, nitrate, ammonium and other aerosol sensitivities to elevated point source NO_x emissions;
- Ozone, sulfate, nitrate, ammonium and other aerosol sensitivities to ground level NO_x and VOC emissions including on-road and non-road mobile and area sources; and
- Sulfate, nitrate, ammonium and other aerosol sensitivities to ammonia.

The need to perform sensitivity experimentation (Levels I, II, or III) will depend on the outcome of the initial St. Louis ozone and PM operational performance evaluations. If such a need arises, the ability to actually carry out selected sensitivity and/or diagnostic experiments will hinge on the availability of resources and sufficient time to carry out the analyses. Clearly, selection of the specific analysis method will depend upon the nature of the technical question(s) being addressed at the time.

1.5.8.2 Diagnostic Tests

A rich variety of diagnostic probing tools are available for investigating model performance issues and devising appropriate means for improving the model and/or its inputs. In the previously section we introduced the suite of "probing tools" available for use in the CMAQ and/or CAMx modeling systems. Where the need exists (i.e., if performance problems are encountered) and assuming the St. Louis modeling study elects to use probing tool applications, these techniques could be employed as appropriate to assist in the model performance improvement efforts associated with the St. Louis ozone, $PM_{2.5}$ and air toxics base case development. Here we describe an additional diagnostic method – indicator species and species ratios – that is potentially useful not only in model performance improvement activities but also in judging the models reliability in estimating the impacts on air quality from future emissions. This method involves the use of so-called "indicator species" and species ratios. If, during the conducting of the St. Louis ozone and PM simulations we determine that application of indicator species and species ratio techniques would be beneficial to the study (and if existing project resources allow), we will discuss with the AQMP Technical Workgroup the merits of including this additional probing tool as part of additional work efforts.

Beginning in the mid 1990s, considerable interest arose in the calculation of indicator species and species ratios as a means of diagnosing photochemical model performance and in assessing model credibility in estimating the effects of emissions changes. Major contributions to the development and refinement of this general diagnostic method over the past decade have been made many scientists including Milford et al. (1994), Sillman (1995, 1999), Sillman et al. (1997), Blanchard (2000), Blanchard and Fairley (2001), and Arnold et al. (2003). Recent analytical and numerical modeling studies have demonstrated how the use of ambient data and indicator species ratios can be used to corroborate the future year control strategy estimates of Eulerian air quality models. Blanchard et al. (1999), for example used data from environmental (i.e., smog) chambers and photochemical models to devise a method for evaluating the 1-hour ozone predictions of models due to changes in precursor NOx and VOC emissions. Reynolds et al. (2003) followed up this analysis, augmented with process analysis, to assess the reliability of SAQM photochemical model estimate of 8-hour ozone to precursor emissions cutbacks. These researchers used three indicator ratios (or diagnostic "probes") to quantify the model's response to input changes:

- The ozone response surface probe [O3/NOx];
- The chemical aging probe [NOz/NOy]; and
- The ozone production efficiency probe [O3/NOz].

By closely examining the CMAQ's response to key input changes, properly focused in time and spatial location, Arnold et al. (2003) were able to show not only good agreement with measurements but also convincingly demonstrated the utility of the method for diagnosing model performance in a variety of ways.

Traditionally, indicator species analyses have focused on ozone and its precursor and product species. However the method is equally applicable to PM species and species ratios given sufficient measurement data for comparisons. For example, Ansara and Pandis (1998) demonstrated how indicator species ratios could be applied to show how the modeled mass of PM might respond to sulfate, nitrate and ammonia emissions-related reductions. The extension of these techniques to address CMAQ and CAMx predictions for secondary aerosols, in addition to ozone, will doubtless be quite challenging, but the use of indicator species (e.g., ammonia or HNO_3 limitation for nitrate particle formation) and species ratios appears to offer, at this time, the only real opportunity to quantify the expected reliability of the air quality model to correctly simulate the effects of emissions changes. In the St. Louis CMAQ and CAMx model evaluation, we will remain alert to opportunities to extend the indicator species ratio analyses to the problem of fine particulate in addition to ozone. This is one area where technical collaboration between the ENVIRON team and the AQMP Technical Workgroup can be especially fruitful in terms of identifying and testing emergent methods for challenging the model's ability to correctly simulate the effects of future year emissions changes. Finally, we note that this is truly a current research area and as such may fall outside the scope of the current St. Louis ozone and PM modeling effort. However, given its importance, we will remain alert to opportunities to utilize newly available methods should this prove feasible within the St. Louis modeling study resources and schedule.

1.5.9 Weight of Evidence Analyses

EPA's guidance recommends three general types of "weight of evidence (WOE)" analyses in support of the attainment demonstration: (a) use of air quality model output, (b) examination of air quality and emissions trends, and (c) the use of corroborative modeling. We will consider the use of these methods in conducting the CMAQ/CAMx modeling because it could significantly strengthen the credibility and reliability of the modeling available to the states for their subsequent use. The exact details of the WOE analyses must wait until the St. Louis ozone and PM modeling study evolves further. It is premature to prescribe which, if any of the WOE analyses would be performed since the model's level of performance with the base case modeling is obviously not known at this time. We believe it is always a good idea to perform WOE analysis to corroborate the modeled attainment demonstration. Many of the WOE analyses are independent of the photochemical modeling being conducted by the study team and can potentially be performed by the project sponsors or interested stakeholders. Below are thoughts regarding what would likely be considered as part of the WOE analyses.

Use of Emissions and Air Quality Trends: Emissions and air quality trend analysis is always an important component of a WOE analysis. When combined with meteorological analysis of the yearly ozone formation potential, it can be used to determine whether actual trends can corroborate the model projected determination of whether future-year air quality goals are achieved. Traditionally, these types of analyses are performed by the lead agency's own staff. Thus, these activities will likely be performed by the MDNR and/or IEPA as part of their SIP development.

Use of Corroborative Observational Modeling: While regulatory modeling studies for ozone attainment demonstrations have traditionally relied upon photochemical models to evaluate ozone control strategies, there has recently been growing emphasis on the use of data-driven models to corroborate the findings of air quality models. As noted, EPA's guidance (EPA, 2007) now encourages the use of such observation-based (OBM) or observation-driven (OBD) models. These include receptor models such as Chemical Mass Balance (CMB) model and the Positive Matrix Factorization (PMF) model. Another type of observational modeling is indicator species approach which we have discussed above. We will consider the merits of using these techniques as supportive WOE. While the OBD/OBM models cannot predict future year air quality levels, they do provide useful corroborative information on the extent to which ozone formation in specific subregions may be VOC-limited or NOx-limited, for example, or where controls on ammonia or SO_2 emissions might be most influential in reducing $PM_{2.5}$. Information of this type, together with results of DDM, PA, OSAT and PSAT as well as traditional "brute-force" sensitivity simulations, can be extremely helpful in postulating emissions control scenarios since it helps focus on which pollutant(s) to control.

Use of Corroborative Photochemical Modeling: Noteworthy in EPA's ozone, PM, and regional haze guidance documents is the encouragement of the use of alternative modeling methods to corroborate the performance findings and control strategy response of the primary air quality simulation model (EPA, 2007). This endorsement of the use of corroborative methodologies, stems from the common understanding that no single photochemical modeling system can be expected to provide exact predictions of the observed ozone and PM species concentrations, especially over time scales spanning 1-hour to 1 year. Although the photochemical/PM models identified in EPA's modeling guidance document possess many up-to-date science and computational features, there still can be important differences in modeled gas-phase and aerosol predictions when alternative models are exercised with identical and/or similar inputs. Mindful of EPA's endorsement of corroborative modeling methods and the rigorous use of "weight of evidence" investigations, we recommend that the most recent version of CMAQ and CAMx be carried through the study, including potentially the evaluation of emissions control strategies. Among other things, this will permit the more explicit identification the expected range of model uncertainty and to corroborate the general effectiveness of the CMAQ and/or CAMx ozone and PM control strategies.

1.5.10 Assessing Model Reliability in Estimating the Effects of Emissions Changes

EPA identifies three methods (e.g., EPA, 2001, pg. 228) potentially useful in quantifying a model's reliability in predicting air quality response to changes in model inputs, e.g., emissions. These include:

- Examination of conditions for which substantial changes in (accurately estimated) emissions occur;
- Retrospective modeling, that is, modeling before and after historical significant changes in emissions to assess whether the observed air pollution changes are adequately simulated; and
- Use of predicted and observed ratios of "chemical indicator species".

We note that in some urban-scale analyses, the use of weekday/weekend information has been helpful in assessing the model's response to emissions changes. Such analysis should be examined to determine whether it is appropriate for the St Louis area.

The use of indicator species and ratios offers some promise, and was described earlier in Section 1.5.8.2. The first two methods have actually been considered for over 15 years and were the subject of intensive investigations in the early 1990s in Southern California in studies sponsored by the South Coast Air Quality Management District (Tesche, 1991) and the American Petroleum Institute (Reynolds et al., 1996). To date, neither method has proven useful largely because of the great difficulty in developing historical emissions inventories of sufficient quality to make such an analysis credible and the difficulties in removing the influences of different meteorological conditions such that the modeling signal reflects only the model's response to emissions changes. It is difficult enough to construct reliable emissions inventories using today's modeling technology let alone construct retrospective inventories 5-10 years ago prior to the implementation of significant emissions control programs, major land use changes and widespread adoption of Continuous Emissions Monitors (CEMs).

1.5.11 Future Year Control Strategy Modeling

The specific future year has not been determined, but will be specified by the State Air Agencies (MDNR and IEPA) after U.S. EPA's promulgation of the final 8-hour ozone standard. The 2007 base year emissions will be projected to the future year assuming growth and currently on-the-book (OTB) controls. More details on the development of the future year emissions are described in Chapter 8.

1.5.12 Future Year Ozone and $PM_{2.5}$ Attainment Demonstrations

The St. Louis modeling results will be used to demonstrate attainment of the 8-hour ozone and $PM_{2.5}$ standards. The procedures to be used to demonstrate attainment of the two NAAQS will follow EPA guidance (EPA, 2007). A common theme in the 8-hour ozone and $PM_{2.5}$ attainment demonstration modeling approaches is the use of the model in a relative since to scale the observed Design Values using Relative Reduction Factors (RRFs). RRFs are the ratio of the future-year to current-year modeling results and are used to scale the current-year Design Values to project future-year Design Values that are compared against the air quality standards to determine whether attainment has been demonstrated. Chapter 9 of this Protocol provides more details on the 8-hour ozone and $PM_{2.5}$ attainment demonstration modeling approaches.

1.6 Project Participants and Communication

MDNR and IEPA are the lead state agencies in the development and evaluation of control strategies, research, modeling, and other activities under the AQMP3. They form, together with other local agencies including the East-West Gateway Council of Governments (EWGCOG), U.S. EPA Region VII and Region V, the AQMP Technical Workgroup to conduct and manage the technical work necessary to demonstrate attainment of NAAQS in the St. Louis area including emissions processing and photochemical modeling for the base case as well as source apportionment and sensitivity analysis. The Air Quality Advisory Committee inside the EWGCOG serves as a forum to communication and outreach between local government agencies, stakeholders, the state agencies, and the AQMP Technical Workgroup. MDNR has contracted with a team of ENVIRON International Corporation (ENVIRON), Eastern Research Group (ERG) and Washington University (WU) to provide support for the technical work related to the St. Louis ozone, $PM_{2.5}$ and air toxics modeling activity performed by the AQMP Technical Workgroup. Key participants in the St. Louis modeling study and their contact information are provided in Table 1-1.

An overview of the management organization for the modeling project is provided in Figure 1-1 that shows the lines of responsibility and information flow for activities under this project. Mr. Ralph Morris of ENVIRON will serve as the Principal Investigator, working closely with and under the direction of MDNR. Each specific task has been assigned to managers at ENVIRON and ERG.

Frequent communication between the AQMP Technical Workgroup and the ENVIRON/ERG team as needed, is anticipated. These communications will include e-mails, conference calls, webinars, and face-to-face meetings. Three face-to-face meetings are anticipated to occur in St. Louis or Jefferson City, but other cities could also be accommodated. The AQMP Technical Workgroup will review interim products as they become available so that comments can be received during the study to allow for corrective action as necessary. These interim deliverables would include, but not be limited to, preliminary WRF evaluation, preliminary current and future-year emissions assumptions and results, and preliminary CMAQ and CAMx model performance evaluations.

1.7 Schedule

Table 1-2 lists the schedule for key deliverables under the St. Louis modeling study. The schedule indicates our assumptions about timing and duration of SMOKE and CMAQ/CAMx modeling that will be conducted by the AQMP Technical Workgroup. We understand that it may be necessary to adjust the deliverable deadlines laid out here depending on changing needs of the Workgroup and timing of the availability of various pieces of data needed to conduct the work.

Table 1-1. Key participants and contact information for the St. Louis modeling study.

	Person / Role	**Affiliation / Address**	**Contact Information**
AQMP Technical Workgroup	Adel Alsharafi (MDNR Project Manager)	MDNR P.O. Box 176 Jefferson City, MO 65012	(573) 751-4817 adel.alsharafi@dnr.mo.gov
	Rob Kaleel (IEPA Project Manager)	IEPA 1340 N. 9th Street Springfield, IL 62702	(217) 524-4387 Rob.Kaleel@Illinois.gov
Contracting Team	Ralph Morris (Principal Investigator)	ENVIRON 773 San Marin Drive Novato, CA 94998	(415) 899-0708 rmorris@environcorp.com
	Bonyoung Koo (ENVIRON Project Manager)	ENVIRON 773 San Marin Drive Novato, CA 94998	(415) 899-0722 bkoo@environcorp.com
	Marty Wolf (ERG Project Manager)	ERG 10860 Gold Center Drive Rancho Cordova, CA 95670	(916) 635-6594 marty.wolf@erg.com
	Jay Turner (WU Project Manager)	WU Campus Box 1180 One Brookings Drive St. Louis, MO 63130	(314) 935-5480 jrturner@wustl.edu

Table 1-2. Key deliverables and dates for the St. Louis modeling study.

Deliverables	Date
Draft Modeling Protocol submitted.	May 3, 2011
Approval of Revised Modeling Protocol.	August 31, 2011
PGM-Ready On-road Mobile Emissions for Jun-Sep 2007; SMOKE & SMOKE-MOVES Set-ups.	September 30, 2011[1]
SMOKE-Ready Point/Area/Non-road Emissions for Jun-Sep 2007.	September 30, 2011[1]
SMOKE-BEIS-Ready Landcover Data.	September 30, 2011
SMOKE Speciation Profiles for Air Toxics.	September 30, 2011
PGM-Ready Meteorological Inputs for Jun-Sep 2007.	September 30, 2011
Other PGM Inputs (IC/BC/AHOMAP/TUV/Runscripts).	September 30, 2011
Documentation of Emissions QA/QC.	TBD[2]
Model Performance Evaluation; Recommendations for Sensitivity Analyses.	TBD[3]
SMOKE-Ready Future Year Growth/Control Factors; SMOKE-MOVES Set-up for Future Year On-road Mobile Emissions.	TBD[4]
Draft Final Report	June 30, 2012
Revised Final Report	TBD[5]
Oral Presentation on the Final Results	TBD[6]

[1]Assumes all required external data availability by August 31, 2011. Note that it is still unclear when the SEMAP 2007 inventory will be available. If it won't be available by the end of August 2011, we will discuss the issue with the Technical Workgroup and decide whether to prepare the inventory for the SEMAP states using the 2008 NEI data instead.
[2]Within 60 days of receipt of emissions files from MDNR.
[3]Within 60 days of receipt of modeling results from MDNR.
[4]Within 90 days of selection of the future year to model. MDNR will determine the future year after EPA finalizes the new ozone standard.
[5]Within 30 days of receipt of MDNR comments on the Draft Final Report.
[6]Requires minimum of 15 days advance notice from MDNR.

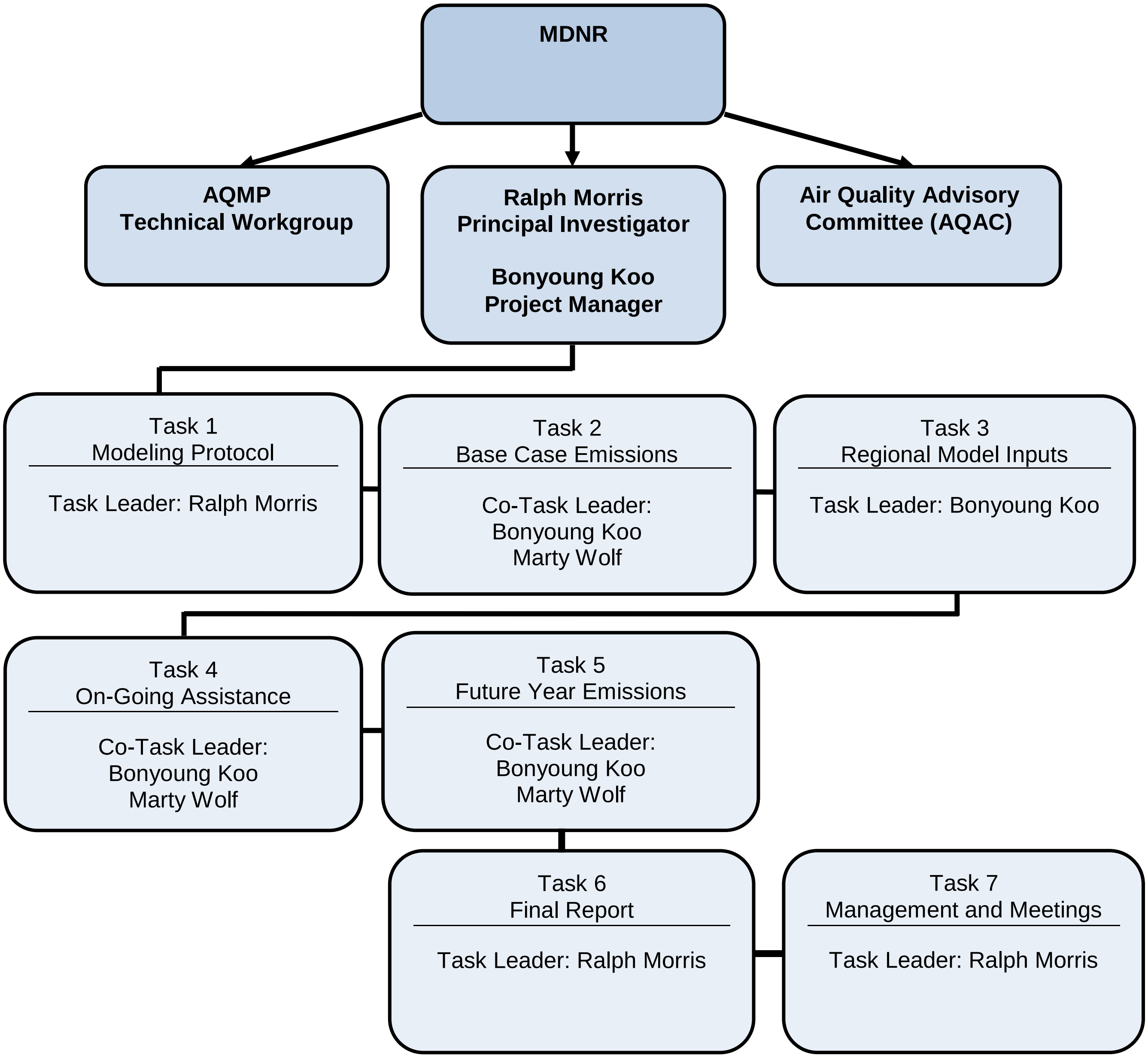


Figure 1-1. Management organizational chart showing key contractor personnel and their duties for the St. Louis modeling study.

2.0 MODEL SELECTION

This section introduces the models to be used in the St. Louis criteria and air toxics modeling study. The selection methodology presented in this chapter rigorously adheres to EPA's guidance for regulatory modeling in support of ozone and fine particulate attainment demonstrations (EPA, 2007). Unlike previous ozone 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.

All of these considerations should be examined for each class of models to be used (e.g., emissions, meteorological, and photochemical) in part because EPA no longer recommends a specific model or suite of photochemical models for regulatory application as it did twenty years ago (EPA, 1991). After identifying the models we believe are best suited to the requirements of the St. Louis criteria and air toxics modeling study, the justification for their selection is discussed. The actual science configurations we recommend for each model in this study are introduced in Chapter 5.

EPA's new guidance on model selection and justification requires a substantial effort to document the past evaluation studies, peer-reviews and application efforts associated with the models recommended for use. Many of the relevant citations are presented in the References section of this report.

2.1 Regulatory Context for Model Selection

A comprehensive modeling protocol for the St. Louis ozone, $PM_{2.5}$ and air toxics study consists of many elements. Its main function is to serve as a means for planning and communicating how a modeled attainment demonstration will be performed *before* it occurs (EPA, 1999; 2007). The protocol guides the technical details of a modeling study and provides a formal framework within which the scientific assumptions, operational details, commitments and expectations of the various participants can be set forth explicitly and means for resolution of potential differences of technical and policy opinion can be worked out openly and within prescribed time and budget constraints.

2.1.1 Summary of Recommended Models

To develop new ozone, $PM_{2.5}$ and air toxics modeling episodes for the St. Louis area, the following state-of-science regional meteorological, emissions and air quality models will be used. The science features of these models and the justification for their selection are given later in this section.

WRF: The Weather Research and Forecasting (WRF) Model is a next-generation mesoscale prognostic meteorological model routinely used for urban- and regional-scale photochemical, fine particulate, and regional haze regulatory modeling studies.

Developed jointly by the National Center for Atmospheric Research and the National Centers for Environmental Prediction, WRF is maintained and supported as a community model by researchers and practitioners around the globe. The code supports two modes: the Advanced Research WRF (ARW) version and the Non-hydrostatic Mesoscale Model (NMM) version. WRF-ARW has become the new standard model used in place of the older Mesoscale Meteorological Model (MM5) for regulatory air quality applications in the U.S. It is suitable for use in a broad spectrum of applications across scales ranging from meters to thousands of kilometers.

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 an existing base emissions inventory data into the hourly gridded and speciated 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.

MOVES: The MOtor Vehicle Emission Simulator model (MOVES) is a multi-scale emissions modeling system that generates emission inventories or emission rate lookup tables for on-road mobile sources. MOVES is capable of creating inventories or lookup tables at the national, state, county, or project scales. MOVES was designed by EPA's Office of Transportation and Air Quality (OTAQ) and their latest release version as of August 2010 is MOVES2010a. MOVES is principally an emissions modeling system where emissions estimates are simulated from 'first principles' taking into account the effects of fleet age deterioration, ambient temperature and humidity, activity patterns, fuel properties, and inspection and maintenance programs on emissions from all types of motor vehicles. MOVES outputs can be input to emissions processing systems such as SMOKE.

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, 2010). CAMx 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 (a) simulate air quality over many geographic scales, (b) 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, (c) provide source-receptor, sensitivity, and process analyses and (d) be computationally efficient and easy to use. The U.S. EPA has approved the use of CAMx for numerous ozone and PM State Implementation Plans throughout the U.S, and has used this model to evaluate regional mitigation strategies including those for recent regional rules (e.g., CAIR, NOx SIP Call, etc.).

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) a meteorological module for the description of atmospheric states and motions, (b) an emission models for man-made and natural emissions that are injected into the atmosphere, and (c) a chemistry-transport modeling system for simulation of the chemical transformation and fate.

2.1.2 Rationale for Use of Parallel, Corroborative Modeling Systems

EPA's guidance on model selection for SIP modeling (EPA, 2007) does not identify a preferred photochemical modeling system, recognizing that there is no single model which has been extensively tested and shown to be clearly superior or easier to use than several alternatives. The agency recommends that models used for SIPs should meet the requirements for alternative models. The models we recommend for the St. Louis 8-hr ozone and $PM_{2.5}$ SIP modeling (e.g., CAMx, CMAQ) meet these requirements.

From recent experience in the RPO regional haze modeling for VISTAS, CENRAP, WRAP and MRPO, there is significant value in including parallel regional models in favor of just one air quality modeling platform. For example, in an operational and diagnostic evaluation of the CAMx and CMAQ models in the VISTAS regional haze program (Tesche et al., 2006) revealed that while both models produce results of comparable accuracy and reliability, some particular features of model response invited more detailed diagnostic efforts, culminating in improvements to the chemistry and physics of both models (Morris et al., 2005a,b).

This parallel application of models, including preparing model inputs, diagnosing and improving model performance and in conducting weight-of-evidence investigations leads to a strengthening of the overall modeling effort. Thus, for St. Louis, we recommend joint, integrated use of CAMx and CMAQ together to achieve following seven specific purposes:

Diagnosis: To serve as an efficient diagnostic tool addressing model performance issues that may arise in the simulation of the 8-hr ozone modeling episodes. CAMx's suite of diagnostic probing tools plus its flexi-nesting algorithms make it an attractive tool for assisting in the diagnosis of CMAQ performance should unexpected situation arise;

Model Evaluation Corroboration: To provide corroboration of the base case model performance evaluation exercises to be performed with CAMx and CMAQ and help identify any compensatory errors in the modeling systems;

Emissions Control Response Corroboration: To provide corroboration of the response of the two modeling systems to generic and specific future year emissions changes on modeled gas-phase concentrations;

Quantification of Model Uncertainty: To provide one estimate of the range of uncertainty that attends statements of air quality model performance in the episodic base case simulations and in the estimate of 8-hr ozone reductions associated with future emissions change scenarios;

Alternative Science: CMAQ contains alternative science algorithms that may elucidate model performance issues with CAMx (or vice versa);

Consistency with Other Modeling Studies: The Midwest RPO is using CAMx for their ozone, $PM_{2.5}$ and regional haze modeling whereas the southeastern states (SEMAP) are primarily using CMAQ. The EPA used the CAMx model and its ozone and PM source apportionment capability in its Transport Rule (TR). The CAMx source apportionment may also be useful in the St. Louis modeling for the Transport SIP component.

Backup Contingency: To provide a 'backstop' model in the event that unforeseen difficulties or schedule/resource constraints make it necessary to switch to the use of a single modeling system at some point in the study.

The benefits of employing a pair of complimentary state-of-science air quality models are thus quite significant and well worth considering. Especially considering that the same WRF output (through WRFCAMx and MCIP) and SMOKE output can be used to operate both models without performing significant, additional meteorological or emissions modeling. In particular, ENVIRON has developed CAMx2CMAQ and CMAQ2CAMx processing tools that can convert inputs from one modeling system to the other.

2.2 Details of the Recommended Models

Further details of the models we propose for use in the St. Louis ozone, $PM_{2.5}$ and toxics modeling effort are described below. More information on these models may be obtained from the WRAP, VISTAS, CENRAP, and other modeling protocols (Morris et al., 2004a,b; Tesche et al., 2005b) and the literature references cited therein.

2.2.1 The WRF Meteorological Model

The non-hydrostatic version of the WRF model (WRF-ARW; Skamarock et al. 2008; Michalakes et al. 2001) is a three-dimensional, limited-area, primitive equation, prognostic model that has been used widely in regional air quality model applications. The basic model has been under continuous development, improvement, testing and open peer-review for more than 10 years and has been used world-wide by hundreds of scientists for a variety of mesoscale studies, including cyclogenesis, polar lows, cold-air damming, coastal fronts, severe thunderstorms, tropical storms, subtropical easterly jets, mesoscale convective complexes, desert mixed layers, urban-scale modeling, air quality studies, frontal weather, lake-effect snows, sea-breezes, orographically induced flows, and operational mesoscale forecasting.

WRF is based on the prognostic equations for three-dimensional wind components (u, v, and w), temperature (T), water vapor mixing ratio (q_v), and the perturbation pressure (p'). Use of a constant reference-state pressure increases the accuracy of the calculations in the vicinity of steep terrain. The model uses an efficient semi-implicit temporal integration scheme and has a nested-grid capability that can use multiple domains of arbitrary horizontal and vertical resolution. The interfaces of the nested grids can be either one-way or two-way interactive.

WRF uses a terrain-following non-dimensionalized pressure, or "eta", vertical coordinate similar to that used in many operational and research models. The gridded meteorological fields produced by WRF are directly compatible with the input requirements of ‘one atmosphere’ air-quality models using this coordinate (e.g., CMAQ). WRF fields can be easily used in other regional air quality models with different coordinate systems (e.g., CAMx) by performing a vertical interpolation, followed by a mass-conservation re-adjustment.

Distinct planetary boundary layer (PBL) parameterizations are available for air-quality applications, both of which represent sub-grid-scale turbulent fluxes of heat, moisture and momentum. These parameterizations employ various surface energy budget equations to estimate ground temperature (T_g), based on the insolation, atmospheric path length, water vapor, cloud cover and longwave radiation. The surface physical properties of albedo, roughness length, moisture availability, emissivity and thermal inertia are defined as functions of land-use for numerous categories via a look-up table. One scheme uses a first-order eddy diffusivity formulation for stable and neutral environments and a modified first-order scheme for unstable regimes. Other schemes use a prognostic equation for the second-order turbulent kinetic energy, while diagnosing the other key boundary layer terms.

Initial and lateral boundary conditions are specified from mesoscale three-dimensional analyses performed at regular intervals (12 hours, 6 hours, etc.) on the outermost grid mesh selected by the user. Additional surface fields are analyzed at shorter intervals. A Cressman-based technique is used to analyze standard surface and radiosonde observations, using the National Meteorological Center's (NMC) spectral analysis as a first guess. The lateral boundary data are introduced into WRF using a relaxation technique applied in the outermost five rows and columns of the most coarse grid domain. The top boundary is set at a constant pressure level, with gravity wave absorption via diffusion or Rayleigh damping.

Results of detailed performance evaluations of the WRF modeling system in regulatory air quality application studies have been reported in the literature (e.g., EPA 2007; Gilliam et. al., 2009) and many have involved comparisons with other prognostic models such as MM5. Although WRF includes many of the same physics parameterizations as MM5, many newer physics choices have been developed since MM5 development ceased in 2004. We expect WRF to perform as well or better than MM5 in almost all situations.

2.2.2 The SMOKE Emissions Modeling System

Emissions modeling for the St. Louis SIP modeling will be performed primarily with SMOKE (version 2.7). The Sparse Matrix Operator Kernel Emissions (SMOKE) Emissions Processing System Prototype was originally developed at MCNC (Coats, 1995). 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 sometimes output from transportation travel-demand models.

SMOKE was originally designed to allow emissions data processing methods to utilize emergent high-performance-computing (HPC) as applied to sparse-matrix algorithms. Indeed, SMOKE is the fastest emissions processing tool currently available to the air quality modeling community. The sparse matrix approach utilized throughout SMOKE permits both rapid and flexible processing of emissions data. The processing is rapid because SMOKE utilizes a series of matrix calculations instead of less efficient algorithms used in previous systems such as EPS and EMS. The processing is flexible because the steps of temporal projection, controls, chemical speciation, temporal allocation, and spatial allocation are separated into independent operations wherever possible. The results from these steps are merged together at a final stage of processing.

SMOKE supports area, mobile, fire and point source emission processing and also includes biogenic emissions modeling through a rewrite of the Biogenic Emission Inventory System, Version 3 (BEIS3). SMOKE has been available since 1996, and it has been used for emissions processing in a number of regional air quality modeling applications. In 1998 and 1999, SMOKE was redesigned and improved for EPA for use CMAQ. The primary purposes of the SMOKE redesign were support of: (a) emissions processing with user-selected chemical mechanisms and (b) emissions processing for reactivity assessments.

SMOKE contains a number of major features that make it an attractive component of the HC-2 modeling system (Seppanen, 2005). The model supports a variety of input formats from other emissions processing systems and models including the Inventory Data Analyzer (IDA), Emissions Modeling System-2003 (EMS-2003), and the Emissions Preprocessor System (EPS2.x and EPS3). It supports both gridded and county total land use schemes for biogenic emissions modeling. Although not necessary in St. Louis, SMOKE can accommodate emissions files from up to 10 countries and any pollutant can be processed by the system.

Recent computational improvements to SMOKE include: (a) enhanced disk space requirements compared with other emissions processing software, (b) run-time memory allocation, eliminating any need to recompile the programs for different inventories, grids, or chemical mechanisms, and (c) updated I/O API libraries. A number of science features have been incorporated into the "current" version of SMOKE (version 2.7) including: (a) any chemical mechanism can be used to partition pollutants to model species, as long as the appropriate input data are supplied, (b) integration with the MOVES on-road mobile source emissions model using the SMOKE-MOVES Integration Tool, (c) support of plume-in-grid (PiG) processing (note that CMAQ no longer supports the plume-in-grid processing; CAMx does), (d) integration of the BEIS3 emissions factors in SMOKE.

Notable features of SMOKE from an applications standpoint include: (a) improved control strategy input formats and designs, (b) control strategies can include changes in the reactivity of emitted pollutants, a useful capability, for example, when a solvent is changed in an industrial process, (c) no third party software is required to run SMOKE, although some input file preparation may require other software, (d) fewer SMOKE programs than the SMOKE prototype because programs were combined where possible to be used for multiple source categories, (e) integration with Models-3 file formats and settings, (f) improved data file formats, (g) support of various air quality model emissions input formats (e.g., CMAQ, MAQSIP, UAM-IV, UAM-V, REMSAD and CAMx), (h) enhanced quality assurance pre- and post-processing, (h) fully integrated with Models-3, which will provide the SMOKE Tool for SMOKE input file preparation, (i) enhanced treatment of growth and control factors, (j) improved emissions reporting and QA capabilities, and (k) improved temporal allocation.

Continuing model development activities with SMOKE now occur at the University of North Carolina (UNC) Carolina Environmental Program (CEP). SMOKE 2.7 is the latest version that is recommended for the various St. Louis modeling episodes. The SMOKE executables, scripts and databases may be downloaded through the Community Modeling and Analysis (CMAS) center's Software Clearinghouse[1]. The SMOKE user's guide is also available online at the main SMOKE website[2].

2.2.3 The MOVES Motor Vehicle Emission Model

MOVES is the U.S. EPA's Motor Vehicle Emission Simulator[3]. The purpose of the tool is to provide an accurate estimate of emissions from mobile sources under a wide range of user-defined conditions. In the modeling process, the user specifies vehicle types, time periods, geographical areas, pollutants, vehicle operating characteristics, and road types to be modeled. The model then performs a series of calculations, which have been carefully developed to accurately reflect vehicle operating processes, such as cold start or extended idle, and provide estimates of bulk emissions or emission rates. Specifying the characteristics of the particular scenario to be modeled is done by creating a Run Specification, or RunSpec.

In December 2009, the EPA Office of Transportation and Air Quality (OTAQ) publicly released the first version of the MOVES model as a replacement to EPA's previous model for estimating on-road mobile source emissions, MOBILE6, which must be used for generating on-road mobile source emissions in future SIPs, including those being developed as part of the St. Louis study. MOVES is different from MOBILE6 in that it was deliberately designed to work with databases. With this design, new data that may become available can be more easily incorporated into the model. In addition, MOVES allows and facilitates the import of data specific to a user's unique needs.

The MOVES model includes a "default" database that summarizes emission relevant information for the entire United States. The data for this database comes from many sources including EPA research studies, Census Bureau vehicle surveys, Federal Highway Administration travel data, and other federal, state, local, industry and academic sources. The MOVES team continually works to improve this database, but, for many uses, up-to-date local inputs will be more appropriate, especially for analyses supporting State Implementation Plans (SIPs) and conformity determinations.

MOVES2010a is the latest version of the MOVES emissions modeling tool. MOVES2010a builds on the functionality of previous MOVES versions: MOVES2004, MOVESDemo, DraftMOVES2009, and MOVES2010. MOVES can be used to estimate national, state, and county level inventories of criteria air pollutants, greenhouse gas emissions, and some mobile source air toxics from highway vehicles. Additionally, MOVES can make projections for energy consumption (total, petroleum-based, and fossil-based).

[1] http://www.cmascenter.org/download/software.cfm
[2] http://www.smoke-model.org/version2.7/
[3] http://www.epa.gov/otaq/models/moves/index.htm

While MOVES provides more detailed approach to modeling mobile emissions than MOBILE6, it is also much more computationally demanding. To address this issue, the EPA Office of Air Quality Planning and Standards (OAQPS) contracted with ENVIRON and UNC to implement a computationally efficient MOVES emissions capability in SMOKE, that is, SMOKE-MOVES. There are three steps to the SMOKE-MOVES modeling system:

1. Meteorological preprocessing of grid cell temperature and humidity using a tool developed by UNC.
2. Running a driver script for MOVES, which assembles the RunSpec files, builds county data input MySQL tables, and launches the MOVES RunSpec files for multiple counties in batch, developed by ENVIRON.
3. Running a post-processing script that speciates the PM emission rates, drops unnecessary fields to control file size, and formats other aspects of the lookup tables so they are transformed into SMOKE-ready files, developed by ENVIRON.

The new SMOKE-MOVES Integration Tool was released in July 2010 through the CMAS center's Software Clearinghouse and the User's Guide is available online at the main SMOKE website[4].

2.2.4 The CAMx Regional Photochemical Model

The Comprehensive Model with Extensions (CAMx) modeling system is a publicly available[5] three-dimensional multi-scale photochemical/aerosol grid modeling system that is developed and maintained by ENVIRON International Corporation. CAMx was developed with all new code during the late 1990s using modern and modular coding practices. This has made the model an ideal platform for the extension to treat a variety of air quality issues including ozone, particulate matter (PM), visibility, acid deposition, and air toxics. The flexible CAMx framework has also made it a convenient and robust host model for the implementation of a variety of mass balance and sensitivity analysis techniques including Process Analysis (IPR, IRR, and CPA), Decoupled Direct Method (DDM), and the Ozone/Particulate Source Apportionment Technology (OSAT/PSAT). Designed originally to address multiscale ozone issues from the urban- to regional-scale, CAMx has been widely used in recent years by a variety regulatory agencies for 1-hour and 8-hour ozone SIP modeling studies. Key attributes of the CAMx model for simulating gas-phase chemistry include the following:

- Two-way grid nesting that supports multi-levels of fully interactive grid nesting (e.g., 36/12/4/1.333 km);
- CB05, CB4 or SAPRC99 Chemical Mechanisms. ENVIRON has recently developed the CB6 chemical mechanism that is implemented in an internal version of CAMx;
- Two chemical solvers, the Euler Backward Iterative (EBI) solver and the Implicit Explicit Hybrid (IEH) solver (the Livermore Solver for Ordinary Differential Equations (LSODE) is also available as a reference method);
- Multiple numerical algorithms for horizontal transport including the Piecewise Parabolic Method (PPM) and Bott advection solvers;
- Subgrid-scale Plume-in-Grid (PiG) algorithm to treat the near-source plume dynamics and chemistry from large NOx, VOC, SOx, and/or PM point source plumes;

[4] http://www.smoke-model.org/smoke_moves_tool/
[5] http://www.camx.com

- Ability to interface with a variety of meteorological models including the MM5, WRF and RAMS prognostic hydrostatic meteorological models and the CALMET diagnostic meteorological model (others also compatible);
- The Ozone Source Apportionment Technology (OSAT) and Particulate Source Apportionment Technology (PSAT) that identifies the ozone or PM contribution due to geographic source regions and source categories (e.g., mobile, point, biogenic, etc.); and
- The Higher-order Decoupled Direct Method (HDDM) sensitivity analysis tool is implemented for emissions, IC/BC, and reaction rates to obtain first- and second-order sensitivity coefficients for all gas-phase species.

Culminating extensive model development efforts at ENVIRON and other participating groups, the CAMx Version 5.30 was released in March 2010 as a truly "One-Atmosphere" models that rigorously integrates the gas-phase ozone chemistry with the simulation of primary and secondary fine and course particulate aerosols. This extension of CAMx to treat PM involved the addition of several science modules to represent important physical processes for aerosols, including RADM aqueous-phase chemistry module, SOAP secondary organic aerosol partitioning module, and ISORROPIA inorganic aerosol thermodynamics module.

We recommend exercising CAMx (version 5.3) in parallel with CMAQ for the St. Louis modeling, using as many similar science options and input data sets as possible. However, in some instances, the CMAQ and CAMx model development teams chose different options for characterizing physical and chemical processes, or for implementing the governing equations on modern parallel computers. In these cases, we will utilize the science configurations embodied in the current release of CAMx. Note that ENVIRON has recently implemented CB6 in CAMx v5.3. CB6 reflects the latest chemical kinetic data and updated aromatic chemistry that may be important for simulating ozone in the St. Louis urban area. CB6 is backward compatible with CB05, thus existing emission speciation profiles for CB05 can be used. Even with the emissions speciated for CB05, we can still benefit from CB6's updated reactions of aromatics, isoprene, ketones and production of HO_2 radicals from RO_2 radicals.

2.2.5 The CMAQ Regional Photochemical Model

For more than a decade, EPA has been developing the Models-3 Community Multiscale Air Quality (CMAQ) modeling system with the overarching aim of producing a "One-Atmosphere" air quality modeling system capable of addressing ozone, particulate matter (PM), visibility and acid deposition within a common platform (Dennis et al., 1996; Byun et al., 1998; Byun and Ching, 1999; Pleim et al., 2003, 2004, 2005, 2006; Roselle et al., 2008). The original justification for the Models-3 development emerged from the challenges posed by the 1990 Clean Air Act Amendments and EPA's desire to develop an advanced modeling framework for 'holistic' environmental modeling utilizing state-of-science representations of atmospheric processes in a high performance computing environment. EPA completed the initial stage of development with Models-3 and released CMAQ in mid-1999 as the initial operating science model under the Models-3 framework (Byun and Ching, 1999).

CMAQ consists of a core Chemical Transport Model (CTM) and several pre-processors including the Meteorological-Chemistry Interface Processor (MCIP), initial and boundary conditions processors (ICON and BCON) and a photolysis rates processor (JPROC). EPA is continuing to improve and develop new modules for the CMAQ model and typically provides a new release each year. In the past EPA has also provides patches for CMAQ as errors are discovered and corrected. EPA has funded the Community Modeling and Analysis Systems (CMAS) center to support the coordination, update and distribution of the Models-3 system.

A number of features in CMAQ's theoretical formulation and technical implementation make the model well-suited for regional 8-hr ozone and annual PM modeling in St. Louis. In CMAQ, the modal approach has been adapted to dynamically represent the PM size distribution using three log-normal modes (two fine, and one coarse). The thermodynamics of inorganic aerosol composition are treated using the ISORROPIA module. Aerosol composition is coupled to mass transfer between the aerosol and gas phases. For aqueous phase chemistry, the RADM model is currently employed. This scheme includes oxidation of SO_2 to sulfate by ozone, hydrogen peroxide, oxygen catalyzed by metals and radicals. The impact of clouds on the PM size distribution is treated empirically. For wet deposition processes, CMAQ uses the RADM/RPM approach. Particle dry deposition is included as well. CMAQ models secondary organic aerosol (SOA) based on the Secondary Organic Aerosol Model (SORGAM) which is a reversible semi-volatile scheme whereby VOCs can be converted to condensable gases that can then form SOA and then evaporate back into condensable gases depending on atmospheric conditions.

Roselle et al., (2008) describes new features implemented in CMAQ ver 4.7. Notable updates include: (a) additional SOA forming pathways (SOA from isoprene and sesquiterpenes, acid-catalyzed SOA formation, in-cloud SOA formation); (b) multi-pollutant capability (hazardous air pollutants (HAPs) and mercury in single modeling platform); (c) enhanced heterogeneous HONO reaction; and (d) new diagnostic tools (Decoupled Direct Method in 3 dimensions (DDM-3D), Sulfur Tracking, Primary Carbon Apportionment).

The CMAQ model code is released through the CMAS center's Software Clearinghouse. The most recent rendition is CMAQ version 4.7.1 released in June 2010. EPA is in the process of completely revamping the CMAQ code to make it more modular and plans to release CMAQ version 5 later in 2011.

2.3 Justification for Model Selection

2.3.1 WRF (v3)

The most commonly used prognostic meteorological models to support air quality modeling are WRF and MM5. A number of recent studies inter-compare the theoretical formulations and operational features of these models and evaluate their performance capabilities under a range of atmospheric conditions. However, development of MM5 ceased in December 2004, and users are strongly encouraged by NCAR to move to the new model, WRF. WRF is therefore recommended as the prognostic meteorological modeling component for the St. Louis study for the following reasons:

- All of the available state-of-science regional photochemical models identified in EPA's 8-hour modeling guidance can be operated without difficulty using inputs supplied by the WRF;
- The WRF model has at least an equivalent application history in regulatory ozone modeling studies compared with MM5;

- While the study team has extensive experience exercising both WRF and MM5 in different urban and regional-scale studies, in most recent regulatory ozone applications the WRF model has been the preferred system.
- A WRF run (36-/12-km domain) has already been performed by the states of Iowa and North Carolina, and can be used to initialize the finer domains for ozone and PM modeling.

2.3.2 SMOKE (v2.7)

The SMOKE modeling system is recommended as the emissions model for the St. Louis modeling study for the following reasons:

- SMOKE is a mature, thoroughly-tested emissions modeling system and has been employed by a wide variety of governmental, commercial, academic, and private users in numerous regions throughout the U.S. and abroad.
- The science team has considerable experience with the model, in part because ENVIRON staff members have been using SMOKE for many years to develop the regional modeling inventories for WRAP, CENRAP, VISTAS, and Houston.
- SMOKE provides several quality assurance and error checking routines, thereby allowing the study team to perform an independent verification of the base year and future year emissions inventories developed for this project.

2.3.3 MOVES (v2010a)

The MOVES model is required for the St. Louis modeling study because it is the current official regulatory tool for use with State Implementation Plans. The ENVIRON/ERG team has considerable experience with the MOVES model. ENVIRON was part of a team that developed the SMOKE-MOVES Integration Tool for EPA's Office of Air Quality Planning and Standards and thus has an intimate knowledge of the model.

2.3.4 CAMx (v5.3)

During the NARSTO Critical Tropospheric Ozone Assessment, two major reviews of photochemical modeling were performed. Russell and Dennis (2000) compared the scientific and operational features of essentially all current recent Eulerian photochemical models in use up to that time. In parallel, Roth et al., (1998, 2005) reviewed more than twenty regulatory applications of photochemical models in the U.S. and Canada. From these reviews, and the modeling team's experience with each of these models, we recommend CAMx as one of the two ozone modeling tools for the St. Louis study the following reasons:

- CAMx is a state-of-science "one-atmosphere" model.
- CAMx has undergone extensive successful testing by a variety of groups for nearly a decade.
- CAMx is unique among state-of-science "one-atmosphere" air quality models in its ability to offer ozone and particulate source apportionment technology (OSAT, PSAT), Process Analysis, and the DDM sensitivity analysis scheme.
- CAMx has been used extensively for numerous recent 8-hour ozone SIPs including Denver, Oklahoma, St. Louis, and areas in Texas and other regulatory modeling

including the EPA to support for regulatory decision making (e.g., CAIR, NOx SIP Call, etc.).
- CAMx is a public-domain model, available free of charge, without restriction.
- We will also consider using an internal version (publicly available on request) of CAMx v5.3 that uses the CB6 chemical mechanism.

2.3.5 CMAQ (v4.7.1)

Many of the reasons justifying the choice of CAMx also apply to CMAQ. In particular,

- CMAQ is a state-of-science "one-atmosphere" model for gas phase photochemistry and fine particulate aerosol.
- CMAQ has undergone extensive testing within EPA ORD/OAQPS (Arnold et al., 2003) and by external State regulatory agencies (e.g., Sistla et al., 2001), and scientific groups (Tesche et al., 2006; Morris et al., 2005a,b).
- CMAQ has been successfully applied in Houston for the Aug-Sept 2000 episode (Byun et al., 2004, 2005) and used by many RPOs including CENRAP, WRAP,and VISTAS.
- CMAQ is a public-domain model, available free of charge, without restriction.

2.4 Model Limitations

All mathematical models possess inherent limitations owing to the necessary simplifications and approximations made in formulating the governing equations, implementing them for numerical solution on fast computers, and in supplying them with input data sets and parameters that are themselves approximations of the full state of the atmosphere and emissions processes. Below, we list the more important limitations of the various modeling systems to be employed in the St. Louis study.

2.4.1 WRF

Because WRF shares with MM5 a number of physics parameterizations (e.g. both contain the Pleim-Xiu PBL scheme) both would suffer from similar science limitations. For example, the proper treatment of vertical turbulent mixing and the estimate of the PBL heights are among the important current science limitations in models like MM5 and WRF. In general, numerous meteorological processes are microscale in nature and cannot be captured by a prognostic meteorological model using a grid resolution of kilometers. Convective precipitation, in particular, is difficult to correctly simulate. When coarser resolution is used (e.g., 36 and 12 km) the convective precipitation can be subgrid-scale so is parameterized. At resolutions less than 10 km it can be explicitly modeled. In the past MM5 has had difficulty in correctly simulating convective precipitation and is an area that will have to be closely examined and evaluated in WRF.

2.4.2 SMOKE

All emissions modeling systems have uncertainties and limitations. Foremost among these are the initial emissions estimates provided as input to the emissions models. However, even with exact emission estimates as inputs (an unlikely event) the emissions models still have numerous limitations just because of the sheer volume of data that needs to be characterized and processed and the limited amount of data available to make the characterization:

> **Spatial Allocation**: Emissions modeling system use surrogate distributions to spatially distribute county-level emissions. For example agricultural land use category would be used to spatially distribute agricultural equipment emissions, population may be used for a variety of home related emissions (e.g., home heating, aerosol sprays, etc.). The accuracy of these surrogate distributions will likely vary by source category.
>
> **Temporal Allocation**: The allocation of annual average emissions to months and across the diurnal cycle use typical distributions by source category. The accuracy of these temporal allocations varies by source type within broader categories (e.g., heavy-duty diesel vs. light duty gas within the on-road category). They may also vary over different days. For example, a typical temporal distribution for a Sunday may be quite different on days when the St. Louis Rams are in town.
>
> **Chemical Speciation**: Emission models need to chemically speciate the VOC emissions into the photochemical mechanism (e.g., CB05) used in the photochemical grid model based on industrial codes. There are actually a limited number of speciation profiles and individual source tests have not been conducted for all different types of sources; consequently speciation profiles are assigned to "similar" sources that have source profile measurements.
>
> **Emission Projections**: Projecting emissions introduce the largest layer of uncertainty. Emission projections include growing emissions from a current (e.g., 2007) to future (e.g., 2020) year and then the application of any appropriate controls. Both of these steps are characterized by potentially huge limitations.

2.4.3 MOVES

Due in part to its database platform, MOVES run time duration can be quite long. In order to speed up processing time, ENVIRON has a dedicated cluster of machines solely for running MOVES, both in Windows and more recently on Linux. ENVIRON has experimented with parallel computing, utilizing the model's master-worker architecture to divide large MOVES runs into multiple sets of master-worker configurations. Parallel computing has proven to be an effective strategy for larger scale runs. Additionally, ENVIRON has configured MOVES2010a to run in the Linux environment and we are seeing additional improvements in computation time for this operating system. Aside from run time considerations, the MOVES model is relatively new and some model features are still not fully tested. ENVIRON was recently tasked with overseeing the MOVES emissions development efforts for SESARM states and found conflicts between the MOVES default database and the new SMOKE-MOVES Integration Tool approach of using representative counties. We have developed and tested an effective workaround approach that will be used in the St. Louis modeling study to prevent scheduling delays and ensure high quality results.

2.4.4 CAMx

Like all air quality models, there are a number of conceptual, physical, chemical, computational and operational challenges that CAMx model developers and the user community face to one extent or another. Indeed, many of these are common to CMAQ as well (see below). One current limitation is the treatment of vertical turbulent mixing where there are alternative means for estimating the time and space variation in turbulent mixing. By default, CAMx employs a standard "K-theory" approach for vertical diffusion to account for sub-grid scale mixing layer-to-layer. A recent update to CAMx (version 5.10) implemented the Asymmetric Convective Model Version 2 (ACM2; Pleim, 2007) which uses K-theory for mixing between adjacent layers and includes mixing between non-adjacent layers only for transfer from the surface to layers aloft during convective conditions. Another common drawback of CAMx (and CMAQ as well) is the extensive emissions, meteorological and IC/BC inputs needed to operate the model. Treatment of clouds and wet deposition is an area of current research that needs to be updated. A practical limitation of CAMx is the computational requirements, including the need of significant disk space.

2.4.5 CMAQ

As with CAMx, a major limitation of CMAQ is the substantial emissions, meteorological and IC/BC input data requirements. Unlike most models used in regulatory studies, the CMAQ system has undergone extensive peer review (see, for example, Amar et al., 2004, 2005). A number of the limitations in earlier versions of CMAQ have been rectified and current challenges, many identified by the peer-reviewers but also a number raised by the user community are being assessed by EPA in their current and future work plans (EPA, 2005a, 2007).

One of the operational limitations of CMAQ is lack of any two-way grid nesting, which limits the ability of the model to properly resolve point source plumes or urban photochemistry and their effects on more distant Class I areas without a prohibitive number of grid cells. Like CAMx, another limitation of CMAQ is the computational requirements, including the need of substantial disk space.

None of the current limitations identified in the WRF, SMOKE, MOVES, CAMx and CMAQ models render any of these models inappropriate for their use in this study, and are in fact common to all current models available for this type of application. However, such limitations need to be recognized and accounted for in the interpretation of the modeling results.

2.5 Model Input Requirements

Each of the modeling system components has significant data base requirements. These data needs fall into two categories: those required for model setup and operation, and those required for model evaluation testing. Below, we identify the main input data base requirements for the meteorological, emissions, and air quality models. Details on the sources of the required data and how they will be used to construct model inputs are discussed in Chapter 5.

2.5.1 WRF

The databases required to set up, exercise, and evaluate the WRF model for the July – September 2007 episode consist of various fixed and variable inputs including: (a) topography, (b) vegetation type, (c) land use, (d) atmospheric data, (e) water temperature, (f) clouds and precipitation; and (g) multi-scale FDDA data.

2.5.2 SMOKE

The databases required to set up and operate SMOKE for the St. Louis point, area, and nonroad source emissions modeling are as follows (a) area source emissions in IDA format, (b) nonroad source emissions in IDA format, (c) stationary point source emissions in IDA format, (d) CEM emissions, day specific, and (e) wildfire emissions, day specific. Also required are data files specific for temporal allocation, spatial allocation, and chemical speciation.

2.5.3 MOVES

The detailed modeling approach for Missouri, Illinois, Kansas and Oklahoma requires several types of inputs for MOVES including (1) meteorological conditions specific to the episode and domain, (2) local input data for each representative county, and (3) local input data for annual VMT and population for each group of counties represented by a single county.

ENVIRON will generate the required meteorological conditions for MOVES by processing the MET data using the SMOKE-MOVES Tool pre-processor, *MET4MOVES*. MET4MOVES outputs which are input to MOVES include minimum and maximum temperature in any grid cell by representative county group, as well as a range of diurnal temperature profiles. ENVIRON will request the required MOVES county level input data from EWGCOG, MDNR and IEPA.

2.5.4 CAMx

Major CAMx model inputs include: (a) three-dimensional hourly meteorological fields generated by WRFCAMx processing of the WRF output, (b) three-dimensional hourly emissions generated by SMOKE, (c) initial conditions and boundary conditions (IC/BC), (d) photolysis rates look up table, (e) albedo/haze/ozone column input file, and (f) land use input file.

2.5.5 CMAQ

As described in more detail in Chapter 5, the CMAQ Chemical Transport Model (CTM) requires the following inputs: (a) three-dimensional hourly meteorological fields generated by the CMAQ MCIP processing of the WRF output, (b) three-dimensional hourly emissions generated by SMOKE, (c) IC/BC, (d) topographic information, (e) land use categories; and (e) photolysis rates generated by the CMAQ JPROC processor.

2.6 Summary of Model Selection and Justification

In summary, we recommend the WRF, SMOKE, and CAMx and CMAQ regional models for use in the St. Louis ozone, $PM_{2.5}$ and air toxics modeling study. The MOVES model is required for any new ozone, CO, PM, and NO_2 SIP development outside of California (EMFAC2007 is the current approved model in California) because it is EPA’s official regulatory tool for estimating motor vehicle emissions and based on the best information currently available.

In this chapter, we have introduced the models in the context of the current state-of-science in emissions, meteorological, and photochemical modeling and have provided brief technical summaries of each one. In addition, we have presented the rationale underpinning the selection of this specific suite of models for the St. Louis modeling study.

We conclude the model selection discussion by presenting in Tables 2-1 through 2-4 the six (6) criteria set forth in EPA's modeling guidance (EPA, 2005a, 2007) for determining whether a candidate model is *appropriate* for use in an attainment demonstration study. Associated with each of the six criteria are the reasons why we believe the four models are indeed suitable candidates for this application. Tables 2-1 through 2-4 also list the five (5) criteria that EPA has established for actually *justifying* the use of a model in the proposed study. Collectively, the information presented in Tables 2-1 though 2-4 supports our recommendation that the WRF, SMOKE, CAMx, and CMAQ models are logical choices given the specific technical, regulatory, schedule and resource aspects of the St. Louis ozone, $PM_{2.5}$ and air toxic modeling study.

2.7 Availability of Model Codes, Analysis Tools and Related Software

The source codes, user's guides, analysis tools, documentation and related software for all models used in this study are publicly available. These models and their pre- and post-processor programs and test data bases may be obtained at the following websites:

WRF:	http://www.mmm.ucar.edu/wrf/users/
SMOKE:	http://www.smoke-model.org/index.cfm
MOVES:	http://www.epa.gov/otaq/models/moves/
CAMx:	http://www.camx.com/
CMAQ:	http://www.cmaq-model.org/

Table 2-1. Factors qualifying and justifying WRF for use in the St. Louis modeling study.

Consideration	Qualification/Justification
The model has received a scientific peer review.	Formal scientific reviews of the WRF model have been widely carried out in the U.S. and abroad over the past 10+ years. Examples cited in REFERENCES include Skamarock, 2004; Hines and Bromwich 2008. More than one hundred governmental, academic, industrial and private modeling groups in the U.S. and abroad have reviewed the model code as part of training, model set-up, exercise, and quality assurance activities.
The model can be demonstrated to be applicable to the problem on a theoretical basis.	By design, WRF explicitly or implicitly represents the various physical and microphysical processes relevant to the prediction of mesoscale atmospheric phenomena. The model has been used world-wide by hundreds of scientists for a variety of mesoscale studies, including cyclogenesis, polar lows, cold-air damming, coastal fronts, severe thunderstorms, tropical storms, subtropical easterly jets, mesoscale convective complexes, desert mixed layers, urban-scale modeling, air quality studies, frontal weather, lake-effect snows, sea-breezes, orographically induced flows, and operational mesoscale forecasting. The features and capabilities of the WRF modeling system are consistent with the application on a combined urban- and regional-scale, as required in the St. Louis study.
Databases needed to perform the analysis are available and adequate.	The surface and upper air meteorological data required to exercise and evaluate WRF are available routinely from the National Weather Service. Large-scale databases needed for model initialization and boundary conditions are available from the National Center for Environmental Prediction (NCEP) and the National Center for Atmospheric Research (NCAR). These data sets include surface and aloft wind speed, wind direction, temperature, moisture, and pressure. Hourly surface data for model evaluation are available from many 'Class I' airports, i.e., larger-volume civil and military airports operating 24-hour per day. The standard set of upper air data are provided by rawinsonde soundings launched by the NWS every 12 hours from numerous sites across the continent. In addition, NOAA/NCAR operate continuous hourly RADAR profiler sites that report upper-air meteorological measurements at approximately 30 sites throughout the central U.S. Model inputs will be prepared following the guidelines recommended by the model developers and the adequacy of the input data bases will be assessed as part of the WRF model performance evaluation.
Available past appropriate performance evaluations have shown the model is not biased toward underprediction.	A number of studies have examined the theoretical formulation and operational features of the WRF model (see in REFERENCES for example, Klemp et.al., 2007; Knievel et. al., 2007; Moneng et. al., 2007; Skamarock, 2006), the performance of the model under a range of atmospheric conditions (e.g., Gaudet et. al., 2009; Hara et. al., 2008; Hines and Bromwich, 2008). No significant, unexplained bias in the model's estimates of state variables has been encountered. WRF is one of two state-of-science mesoscale prognostic meteorological models actively used in the U.S. and abroad as input to regional photochemical dispersion and emissions models.
A protocol on methods and procedures to be followed has been established.	The protocol is outlined in this document. The WRF modeling will be performed in a manner that is consistent with established practice and EPA guidelines regarding air quality modeling related to the 8-hr ozone standard.
The developer of the model must be willing to make the source code available to users for free or for a reasonable cost, and the model cannot otherwise be proprietary.	WRF has been in the public domain since its original development in the late 1990s. Free copies of the source code, user's guide, and test model inputs can be obtained from the National Center for Atmospheric Research and the U.S. EPA Office of Research and Development. Copies of ancillary data sets and model applications and evaluation software are available from various governmental agencies (e.g., the California Air Resources Board), academic institutions, National Laboratories, and consulting firms.

Consideration	Qualification/Justification
Nature of air quality problem leading to non-attainment of the ozone NAAQS should first be assessed, and the selected model should have the attributes and capabilities consistent with the perceived nature of the problem.	The WRF modeling system is expected to allow a physically realistic, dynamically consistent simulation of the land-gulf-bay breeze circulation regime over the St. Louis study area as well as other mesoscale features including convergence zones, cumulus convection, and so on. The nested grid feature of WRF will directly support the urban-to regional-scale nesting schemes in CAMx and CMAQ.
Availability, documentation and past performance should be satisfactory.	The WRF modeling system is publicly available and has been regularly used in support of CAMx and CMAQ modeling studies across the country. It has also been successfully used for several air quality studies in the western U.S. including work done for the Bay Area Air Quality Management District (BAAQMD) and the Texas Center for Environmental Quality (TCEQ). Results of numerous model evaluation studies with the WRF reveal that the model performs as well or better than any other mesoscale, applications-oriented, public domain model (Chen et. al., 2011; Henmi et. al., 2005).
Relevant experience of available staff and contractors should be consistent with choice of a model.	The WRF modeling will be performed by the study team (ENVIRON staff) who are thoroughly knowledgeable of the use of the model for mesoscale research applications as well as in regulatory photochemical modeling studies.
Time and resource constraints may be considered.	Use of the WRF model is consistent with the St. Louis ozone, $PM_{2.5}$ and air toxics modeling study schedule and budget.
Consistency of the model with what was used in adjacent regional applications should be considered.	WRF is been applied in several concurrent photochemical modeling studies in support of SIPs (e.g., Denver, SEMAP.)

Table 2-2. Factors qualifying and justifying SMOKE for use in the St. Louis modeling study.

Consideration	Qualification/Justification
The model has received scientific peer review.	A formal scientific review of the SMOKE modeling system has been continuous since its first release in 1996 that is now being performed as part of the CMAS Center operations (www.cmascenter.org). Numerous governmental, educational and private modeling groups in the U.S. and abroad have engaged in ongoing review, testing, and evaluation of the SMOKE model code as part of training, model set-up, exercise, and quality assurance activities. In particular, the RPOs have performed extensive testing and peer-review of the SMOKE modeling system and the CMAS Center conducts training on its use.
The model can be demonstrated to be applicable to the problem on a theoretical basis.	The SMOKE modeling system was explicitly designed to treat all categories of anthropogenic and biogenic emissions source in a modeling framework suitable for input to episodic Eulerian photochemical dispersion models. The model provides hourly resolved, gridded, chemically speciatiated, and source category specific emissions estimates for the important known precursors of photochemically produced ozone and PM. SMOKE is one of three state-of-science regional emissions models actively used in the U.S. and abroad (others are EMS and EPS). The features and capabilities of the SMOKE modeling system are consistent with the application on a combined urban- and regional-scale, as required in the St. Louis modeling study.
Databases needed to perform the analysis are available and adequate.	Key input databases to the SMOKE modeling system (e.g., point, area, and motor-vehicle sources plus biogenic sources) are available from the CENRAP, MRPO, VISTAS, MANE-VU, WRAP, and EPA. Model inputs will be prepared following published User's Guidelines, the development of the VISTAS and CENRAP regional inventories, and those used by EPA in the development of the CAIR modeling. The adequacy of the input databases developed by these various sources will be assessed as part of the SMOKE QA process.
Available past appropriate performance evaluations have shown the model is not biased toward underprediction.	There are very limited data sets with which to verify emissions models. Major point source emissions estimates are commonly based on continuous emissions monitoring (CEM). On-road motor vehicle emissions estimates are based on the EPA MOVES model.
A protocol on methods and procedures to be followed has been established.	The protocol is outlined in this document. The SMOKE modeling will be performed in a manner that is consistent with established practice and EPA guidelines regarding air quality modeling related to the ozone and PM standards.
The developer of the model must be willing to make the source code available to users for free or for a reasonable cost, and the model cannot otherwise be proprietary.	SMOKE has been in the public domain since its original development under EPA contract in the mid 1990s. Copies of the source code, user's guide, and test model inputs can be obtained from the CMAS website: http://www.cmascenter.org/
Nature of air quality problem leading to non-attainment of the ozone NAAQS should first be assessed, and the selected model should have the attributes and capabilities consistent with the perceived nature of the problem.	SMOKE is designed for the preparation of detailed urban- and regional-scale photochemical modeling inventories such as is required for the St. Louis study. EPA's BEIS3 emissions model is state-of-science models widely recommended for use in estimating biogenic emissions, which are expected to play an important role in ozone formation in the study area.
Availability, documentation and past performance should be satisfactory.	SMOKE is publicly available at no charge from the U.S. EPA. These models have been successfully used in a variety of regional modeling studies including OTAG, SAMI, and the EPA NOx SIP Call, CAIR, CAMR and CAVR.
Relevant experience of available staff and contractors should be consistent with choice of a model.	The emissions modeling tasks in the St. Louis study will be performed by ENVIRON/ERG team who have substantial experience in using the model.
Time and resource constraints may be considered.	Use of the SMOKE model is consistent with the St. Louis ozone, $PM_{2.5}$ and air toxics modeling study schedule and budget.

Consideration	Qualification/Justification
Consistency of the model with what was used in adjacent regional applications should be considered.	SMOKE model (or their predecessors) has been applied in several photochemical modeling studies including the OTAG modeling, the EPA NOx SIP Call, the EPA Tier II/Sulfur modeling analysis, the SAMI regional modeling study, the Pittsburgh-Beaver Valley SIP, the Cincinnati-Hamilton SIP, the St. Louis SIP, and in more than a dozen other regional ozone and PM modeling studies. The system has also been used in 8-hr ozone modeling studies in Southeastern States, Colorado and Oklahoma.

Table 2-3. Factors qualifying and justifying CAMx for use in the St. Louis modeling study.

Consideration	Qualification
The model has received a scientific peer review.	Formal scientific reviews of the CAMx model have been widely carried out since the model was first introduced in the mid 1990s (Russell and Dennis, 2000; Roth et al., 2005). Literally dozens of governmental, academic, industrial and private modeling groups have reviewed the model code as part of training, model set-up, performance evaluations, regulatory applications, and quality assurance activities.
The model can be demonstrated to be applicable to the problem on a theoretical basis.	The CAMx modeling system represents either explicitly or implicitly the physical and chemical processes that are currently known to influence the formation and transport of ozone and PM as well as the emissions, chemical transformation, and dispersion of ozone and PM precursor pollutants. The features and capabilities of the CAMx modeling system are consistent with the application on a combined urban- and regional-scale, as required in the St. Louis study.
Databases needed to perform the analysis are available and adequate.	The CAMx modeling system requires several different types of input data including land use, topographic, air quality, meteorological, and demographic. All of these data sets are routinely available from state or federal agencies. Model inputs will be prepared following EPA guidelines and the adequacy of the input databases will be assessed as part of the CAMx model performance evaluation.
Available past appropriate performance evaluations have shown the model is not biased toward underprediction.	The CAMx modeling system has undergone extensive third party review and performance testing and many prior evaluations and applications. Examples of recent model performance evaluations with CAMx are cited in the references section. Collectively, these evaluation studies do not reveal the presence of significant, unexplained underestimation bias for ground-level ozone concentrations.
A protocol on methods and procedures to be followed has been established.	The protocol is outlined in this document. The CAMx modeling will be performed in a manner that is consistent with established practice and EPA guidelines regarding air quality modeling related to the ozone and PM standards.
The developer of the model must be willing to make the source code available to users for free or for a reasonable cost, and the model cannot otherwise be proprietary.	CAMx has been in the public domain since its original development in the mid 1990s. Free copies of the source code, user's guide, and test model inputs can be obtained from the model developer's website at www.camx.com. Copies of ancillary data sets and model applications and evaluation software are available not only from the model developer (ENVIRON) but also from various governmental agencies (e.g., TCEQ), academic institutions, and consulting firms.
Nature of air quality problem leading to non-attainment of the ozone NAAQS should first be assessed, and the selected model should have the attributes and capabilities consistent with the perceived nature of the problem.	Based on an analysis of the observed 1-hr and 8-hr ozone data and the recent review of climatological data sets in south central states (Nielsen-Gammon et al., 2007), the potential 8-hr ozone and $PM_{2.5}$ nonattainment problems in the region include both regional and local components and is strongly influenced by the complex coastal meteorology of the region. The CAMx photochemical modeling system is well suited for this application in that its urban- and regional-scale grid nesting scheme appropriately addresses the various time and space scales relevant to the mesoscale processes involved in 8-hr ozone episodes. Utilizing meteorological inputs from a nested prognostic model (WRF), CAMx can directly simulate the local processes involved in ozone/PM problems together with the influence of imported ozone/PM and their precursor species from upwind (regional-scale) source regions. The use of detailed meteorological inputs and grid nesting will allow proper treatment of the gulf breeze, convective circulations, vertical mixing and cloud processes. The process-analysis, ozone/particulate source apportionment, and decoupled direct sensitivity analysis algorithms in CAMx will allow a more rigorous evaluation of model performance and aid in diagnostic analysis.
Availability, documentation and past performance should be satisfactory.	The CAMx modeling system is publicly available at no cost. Full user documentation can be obtained from the website: www.camx.com. The CAMx model has been widely evaluated by numerous groups in the U.S. The model has undergone extensive successful testing by a variety of groups (see, for example, Lurmann and Kumar, 1997; McNally et al., 1998a-c; Tesche and McNally, 1998). Model performance has consistently been comparable to or better than that of other contemporary model such as the UAM-V, SAQM, and URM.

Consideration	Qualification
Relevant experience of available staff and contractors should be consistent with choice of a model.	The CAMx modeling will be performed by the AQMP Technical Workgroup with technical support from the ENVIRON scientists who are thoroughly knowledgeable of the use of the model for regulatory photochemical modeling studies. Examples of relevant recent experience with CAMx listed in REFERENCES include Morris et al. (1999, 2004, 2005, 2006, 2008, 2009). Other examples are cited in the references.
Time and resource constraints may be considered.	Use of the CAMx model is consistent with the St. Louis ozone, $PM_{2.5}$ and air toxics modeling study schedule and budget.
Consistency of the model with what was used in adjacent regional applications should be considered.	CAMx has been applied in several recent photochemical modeling studies including the CRC Comparative Model Evaluation Study in Lower Lake Michigan (Tesche et al., 2000), the OTAG, EPA NOx SIP Call, and EPA Tier II/Sulfur modeling analyses, the Pittsburgh-Beaver Valley SIP, the Cincinnati-Hamilton SIP, St. Louis SIP and more than two dozen other regional ozone modeling studies in the eastern U.S. The system was also used in the Kansas City/Missouri, Oklahoma, East Texas, and Peninsular Florida 8-hr ozone modeling studies.

Table 2-4. Factors qualifying and justifying CMAQ for use in the St. Louis modeling study.

Consideration	Qualification/Justification
The model has received a scientific peer review.	Formal scientific reviews of the CMAQ model have been widely carried out since the model was first introduced in the mid 1990s. Examples include Amar et al., (2004, 2005), Kumar and Lurmann (1997); Russell and Dennis (2000); Literally dozens of governmental, academic, industrial and private modeling groups worldwide have reviewed the model code as part of training, model set-up, performance evaluations, regulatory applications, and quality assurance activities.
The model can be demonstrated to be applicable to the problem on a theoretical basis.	The CMAQ modeling system represents either explicitly or implicitly the physical and chemical processes that are currently known to influence the formation and transport of ozone as well as the emissions, chemical transformation, and dispersion of ozone precursor pollutants. The features and capabilities of the CMAQ modeling system are consistent with the application on a combined urban- and regional-scale, as required in the St. Louis study.
Databases needed to perform the analysis are available and adequate.	The CMAQ modeling system requires several different types of input data including land use, topographic, air quality, meteorological, and demographic. All of these data sets are routinely available from state or federal agencies. Model inputs will be prepared following EPA guidelines and the adequacy of the input databases will be assessed as part of the CMAQ model performance evaluation.
Available past appropriate performance evaluations have shown the model is not biased toward underprediction.	The CMAQ modeling system has undergone extensive third party review and performance testing and many prior evaluations and applications. Formal peer reviews and responses are presented by Amar et al., (2004, 2005) and EPA (2005c). Other examples of CMAQ model performance evaluations are included in the reference section. Collectively, these evaluation studies do not reveal the presence of significant, unexplained underestimation bias for ground-level ozone concentrations.
A protocol on methods and procedures to be followed has been established.	The protocol is outlined in this document. The CMAQ modeling will be performed in a manner that is consistent with established practice and EPA guidelines regarding air quality modeling related to the ozone and PM standards.
The developer of the model must be willing to make the source code available to users for free or for a reasonable cost, and the model cannot otherwise be proprietary.	CMAQ has been in the public domain since its original development in the mid 1990s. Free copies of the source code, user's guide, and test model inputs can be obtained from the CMAQ website: http://www.cmascenter.org/. Copies of ancillary data sets and model applications and evaluation software are available not only from EPA but also from State governmental agencies, academic institutions, and consulting firms. See the CMAS website for details and links. See also the annual CMAS-Models-3 CMAQ conference proceedings included on the CMAS site.
Nature of air quality problem leading to non-attainment of the ozone NAAQS should first be assessed, and the selected model should have the attributes and capabilities consistent with the perceived nature of the problem.	Based on an analysis of the observed 1-hr and 8-hr ozone data and the recent review of climatological data sets in the south central U.S. region (Nielsen-Gammon et al., 2007) the potential 8-hr ozone and annual $PM_{2.5}$ nonattainment problems in the region include both regional and local components and is strongly influenced by the complex coastal meteorology of the region. The CMAQ photochemical modeling system is well suited for this application in that its urban- and regional-scale grid nesting scheme appropriately addresses the various time and space scales relevant to the mesoscale processes involved in 8-hr ozone episodes. Utilizing meteorological inputs from a nested prognostic model (WRF), CMAQ can directly simulate the local processes involved in ozone/PM problems together with the influence of imported ozone/PM and their precursor species from upwind (regional-scale) source regions. The use of detailed meteorological inputs and grid nesting will allow proper treatment of the gulf breeze, convective circulations, vertical mixing and cloud processes. The process-analysis and decoupled direct sensitivity analysis algorithms in CMAQ will allow a more rigorous evaluation of model performance and aid in diagnostic analysis.
Availability, documentation and past performance should be satisfactory.	The CMAQ modeling system is publicly available at no cost. Full user documentation can be obtained from the website: http://www.cmascenter.org/. CMAQ has been widely exercised by numerous groups in the U.S. and has undergone extensive successful testing by a variety of groups as indicated in the references.

Consideration	Qualification/Justification
Relevant experience of available staff and contractors should be consistent with choice of a model.	The CMAQ modeling will be performed by the AQMP Technical Workgroup with technical support from the ENVIRON scientists who are thoroughly knowledgeable of the use of the model for regulatory photochemical modeling studies. Relevant recent experience with CMAQ include: Morris et al., 2005,2006; Tesche et al., 2005a,b; Tesche et al., 2003a,b.
Time and resource constraints may be considered.	Use of the CMAQ model is consistent with the St. Louis ozone, $PM_{2.5}$ and air toxics modeling study schedule and budget.
Consistency of the model with what was used in adjacent regional applications should be considered.	CMAQ has been applied in several recent photochemical modeling studies including the CRC Comparative Model Evaluation Study in Lower Lake Michigan (Tesche et al., 2000), the EPA Clear Air Interstate Rule (CAIR), the Clean Air Mercury Rule (CAMR) and dozens other regional ozone and fine particulate (Fan et al., 2005; Morris et al., 2005; Tesche et al., 2005a,b) modeling studies covering Texas and elsewhere in the eastern U.S. The model has also been used in the St. Louis 8-hr ozone and $PM_{2.5}$ SIP development study (Tesche et al., 2005a,b).

3.0 EPISODE SELECTION

EPA's 8-hour ozone and $PM_{2.5}$ modeling guidance (EPA, 2007)[1] contains recommended procedures for selecting modeling episodes, while also referencing EPA's 1-hour ozone modeling guidance for episode selection (EPA, 1991)[2]. This Chapter presents the modeling period selected for performing the new St. Louis ozone attainment demonstration SIP modeling and the justification and rationale for its selection.

3.1 Episode Selection Criteria

EPA's modeling guidance lists primary criteria for selecting episodes for SIP ozone modeling along with a set of secondary criteria that should also be considered.

3.1.1 Primary Episode Selection Criteria

EPA's guidance on 8-hour ozone modeling (EPA, 2007) identifies four specific criteria to consider when selecting one or more episodes for use in demonstrating attainment of the 8-hour ozone NAAQS:

1. A variety of meteorological conditions should be covered, including the types of meteorological conditions that produce 8-hour ozone exceedances in the St. Louis area;
2. Choose episodes having days with monitored 8-hour daily maximum ozone concentrations close to the observed fourth highest value;
3. To the extent possible, the modeling data base should include days for which extensive data bases (i.e. beyond routine aerometric and emissions monitoring) are available; and
4. Sufficient days should be available such that relative response factors (RRFs) can be based on several (i.e., > 10) days with at least 5 days being the absolute minimum.

3.1.2 Secondary Criteria

EPA also lists four "other considerations" to bear in mind when choosing potential 8-hour ozone episodes including:

1. Choose periods which have already been modeled;
2. Choose periods that are drawn from the years upon which the current Design Values are based;
3. Include weekend days among those chosen; and
4. Choose modeling periods that meet as many episode selection criteria as possible in the maximum number of nonattainment areas as possible.

EPA suggests that modeling an entire summer ozone season would be a good way to assure that a variety of meteorological conditions are captured and that sufficient days are available to construct robust relative response factors (RRFs) for the 8-hour ozone Design Value projections.

[1] http://www.epa.gov/ttn/scram/guidance/guide/final-03-pm-rh-guidance.pdf
[2] http://www.epa.gov/ttn/scram/guidance/guide/uamreg.pdf

3.2 Episode Selection for St. Louis SIP Modeling

For the previous St. Louis ozone and $PM_{2.5}$ SIP modeling study, the 2002 year was selected for the photochemical modeling. 2002 was selected due to the occurrence of high ozone and $PM_{2.5}$ concentrations as well as a wealth of supporting meteorological, emissions and air quality modeling data developed by the Regional Planning Organizations (RPOs) in support of preparation of regional haze SIPs and the regional component of 8-hour ozone and $PM_{2.5}$ SIPs.

Figure 3-1 displays the maximum 8-hour ozone Design Value in the St. Louis nonattainment area (NAA) from 2001 to 2009. Shown are the 8-hour ozone Design Values that we calculated in a trends study and the official ones published by EPA[3]. There is a discrepancy in the 2007-2009 8-hour ozone Design Value that we calculated (0.087 ppm) versus EPA's published value (0.078 ppm). However, EPA's published value includes a footnote that not all monitoring sites were included in their calculation including ones that had violated the ozone NAAQS in the past, which is likely the cause for the discrepancy. Figure 3-2 displays an average of 8-hour ozone Design Values across monitoring sites in the St. Louis NAA. Similar figures for the annual $PM_{2.5}$ Design Values are given in Figures 3-3 and 3-4. The 2007 8-hour ozone and annual $PM_{2.5}$ Design Values are the highest values in recent history.

Based on the higher ozone conditions in 2007 than other recent years, we proposed to use the June through September 2007 modeling period for the St. Louis ozone attainment demonstration modeling. The justification for the June-September, 2007 modeling period using EPA's primary and secondary episode selection criteria are as follows:

Primary Criteria

1. Variety of Meteorological Conditions: By modeling an entire four month ozone season from the most severe ozone year seen in recent times (2007) we are assured of obtaining a variety of meteorological conditions that produce elevated ozone concentrations in the St. Louis area.
2. Days with Monitored Ozone near Design Value: 2007 most likely to have more high days with daily maximum 8-hour ozone concentration near the ozone Design Value than other recent years due to the more adverse ozone formation conditions.
3. Include Days with Extensive Databases: Recent extensive databases during high ozone conditions are not available for St. Louis.
4. Make Sure Have Sufficient days for RRFs: The summer of 2007 has more high ozone days than any recent year so is more likely to have more high ozone days that are used to develop RRFs.

Secondary Criteria

1. Choose Periods Which Have Already Been Modeled: 2007 is being modeled by the
2. Choose Periods from current Design Values: The most current ozone Design Values are based on 2008-2010 monitoring data, which does not include the proposed 2007 modeling period. However, the 2008-2010 years were cleaner ozone years than 2007 so would not be better choices given the other episode selection criteria.

[3] http://www.epa.gov/airtrends/values.html

3. Include Weekend Days: By modeling a full ozone season in 2007, we are assured to have many weekend days in the analysis.
4. Choose Modeling Periods That Meet as Many Episode Selection Criteria as Possible: Of the recent years, the summer of 2007 satisfies the most episode selection criteria so is the period selected for ozone attainment demonstration modeling of St. Louis

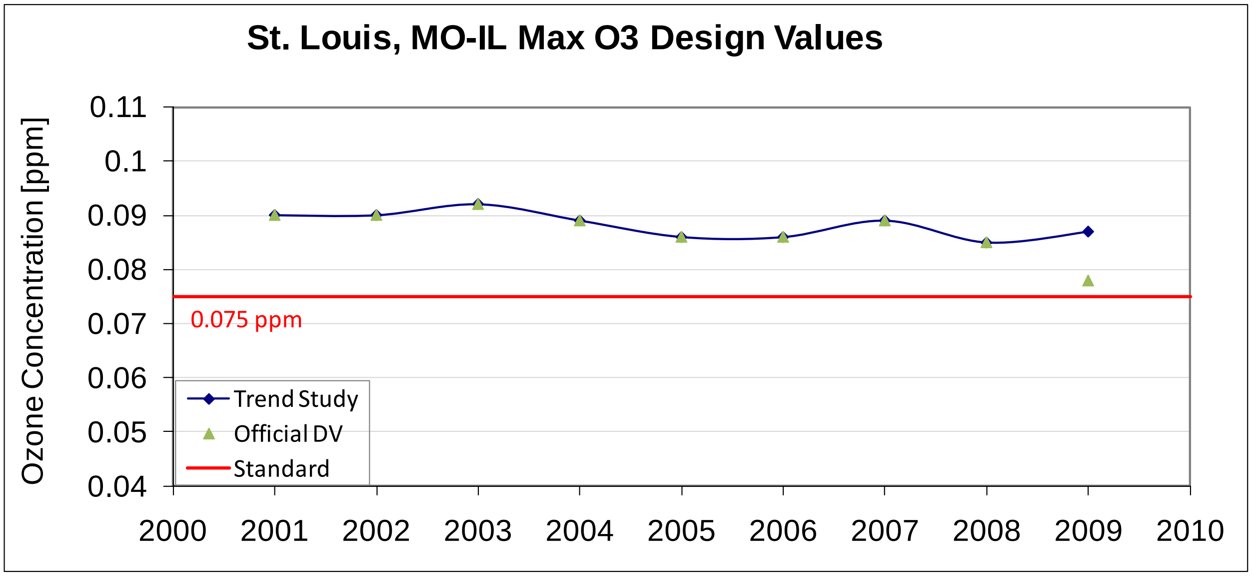


Figure 3-1. Maximum 8-hour ozone Design Values from 2001 to 2009 at any monitor in the St. Louis NAA calculated in a Trend Study and published by EPA.

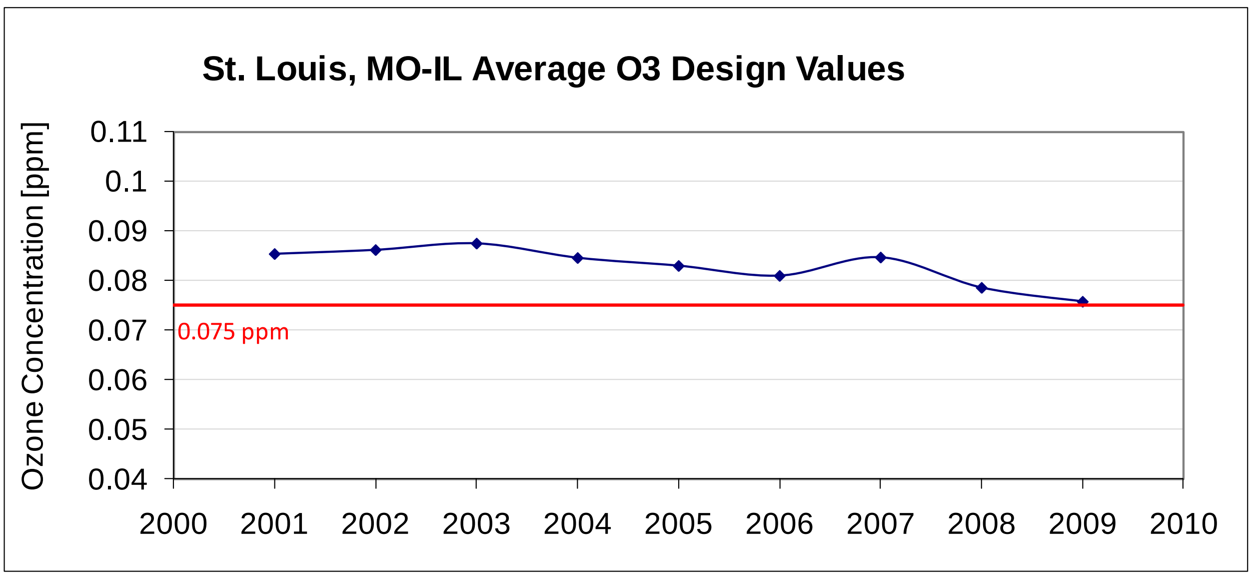


Figure 3-2. Average 8-hour ozone Design Values from 2001 to 2009 across the St. Louis NAA calculated in a Trend Study and published by EPA.

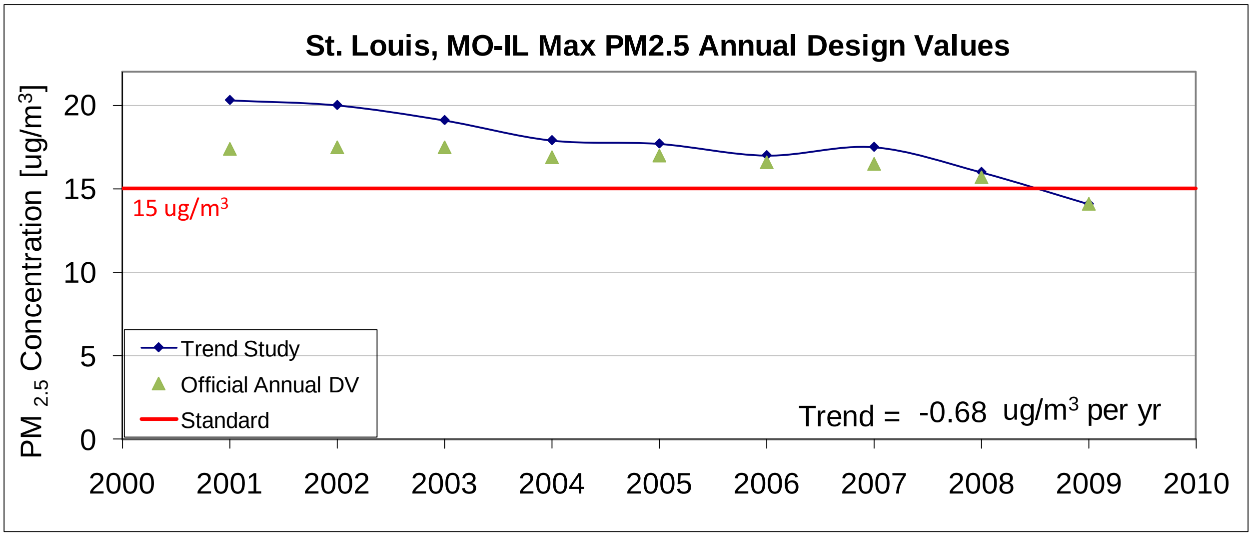


Figure 3-3. Maximum annual $PM_{2.5}$ Design Values from 2001 to 2009 at any monitor in the St. Louis NAA calculated in a Trend Study and published by EPA.

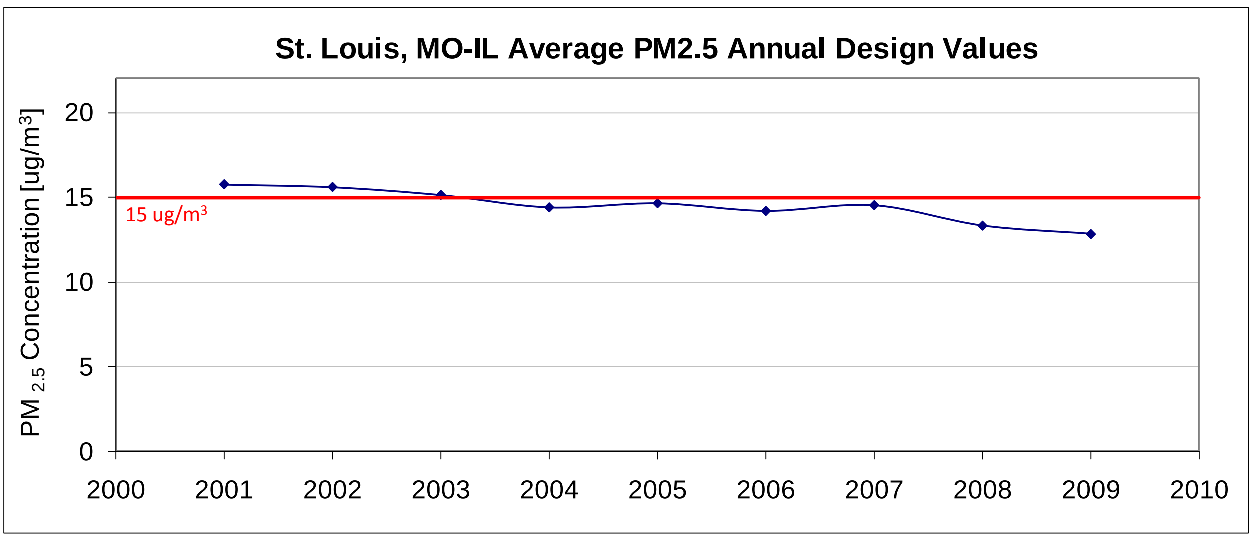


Figure 3-4. Average annual $PM_{2.5}$ Design Values from 2001 to 2009 across monitors in the St. Louis NAA calculated in a Trend Study and published by EPA.

4.0 MODELING DOMAINS AND DATA AVAILABILITY

This chapter summarizes the model domain definitions for the St. Louis ozone, $PM_{2.5}$ and air toxics modeling study including the model domain, resolution, map projections and nesting schemes for high resolution sub-domains. It also discusses the emissions and aerometric data available from various State and federal agencies for use in model input preparation and performance testing.

4.1 Horizontal Modeling Domain

Regional modeling studies of ozone and/or PM frequently use horizontal grid resolutions of 36 km and 12 km. Urban-scale modeling studies use finer resolution such as 4 km to more accurately represent urban plumes and the source-receptor relationships between urban emissions and population. Modeling urban air toxics may require even finer grid resolution (e.g., 1 or 1.333 km) to represent the dispersion of emissions near major sources such as industrial point sources. Grid-nesting enables the simultaneous use of fine and coarse grids to model both local and regional air pollution impacts. A plume-in-grid (PiG) model, where a Lagrangian plume model is embedded within an Eulerian grid model, is another approach to simultaneously modeling local and regional impacts. The impact of grid resolution on the modeling result has been discussed in a previous modeling study for the Detroit area (Nopmongcol et al., 2009). General conclusions from the study include:

- Fine resolution has more impact for primary pollutants than secondary pollutants
- Fine resolution produces more structure and higher peaks for primary pollutants
- Fine resolution can either increase or decrease peak concentrations for secondary pollutants

The above study also showed that even a fine-scale 1 km grid might overly disperse near source influence of primary PM emissions and that this could be mitigated by using the PiG approach (see Figure 4-1).

The 36 km continental U.S. (CONUS) horizontal domain for each of the models will be identical to those used by WRAP, CENRAP, VISTAS and numerous other modeling studies. The CMAQ and CAMx air quality modeling domain is nested in the WRF domain. Figure 4-2 shows the proposed nested 36/12/4/1.333 km domains for photochemical modeling and emissions modeling. Both CAMx and CMAQ will employ the Regional Planning Organization (RPO) unified grid definition for the 36 km CONUS domain for the annual modeling. The RPO unified grid consists of a Lambert-Conformal map projection using the projection parameters listed in Table 4-1. The 12 km modeling domain is made to cover the CENRAP states as much as possible given the definition of the 12 km WRF domain and the need to offset the CMAQ/CAMx domain boundaries by at least 5 grid cells to void numerical artifacts that can occur near the boundaries of the WRF modeling domain. The 4 km modeling domain was made big enough to address ozone and $PM_{2.5}$ issues in both St. Louis and Kansas City areas. The 1.333 km domain is focused on the St. Louis urban area.

The 2007 WRF simulation with nested 36/12 km modeling domains has already been performed by the states of Iowa and North Carolina, which will be used for the St. Louis modeling study. The WRF 36 km grid includes 164 cells in the east-west dimension and 128 cells in the north-south dimension. The CMAQ/CAMx 36 km grid includes 148 cells in the east-west dimension and 112 cells in the north-south dimension. Because the WRF model is also nested in the Eta model, there is a possibility of boundary effects near the WRF boundary that occur as the Eta meteorological variables are being simulated by WRF and must come into dynamic balance with WRF's algorithms. Thus, a larger WRF domain was selected to provide a buffer of 8 grid cells around each boundary of the CMAQ/CAMx 36 km domain. This is designed to eliminate any errors in the meteorology from boundary effects in the WRF simulation at the interface of the WRF and Eta models. The buffer region used here exceeds the EPA suggestion of at least 5 grid cell buffers at each boundary. The WRF 4/1.333 km domains are set to give 5 grid cell buffers at each boundary of the CMAQ/CAMx 4/1.333 km domains. Figure 4-3 shows nested 36/12/4/1.333 km domains for the WRF simulation.

Table 4-2 lists the number of rows and columns and the definition of the X and Y origin (i.e., the southwest corner) for the 36/12/4/1.333 km domains used by WRF and SMOKE/CMAQ/CAMx. In Table 4-2 "Dot" refers to the grid mesh defined at the vertices of the grid cells while "Cross" refers to the grid mesh defined by the grid cell centers. Thus, the dimension of the dot mesh is equal to the cross mesh plus one.

4.2 Vertical Modeling Domain

The CMAQ and CAMx vertical structure is primarily defined by the vertical grid used in the WRF modeling. The WRF model employed a terrain following coordinate system defined by pressure, using 34 layers that extend from the surface to 100 mb. We will use the exactly same vertical layer structure in CAMx as in CMAQ. A layer averaging scheme is adopted for CMAQ/CAMx to reduce the computational cost of the CMAQ and CAMx simulations. The effects of layer averaging were evaluated by WRAP and VISTAS and found to have a relatively minor effect on the model performance metrics when both the 34-layer and 19-layer CMAQ model simulations were compared to ambient monitoring data (Morris et al., 2004a). For the St. Louis ozone, $PM_{2.5}$ and air toxics modeling, 24 vertical layers are used. Table 4-3 lists the mapping from the 34 vertical layers used by WRF to the 24 vertical layers used by CMAQ and CAMx.

4.3 Data Availability

The CMAQ and CAMx modeling systems require emissions, meteorological, initial and boundary condition (IC/BC) and ozone column data for defining the inputs.

4.3.1 Emissions Data

Since the proposed modeling domains for the St. Louis ozone, $PM_{2.5}$ and air toxics modeling study are very extensive (e.g., the 36 km domain covers the entire contiguous U.S. and large portions of Canada and Mexico, etc.), a large quantity of emissions data is needed to accurately represent these domain. However, given project resources and constraints, it is not feasible to develop these county-level emissions data "from scratch" on a state-by-state basis. To the greatest extent possible, the ENVIRON/ERG team will develop the emissions data from the latest existing emissions inventories. Broadly speaking, the St. Louis modeling domains encompasses seven regions:

- Central States Air Resource Agencies (CenSARA) and Central Regional Air Planning Association (CENRAP) – including AR, IA, KS, LA, MN, MO, NE, OK, TX
- Midwest Regional Planning Organization (Midwest RPO) and Lake Michigan Air Directors Consortium (LADCO) – including IL, IN, MI, OH, WI
- Southeastern Modeling, Analysis and Planning (SEMAP) that was formally the Visibility Improvement State and Tribal Association of the Southeast (VISTAS) – including AL, FL, GA, KY, MS, NC, SC, TN, VA, WV
- Mid-Atlantic Regional Air Management Association (MARAMA) and Mid-Atlantic/Northeast Visibility Union (MANE-VU) – including CT, DC, DE, MA, MD, ME, NH, NJ, NY, PA, RI, VA, VT
- Western Regional Air Partnership (WRAP) – including AZ, CA, CO, ID, MT, ND, NM, NV, OR, SD, UT, WA, WY
- Canada
- Mexico

A brief explanation of the known available data (for point, area and nonroad sources) for each of these regions is provided below:

- CENRAP – CENRAP is currently developing a 2007 point source inventory and has agreed to make the inventory data available for the St. Louis modeling study. An FTP drop-off folder has been established to facilitate the data transfer.
- Midwest RPO/LADCO – The 2007 draft base C inventory is nearing completion. The inventory includes all sectors, except fires and consists of a mixture of 2007 and 2008 inventory data (Janssen, 2011). These data will be used as a reasonable approximation of the 2007 emissions.
- VISTAS – The 2007 base year Southeastern Modeling, Analysis, and Planning (SEMAP) Project emissions inventory is nearing completion. As of April 4, the only portions of the inventory that had not been completed were the point sources (limited to partial reporting EGUs) and area sources (remaining reconciliation between point and area sources due to the uncompleted partial reporting EGU point sources). It is expected that the SEMAP inventory will be completed by the end of April 2011 (Methier, 2011).
- MARAMA/MANE-VU – With the exception of on-road motor vehicles, the 2007 MARAMA/MANE-VU regional emissions inventory and documentation is posted on the MARAMA website and FTP site (MARAMA, 2011).
- WRAP – Currently, WRAP inventories only exist for the 2002 base year and the 2018 projection year. A 2008 inventory will be developed as part of the WestJumpAQMS study; however, this work will not be initiated until July 2011. In lieu of the 2008 WestJumpAQMS inventory, it was recommended that data from version 1 of the 2008 National Emissions Inventory (NEI) be used (Moore, 2011).
- Canada – As far as can be determined, a comprehensive 2007 inventory for Canada is not available. It is proposed that an existing 2006 inventory be used as a reasonable approximation of the 2007 Canada emissions.
- Mexico – ERG previously developed the first-ever county-level national emissions inventory for Mexico (ERG, 2006). ERG subsequently developed future year county-level emission projections for the years 2008, 2012, and 2030 (ERG, 2009). It is proposed that the 2008 projections be used as a reasonable approximation of the 2007

Mexico emissions. Only emissions from those Mexican states which lie within the St. Louis modeling domain will be used.

Although the data above have been tentatively identified for use in the St. Louis ozone, $PM_{2.5}$ and air toxics modeling study, in the course of inventory development, some data may turn out to be unavailable or otherwise unusable for the inventory development process. In such instances, the ENVIRON/ERG team will rely upon U.S. EPA's 2008 National Emissions Inventory (NEI). In addition, emissions for the CENRAP states (excluding point source emissions) will likely be obtained from the 2008 NEI. The first iteration (i.e., version 1) of the 2008 NEI was released on April 4, 2011. Version 1 only includes point source emissions (stack parameter type information is missing), on-road motor vehicle emissions, and nonroad mobile source emissions. Area source emissions will be included in version 1.5, which is expected to be released in mid May 2011. It should be noted that emissions data from the 2008 NEI are in an early stage of development and should be considered to be somewhat preliminary.

Data for the detailed SMOKE-MOVES processing for Missouri, Illinois, Kansas and Oklahoma will be obtained from the states. For areas outside these four states, the latest available MOVES-based inventories developed by other entities including EPA (2005 Transport Rule modeling), SESARM (the 2007 calendar year SEMAP project modeling), and potentially other RPO-generated MOVES datasets will be utilized. As default coverage, the EPA Transport Rule modeling provides a comprehensive MOVES-based gridded inventory for 3 calendar years which bracket the 2007 base year for this project and so emissions can be interpolated. The SEMAP project, if completed during a timeframe useful to the St. Louis project, would be a valuable data source due to the detailed SMOKE-MOVES modeling approach and a shared base year.

As necessary, all emissions data will be converted to emission input formats suitable for input to the Sparse Matrix Operating Kernel Emissions (SMOKE) model (i.e., Inventory Data Analyzer (IDA) formats).

4.3.2 Air Quality

Data from ambient monitoring networks for both gas and aerosol species are used in the model performance evaluation. Table 4-4 summarizes routine ambient gaseous, PM and air toxics monitoring networks. Figure 4-4 displays the locations of PM, ozone and air toxics monitoring sites in the St. Louis study domain.

4.3.3 Ozone Column Data

Additional data used in the air quality modeling include the Total Ozone Mapping Spectrometer (TOMS) data which are available for 24-hour average time periods[1]. The TOMS data are used in the CMAQ (JPROC) and CAMx (TUV) radiation models to calculate photolysis rates. Frequently there may be missing periods in the TOMS data that must be filled. Thus, careful QA/QC and range checks need to be performed on the TOMS data to make sure there are no periods of missing or faulty data. Any missing or faulty TOMS data are typically filled in by holding the ozone column data constant from the last day of valid data. Since ozone column

[1] http://toms.gsfc.nasa.gov/ozone/ozone_v8.html

values typically evolve fairly slowly from day to day the filling in of missing data for limited periods does not introduce any significant uncertainties into the model results.

4.3.4 Meteorological Data

Meteorological data are being generated using the WRF prognostic meteorological model. Episodic WRF runs at 5-day increments on the 36/12 km domains have already been performed by the states of Iowa and North Carolina, with a minimum 12 hour spin up period used for each episode. The WRF parameterization and physics choices have been chosen by Iowa Department of Natural Resources (IDNR), and are given in Chapter 5. ENVIRON will run the 4 km WRF simulation as a 1-way nest from IDNR's 12 km WRF outputs. This process is detailed in Chapter 5. ENVIRON will then perform 1-way nesting once again, from the 4 km domain to the 1.333 km domain.

4.3.5 Initial and Boundary Conditions Data

The 36 km simulation will use CMAQ's default initial conditions (ICs) along with a ~15 day spin up period to eliminate any significant influence of the ICs (ICs for the nested grid simulations will be extracted from the 36 km output with a shorter spin up period). The lateral boundary conditions (BCs) for the 36 km grid will be based on results from a 2007 MOZART-4 global model simulation. The 2007 MOZART-4 model output can be downloaded from the MOZART website[2]. The MOZART2CMAQ processor converts the MOZART output to CMAQ BCs. The CMAQ IC/BC inputs for the 36 km grid will be converted to CAMx-ready inputs using the CMAQ2CAMx processor.

[2] http://www.acd.ucar.edu/wrf-chem/mozart.shtml

Table 4-1. RPO unified grid projection definition.

Parameter	Value
Projection	Lambert-Conformal
Center Longitude	-97 degrees
Center Latitude	40 degrees
1st True Latitude	33 degrees
2nd True Latitude	45 degrees

Table 4-2. Grid definitions for WRF and SMOKE/CMAQ/CAMx models.

MODEL	COLUMNS DOT(CROSS)	ROWS DOT(CROSS)	XORIGIN (METERS)	YORIGIN (METERS)
WRF				
36 km grid	165 (164)	129 (128)	-2,952,000	-2,304,000
12 km grid	250 (249)	250 (249)	-612,000	-1,692,000
4 km grid	184 (183)	148 (147)	48,000	-456,000
1.333 km grid	49 (48)	49 (48)	552,000	-160,000
SMOKE/CMAQ/CAMx				
36 km grid	(148)	(112)	-2,736,000	-2,088,000
12 km grid	(239)	(239)	-552,000	-1,632,000
4 km grid	(173)	(137)	68,000	-436,000
1.333 km grid	(38)	(38)	558,667	-153,333

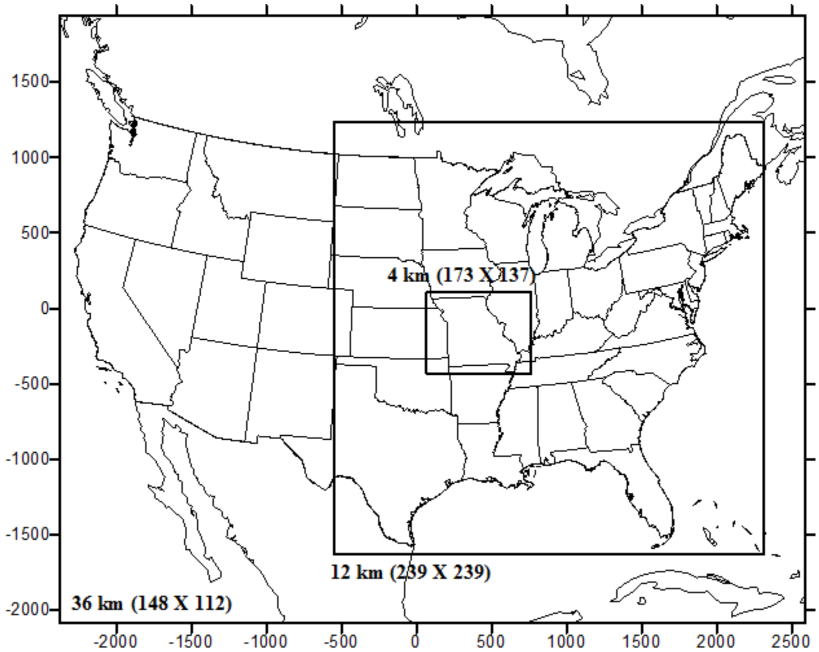
Table 4-3. Vertical layer definition for WRF simulations (left most columns), and approach for reducing CMAQ/CAMx layers by collapsing multiple WRF layers (right columns).

WRF Vertical Layers					CMAQ Vertical Layers		
k	**sigma**	**Pressure (mb)**	**Height (m)**	**Depth (m)**	**k**	**Height (m)**	**Depth (m)**
34	**0.0000**	**100.0**	**16064**	**1472**	**24**	**16064**	**2763**
33	0.0332	129.9	14592	1291			
32	**0.0682**	**161.4**	**13301**	**1177**	**23**	**13301**	**2293**
31	0.1056	195.0	12123	1116			
30	**0.1465**	**231.9**	**11007**	**1056**	**22**	**11007**	**2053**
29	0.1907	271.6	9951	997			
28	**0.2378**	**314.0**	**8954**	**932**	**21**	**8954**	**1799**
27	0.2871	358.4	8022	867			
26	**0.3379**	**404.1**	**7155**	**802**	**20**	**7155**	**1536**
25	0.3895	450.6	6353	734			
24	**0.4409**	**496.8**	**5619**	**669**	**19**	**5619**	**1275**
23	0.4915	542.4	4950	606			
22	**0.5406**	**586.5**	**4344**	**548**	**18**	**4344**	**1037**
21	0.5878	629.0	3796	489			
20	**0.6323**	**669.1**	**3307**	**439**	**17**	**3307**	**831**
19	0.6742	706.8	2868	392			
18	**0.7133**	**742.0**	**2476**	**348**	**16**	**2476**	**660**
17	0.7494	774.5	2128	312			
16	**0.7828**	**804.5**	**1816**	**276**	**15**	**1816**	**520**
15	0.8133	832.0	1540	244			
14	**0.8410**	**856.9**	**1296**	**214**	**14**	**1296**	**214**
13	**0.8659**	**879.3**	**1082**	**188**	**13**	**1082**	**188**
12	**0.8882**	**899.4**	**893**	**163**	**12**	**893**	**163**
11	**0.9079**	**917.1**	**730**	**141**	**11**	**730**	**141**
10	**0.9252**	**932.7**	**589**	**120**	**10**	**589**	**120**
9	**0.9401**	**946.1**	**469**	**101**	**9**	**469**	**101**
8	**0.9528**	**957.5**	**367**	**84**	**8**	**367**	**84**
7	**0.9635**	**967.2**	**283**	**69**	**7**	**283**	**69**
6	**0.9723**	**975.1**	**214**	**57**	**6**	**214**	**57**
5	**0.9796**	**981.6**	**157**	**45**	**5**	**157**	**45**
4	**0.9854**	**986.9**	**112**	**35**	**4**	**112**	**35**
3	**0.9900**	**991.0**	**77**	**31**	**3**	**77**	**31**
2	**0.9940**	**994.6**	**46**	**26**	**2**	**46**	**26**
1	**0.9974**	**997.7**	**20**	**20**	**1**	**20**	**20**
0	**1.0000**	**1000.0**	**0**		**0**	**0**	

Table 4-4. Overview of ambient data monitoring networks.

Monitoring Network	**Chemical Species Measured**	**Sampling Period**	**Data Availability/Source**
Interagency Monitoring of Protected Visual Environments (**IMPROVE**)	Speciated $PM_{2.5}$ and PM_{10}; trace elements (As, Cr, Pb, etc.)	1 in 3 days; 24 hr average	http://vista.cira.colostate.edu/improve/Data/IMPROVE/improve_data.htm
Clean Air Status and Trends Network (**CASTNET**)	Speciated $PM_{2.5}$, O_3, SO_2, HNO_3	Approximately 1-week average	http://java.epa.gov/castnet/
National Atmospheric Deposition Program (**NADP**)	Wet deposition (hydrogen (acidity as pH), sulfate, nitrate, ammonium, chloride, and base cations (such as calcium, magnesium, potassium and sodium)), Mercury	1-week average	http://nadp.sws.uiuc.edu/
Chemical Speciation Network (**CSN**)	Speciated PM	24-hour average	http://www.epa.gov/ttn/amtic/amticpm.html
Southeastern Aerosol Research and Characterization (**SEARCH**) (Southeastern US only)	24-hr $PM_{2.5}$ (FRM Mass, OC, BC, SO_4, NO_3, NH_4, elements); 24-hr PM coarse (SO_4, NO_3, NH_4, elements); Hourly $PM_{2.5}$ (Mass, SO_4, NO_3, NH_4, EC, TC); Hourly gases (O_3, NO, NO_2, NOy, HNO_3, SO_2, CO); trace elements (As, Cr, Pb, etc.)	Hourly or 24-hour average, depending on parameter.	Electric Power Research Institute (EPRI), Southern Company, and other companies. http://www.atmospheric-research.com
Air Quality System (**AQS**) Aka Aerometric Information Retrieval System (**AIRS**)	CO, NO_2, O_3, SO_2, $PM_{2.5}$, PM_{10}, Pb; HAPs	Typically hourly average; 24 hr average for HAPs	http://www.epa.gov/air/data/
National Air Toxics Trends Station (**NATTS**) Network	HAPs	1 in 6 days; 24 hr average	http://www.epa.gov/ttnamti1/natts.html
Photochemical Assessment Monitoring Stations (**PAMS**)	Varies for each of 4 station types.		http://www.epa.gov/ttn/amtic/pamsmain.html
National Park Service Gaseous Pollutant Monitoring Network	O_3, SO_2, meteorological data	Hourly	http://www.nature.nps.gov/air/monitoring/network.cfm

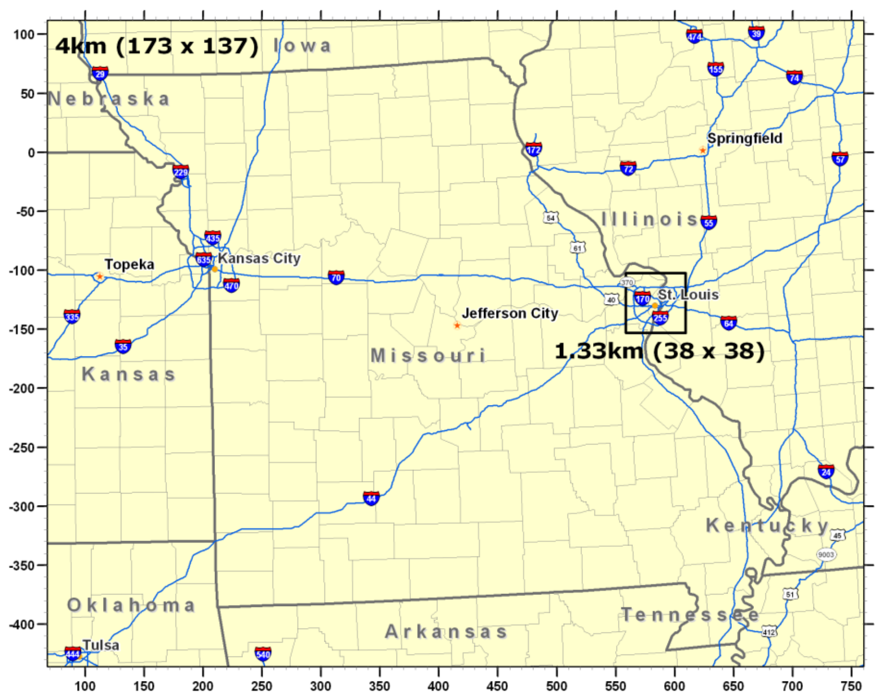
Figure 4-1. Manganese plumes at 2:00 to 3:00 CST on July 8, 2002 superimposed on satellite image of Detroit (the Rouge River area near Dearborn, MI). CAMx model results using a 1 km grid (left) and a 4 km grid with PiG (using a 200 meter sampling grid; right) are shown (Nopmongcol et al., 2009).



36 km Domain
SW Corner: -2736, -2088
NX, NY: 148, 112

12 km Domain
SW Corner: -552, -1632
NX, NY: 239, 239

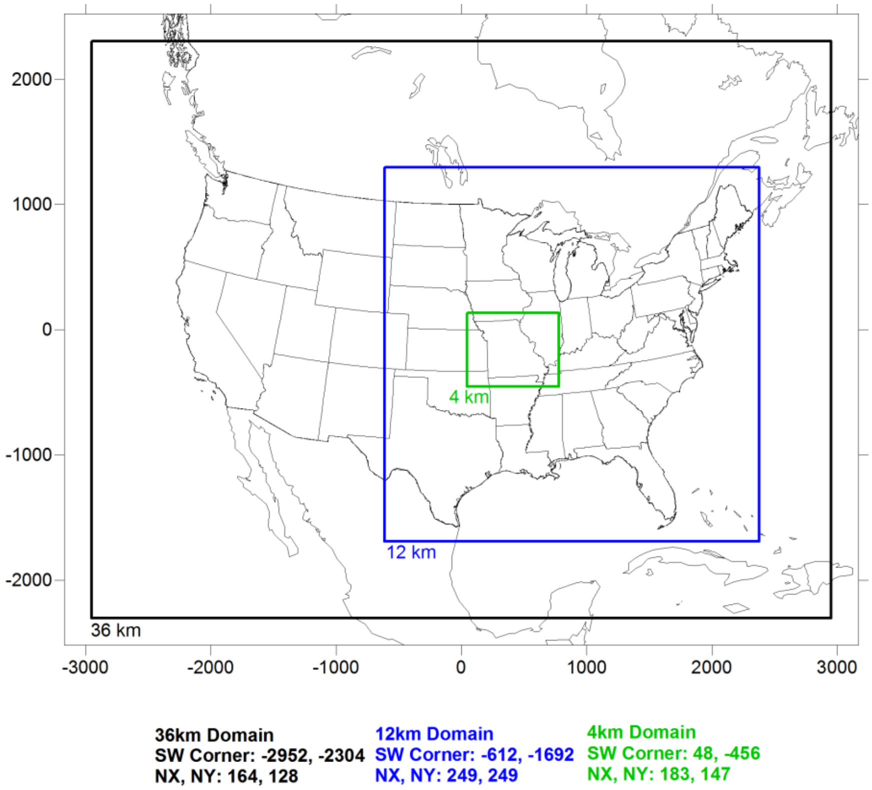
4 km Domain
SW Corner: 68, -436
NX, NY: 173, 137



4 km Domain
SW Corner: 68, -436
NX, NY: 173, 137

1.333 km Domain
SW Corner: 558.667, -153.333
NX, NY: 38, 38

Figure 4-2. 36/12/4 km (top) and 4/1.333 km (bottom) St. Louis SMOKE/CMAQ/CAMx modeling domains.



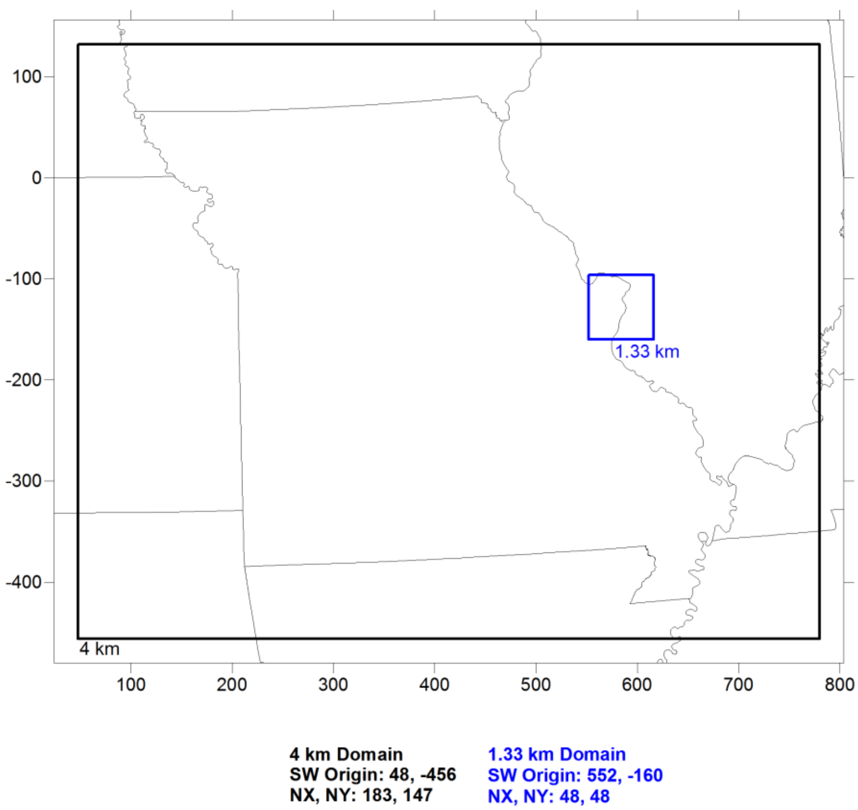


Figure 4-3. 36/12/4 km (top) and 4/1.333 km (bottom) St. Louis WRF modeling domains.

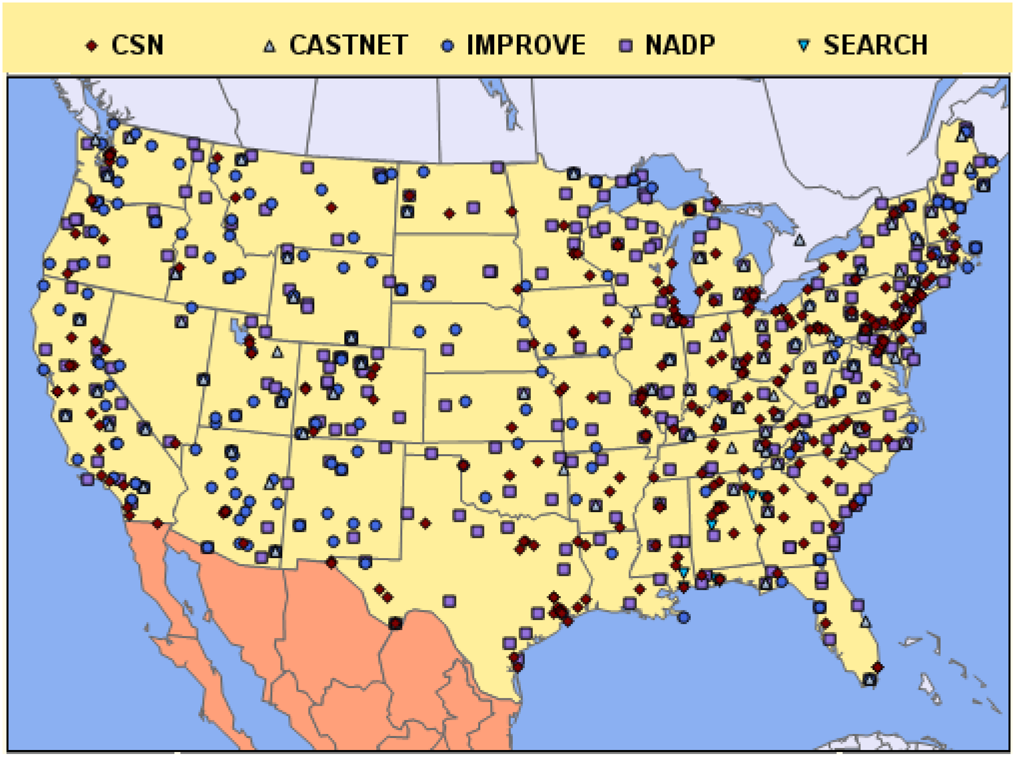


Figure 4-4a. Locations of CSN, CASTNET, IMPROVE, NADP and SEARCH monitoring sites.

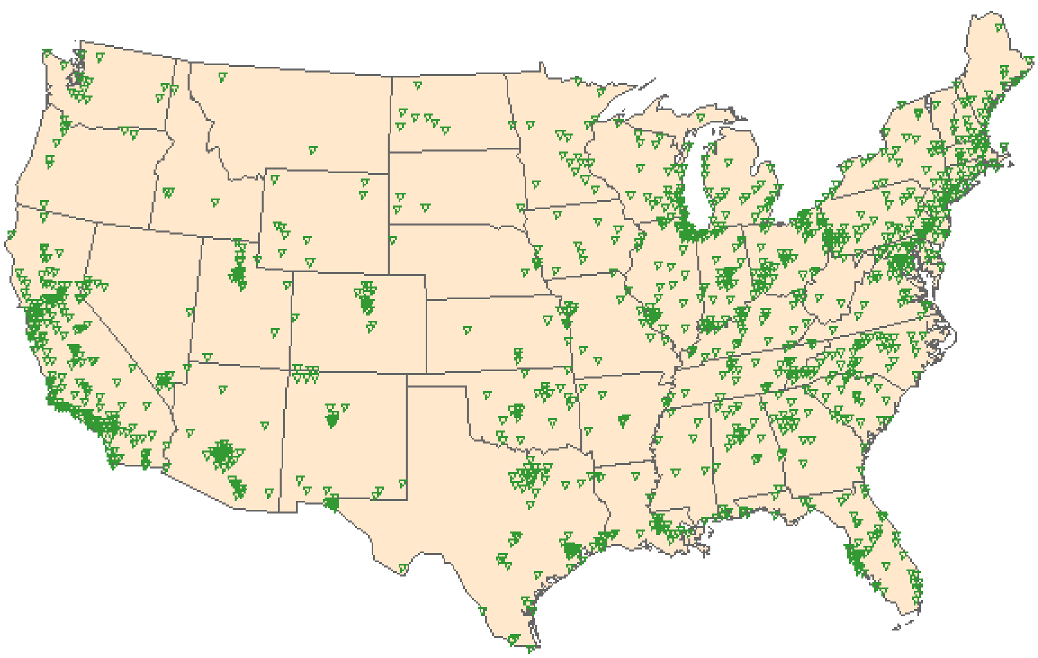


Figure 4-4b. Locations of AQS monitoring sites.

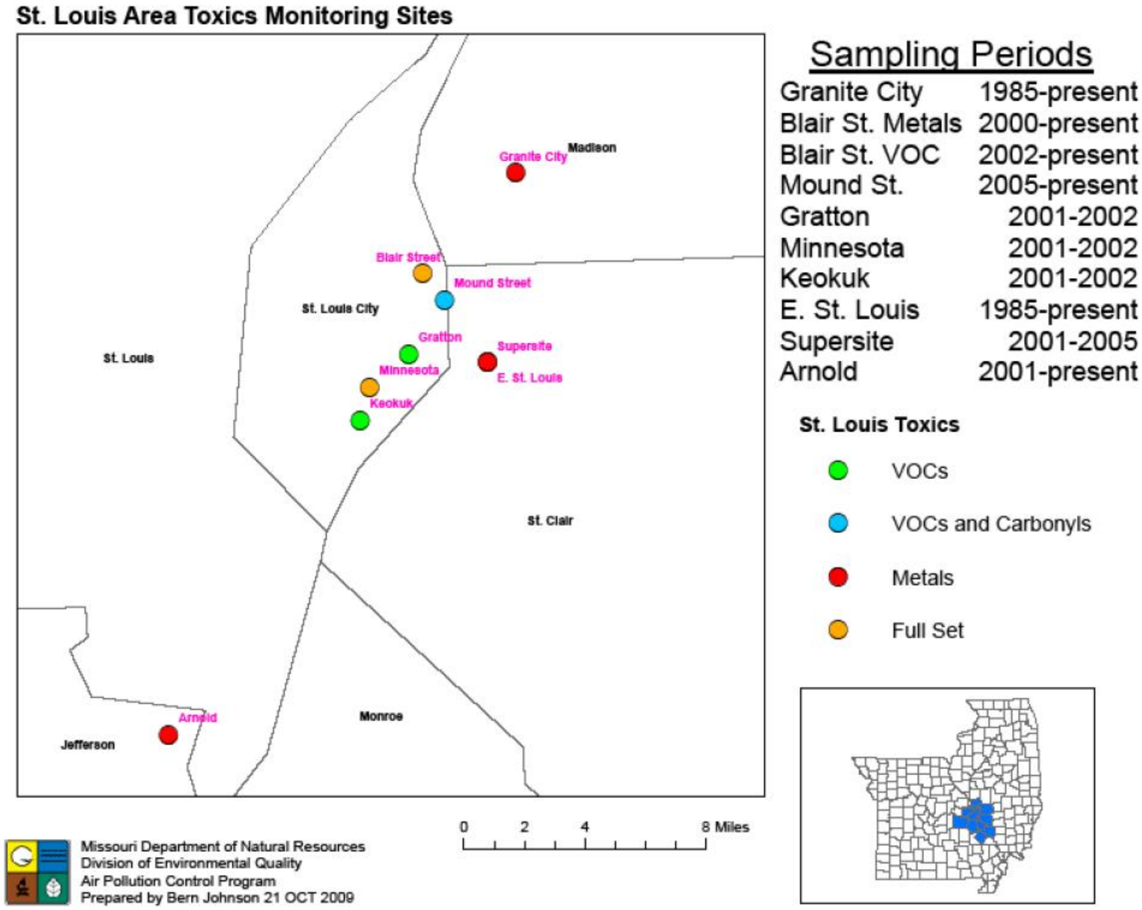


Figure 4-4c. Locations of air toxics monitoring sites in the St. Louis area.

5.0 MODEL INPUT PREPARATION PROCEDURES

This section describes the procedures to be used by the ENVIRON/ERG team in developing the meteorological, emissions, and air quality inputs to the CMAQ and CAMx model inputs for the St. Louis ozone, $PM_{2.5}$ and air toxics modeling. The development of the CMAQ and CAMx meteorological and emissions inputs are discussed together with the science options recommended for CMAQ and CAMx. The procedures for developing the initial and boundary conditions and photolysis rates inputs are also discussed along with the model application procedures.

These procedures recommended here are consistent with EPA guidance (EPA, 2007), other recent 8-hr ozone and $PM_{2.5}$ modeling studies conducted for various State and local agencies using these or other state-of-science modeling tools (see, for example, IEPA, 2007; Morris et al., 2008, 2009; MDNR and ENVIRON, 2009; ENVIRON et al., 2009) as well as the methods used by EPA in support of the recent Transport Rule (EPA, 2010).

5.1 Meteorological Model Inputs

WRF v3.1.1 was used by Iowa Department of Natural Resources (IDNR) for the 36/12 km WRF simulations. Since ENVIRON will be using the 12 km WRF outputs as a 1-way nest for the 4 km WRF simulations, this version will be retained for the 4/1.333 km WRF simulations. This also implies that the same physics options as used in the 36/12 km simulations (aside from cumulus parameterization) must be used for the nested grids as well.

5.1.1 WRF Model Configuration

The physics options utilized by IDNR in their 2007 36/12 km WRF simulations are summarized in Table 5-1. As mentioned above, these options will also be used for the 4/1.333 km WRF simulations performed by ENVIRON. The exception is cumulus parameterization, which can be turned on or off for individual modeling domains. The WRF documentation recommends that cumulus parameterization be turned off for horizontal resolutions < 10 km, since cumulus clouds are likely to be resolved at these resolutions (Skamarock et al., 2008).

5.1.2 WRF Input Data Preparation Procedures

A collection of programs known as the WRF Preprocessing System (WPS) is used to generate inputs for the WRF modeling system. The geogrid, ungrib, metgrid, ndown, and real programs will be used to generate WRF inputs and interpolate the existing 12 km WRF outputs to the 4 km WRF domain. The geogrid program defines the size and location of the model domain and interpolates static terrestrial fields (elevation, land use, soil type, vegetation fraction, etc.) to the model domain. The ungrib program extracts meteorological fields from GRIB files. Since ENVIRON is using the 12 km WRF outputs for initialization and boundary conditions, this step is only needed to run for the first hour of each 5-day segment to initialize soil moisture and temperature values for the 4 km simulation. The metgrid program horizontally interpolates the variables from ungrib to the model domains. The real program vertically interpolates the output from metgrid to the model domain. Finally, the ndown (short for "nest down") program will be used to take the WRF coarse domain outputs (in this case 12 km) and output from the real program to create initial and boundary condition files for the 4 km WRF domain (Wang et. al., 2011).

Surface observation nudging will be used by ENVIRON to improve the performance of the nested domains. This process will utilize surface observation data from the Meteorological Assimilation Data Ingest System (MADIS).

5.1.3 WRFCAMx/MCIP Reformatting Methodology

The WRFCAMx interface program will be used by ENVIRON to translate WRF output meteorological fields to CAMx inputs. The program will generate the files for any duration (from a single hour to several days), but ENVIRON has determined that running WRFCAMx to develop daily input files allows the greatest flexibility, as the meteorological files can become very large. For a single day, 25 hours of meteorology must be present (midnight through midnight, inclusive) as these fields represent hourly instantaneous conditions and CAMx internally time-interpolates these fields to each model time step. Precipitation fields are not time-interpolated, but rather time-accumulated, so cloud/precipitation files contain one less hour than other met files (e.g., 24 hours of clouds / precipitation vs. 25 hours for other meteorology fields).

The CAMx physical height layer structure (meters AGL) is defined from the geopotential heights at each of WRF's "eta" levels, and thus varies in space and time. ENVIRON will perform vertical averaging (“layer collapsing”) of WRF layers to a coarser CAMx layer structure, as CAMx simulations run considerably faster when upper layers are collapsed without a significant difference in resulting CAMx concentrations. The set of WRF layers to combine into CAMx layers is specified in the script file (Table 4-3). Variables in each WRF layer are mass-weighted to each bulk CAMx layer.

Several options are available to derive Kv (vertical diffusivity) fields from WRF output. When TKE (turbulent kinetic energy) is not available from the WRF output (as is the case with the Pleim-Xiu LSM), Kv fields are diagnosed from wind, temperature, and PBL parameters in WRFCAMx. WRFCAMx has the ability to process sub-grid cloud data from WRF fields. Selecting the “DIAG” sub-grid cloud method diagnoses sub-grid cloud fields from WRF gridded thermodynamic fields. For grid spacing less than about 10 km, small-scale convection is likely generated by the grid-resolved cloud physics in WRF. Therefore, the DIAG option will be selected for the St. Louis 12 km WRFCAMx extraction, but not for the 4 or 1.333 km conversion.

The CMAQ Meteorological-Chemistry Interface Processor (MCIP) will be used by ENVIRON to translate WRF output meteorological fields to CMAQ inputs. The selection of the Pleim-Xiu land surface model and ACM2 planetary boundary layer scheme is well-suited for MCIP extraction and CMAQ modeling. ACM2 is the default vertical diffusion scheme (computes stability and vertical mixing) in CMAQ, and the calculation of dry deposition velocities (within MCIP or CMAQ) rely on fields generated by the Pleim-Xiu land surface model (Otte and Pleim, 2010). The extraction process for MCIP is similar to WRFCAMx, in that single files containing 25 hours of meteorological data are generated for each 24-hour simulation period.

When fractional landuse percentages are available (as is the case with the existing IDNR WRF outputs), MCIP can create a PURB (percent of urban landuse) variable that can be used for modifying the minimum eddy diffusivity in CMAQ. This procedure increases the minimum eddy diffusivity (vertical mixing) in urban areas to account for the urban heat island effect.

5.2 Emission Inputs

ENVIRON/ERG team expects to develop the emissions inputs for the St. Louis ozone, $PM_{2.5}$ and air toxics modeling study from pertinent recent urban- and regional-scale modeling programs in the region including continental US, Canadian and Mexican data. The emission inventory data will be obtained from various sources including EPA and other RPOs (see Section 4.3.1 for existing data sources).

5.2.1 Development of Point Source Emissions

As described above, the ENVIRON/ERG team will compile and develop point source emissions data from existing emissions inventories, to the greatest extent possible. In general, these emissions data will be either 2007 or 2008 emissions, depending upon the particular existing inventory that is utilized. Due to project resource constraints, any 2008 point source emissions will be assumed to also be representative of the 2007 inventory year. One exception is that any 2008 point source emissions from electricity generating units (EGUs) will be replaced by actual 2007 emissions data obtained from EPA's Clean Air Markets Division's (CAMD) emissions database (EPA, 2011). In addition to emissions data, associated point source coordinates and stack parameters will also be compiled. The MANE-VU and LADCO states mostly have 2007 inventory, but it is still unknown whether the SEMAP 2007 inventory will be ready in time for this modeling study. Due to delays in the promulgation of the new ozone NAAQS, SEMAP has put their study on hold. An updated status of the inventory year will be provided as we get additional information from the states.

5.2.2 Development of Area and Non-Road Source Emissions

Similar to the point source emissions described above, the ENVIRON/ERG team will also compile and develop area and nonroad mobile source emissions data from existing emissions inventories, to the greatest extent possible. As with the point sources, some of the emissions data will be for 2007, but some of the emissions data might be for other years (i.e., 2006 or 2008), depending upon the particular existing inventory that is utilized. Due to project resource constraints, any area or non-road mobile source emissions for other years will also be assumed to be representative of the 2007 inventory year.

5.2.3 Development of On-Road Mobile Source Emissions

ENVIRON will collect the required data to compile the inputs necessary for developing the on-road mobile source emissions for the June-September 2007 episode in the 4 state area of Missouri, Illinois, Kansas and Oklahoma. ENVIRON will request the following MOVES county level input data from the states:

- For each representative county in Missouri, Illinois, Kansas and Oklahoma,
  - Age Distribution
  - Fuel Supply and Formulation (by month, if a seasonal fuels change occurs during the episode)
  - Inspection and Maintenance Program parameters

- For all counties in Missouri, Illinois, Kansas and Oklahoma,
  - Annual VMT classified by HPMS Vehicle Type
  - Vehicle Population classified by MOVES Source Type
- A crosswalk associating each county to a representative county in the four states.

ENVIRON will also obtain the required data to process MOVES lookup tables in SMOKE. The following files are required SMOKE inputs:

- MBINV: VMT, VPOP, and SPEED inventories in the flat file 2010 (FF10) activity file format
- MCXREF: Reference county cross-reference file
- MEPROC: A list of MOVES emission processes and associated pollutants for SPCMAT
- MFMREF: Reference county fuel month file
- MRCLIST: A list of MOVES lookup tables by reference county
- MOVES emission factor lookup tables: RatePerDistance, RatePerVehicle and RatePerProfile
- MET4MOVES output file for SMOKE
- Other ancillary input files needed for mobile-source emissions modeling including spatial surrogates, surrogate cross-reference file, temporal profiles, temporal cross-reference file, speciation profiles, and speciation cross-reference file.

The MOVESMRG program in SMOKE will be used to develop the base year on-road mobile source estimates for CO, NOx, PM, and VOC emissions. Emission rate lookup tables from MOVES2010a will be combined with meteorology data from MET4MOVES output and county level activity data to calculate the gridded, temporalized emission estimates for the 4 state area.

As previously mentioned, ENVIRON will acquire existing on-road emissions inventories from EPA, SESARM and/or RPOs for coverage of the other 44 states not including Missouri, Illinois, Kansas and Oklahoma. Emissions from other inventories will be grown or interpolated to 2007 if necessary, converted to Inventory Data Analyzer (IDA) emissions data format and then processed through SMOKE. The 4 and 44 state inventories will be carefully merged to avoid double counting.

5.2.4 Development of Biogenic Source Emissions

A revised version of a commonly used biogenic emissions model, the Biogenic Emissions Inventory System (BEIS) will be used to process emissions from biogenic sources. We recommend using BEIS3 which contains several advantages over the previous version, BEIS2:

- Vegetation input data are based on a 1 km Biogenic Emissions Landuse Database (BELD3) vegetation data base,
- Many of the emission factors have been updated including some recent NARSTO modifications,
- Environmental algorithm includes a sunlit/shaded leaf solar radiation model.

The latest BELD3 landuse data provides distributions of 230 vegetation classes at 1 km resolution, and will be used to estimate biogenic emissions for the St. Louis 36/12/4/1.333 km domains and June-September 2007 modeling period. The BEIS model also requires as input hourly, gridded temperature and solar radiation data to estimate biogenic emissions, and these data will be derived from the WRF simulations using MCIP.

ENVIRON will prepare all necessary SMOKE/BEIS3 script files and inputs for the AQMP Technical Workgroup to generate biogenic emissions for the St. Louis modeling study. For a QA, ENVIRON will run SMOKE/BEIS3 for at least one hot summer month and examine the spatial and temporal distribution of biogenic emissions by comparing with other studies (e.g., past RPO and MDNR 2002 biogenic emissions modeling).

Sensitivity tests may be performed using the Model of Emissions of Gases and Aerosols from Nature (MEGAN) as an alternative biogenic emissions model.

5.2.5 Development of Fire Emissions

Emissions from major wild fire events will be developed using Moderate Resolution Imaging Spectroradiometer (MODIS)[1] observed active fire data if the 2007 MODIS data are readily available. We will carefully examine the NEI wildfire data to avoid any "double-counting."

5.2.6 Development of CMAQ-Ready Emissions Inputs

SMOKE version 2.7 will be configured to generate CMAQ-ready emissions inputs for the 36/12/4/1.333 km modeling domains (Figure 4-1) and the June 1 through September 30, 2007 modeling period. For point/area/nonroad source emissions, the ENVIRON/ERG team will compile the inventory data and convert them to SMOKE-ready input files which will be submitted to AQMP Technical Workgroup for the SMOKE processing. On-road mobile source emissions will be prepared by MOVES2010a through the SMOKE-MOVES tool. ENVIRON will perform the SMOKE-MOVES processing and generate CMAQ-ready on-road mobile source emissions that can be readily merged together with the SMOKE outputs for other source categories. Table 5-2 summarizes the emissions modeling configuration to be used.

Producing day-specific input files for all source categories places a burden on available computing facilities, data management systems. Selecting representative model days for some or all of the source categories reduces the processing and file handling requirements to a more manageable level and in most cases does not compromise the accuracy of the emissions files. Other modeling projects undertaken by the EPA, WRAP, VISTAS and LADCO have used a selection approach for all of the source categories (except biogenics) that use a representative weekday/Saturday/Sunday either for each month or each season to model all of the emissions files. In an attempt to better represent the level of temporal and spatial detail available for each source category, we recommend the following strategy:

- Biogenic emissions will be modeled for each episode day, using the daily meteorology.
- Point sources, including CEM and fire emissions, will be modeled for each episode day to take advantage of the available day-specific emissions (if available) and meteorology.

[1] http://rapidfire.sci.gsfc.nasa.gov/

- Area sources, including non-road mobile and dust emissions, with the exception of windblown dust emissions, do not utilize meteorological data, and are temporally allocated by monthly, daily and hourly profiles. Reviewing these profiles indicate that maximum temporal definition can be achieved by selecting representative weekday/Saturday/Sunday/Monday for each month. Holidays will be treated as Sunday.
- Motor vehicle emission factors are influenced by meteorological variability, but the processing requirements for such detailed emission factors for all the modeling domains were determined to be prohibitive under the current schedule. We expect the contributions of the day-specific meteorological effects on mobile source emissions outside of the St. Louis urban area to be much less than from within the St. Louis nonattainment area. Thus, we propose to compute the MOVES emission factors as a function of hourly meteorological data only for the 4/1.333 km domains. Outside the 4 km domain, average day in month emission factors will be processed. VMT data will be processed using the weekday/Saturday/Sunday/Monday scheme.

For ozone modeling alone, hourly emissions are required for NO, NO_2, CO, several classes of VOCs and other pollutants as available. The VOC classes used will depend upon the chemical mechanism selected. For this St. Louis modeling study, the CB05 chemical mechanism will be used. Additional PM and precursor species are needed for PM modeling, which includes SO_2, NH_3, SO_4, NO_3, EC, OMC, other primary $PM_{2.5}$ and coarse PM ($PM_{2.5\text{-}10}$). Also, for the multi-pollutant modeling, the following air toxics as identified in the AQMP3 (MDNR and IEPA, 2010) should be included: lead, acetaldehyde, arsenic compounds, benzene, chromium compounds, formaldehyde and diesel particulate matter. ENVIRON will review EPA's speciation profiles for air toxics and, if necessary, develop new VOC and PM speciation profiles for the air toxics listed above so that SMOKE can generate all the necessary emission input species for the St. Louis ozone, $PM_{2.5}$ and air toxics modeling.

5.2.7 Development of CAMx-Ready Emissions Inputs

Development of the CAMx-ready emissions files follows directly after the CMAQ-ready emissions development process outlined above. Once the CMAQ-ready 3-D emission inputs are generated, the CMAQ-to-CAMx emissions converter would be used to generate the CAMx-ready emission inputs for the same modeling domains and modeling period. This converter performs the following:

- Reads the 3-D CMAQ-ready I/O API emission input file;
- Maps CMAQ species to CAMx species and performs unit conversions;
- Writes out a CAMx-ready low-level emission input file (from the CMAQ emissions in the surface layer) and a CAMx-ready elevated point source input file (from the CMAQ emissions above the surface layer).

5.2.8 QA/QC and Emissions Merging

The emissions will be processed by major source category in several different "streams", including point sources (CEM and non-CEM), area sources, on-road mobile sources, non-road mobile sources, and biogenic sources. Separate Quality Assurance (QA) and Quality Control (QC) will be performed for each stream of emissions processing and in each step.

Prior to inputting emissions inventory data unto the SMOKE input format, the ENVIRON/ERG team will conduct some basic high-level QA on all received emissions data from existing emissions inventories. Since these existing emissions inventories have been released to the public, it is expected that certain level of QA will have already been conducted during the previous development and use of these inventories. As time and resources allow, the ENVIRON/ERG team will conduct the following high-level QA procedures:

- Review of available inventory documentation and metadata;
- Completeness check of source categories and pollutants;
- Identification of sources or source categories that are "outliers" (i.e., emissions that are obviously incorrect by several orders of magnitude);
- Accuracy of point source coordinates (e.g., correspondence between coordinates and counties);
- Completeness check of point source stack parameters.

Data deficiencies identified through the QA procedures outlined above will be discussed with AQMP Technical Workgroup; potential gap filling options, if necessary, will also be discussed. However, due to project limitations, actual gap filling may not be conducted.

For the on-road mobile source emissions, the following additional checks will be performed:

- Review and summary of the 2007 MOVES emissions outputs for each representative county and the county mappings;
- Display of the county level VMT and vehicle population data for 2007 and compare back to the 2002 VMT data used in the previous St. Louis SIP modeling identifying any anomalous growth;
- Graphical visualization of the spatial distribution of the on-road mobile source emissions across the 36/12/4/1.333 km domains and the temporal (monthly, day-of-week and diurnal) distributions of the on-road mobile source emissions.

SMOKE includes advanced quality assurance features that include error logs when emissions are dropped or added. In addition, we will generate visual displays that include:

- Spatial plots of the hourly emissions for each major species (e.g., NOx, VOC, some speciated VOC, SO2, NH3, PM and CO);
- Vertical average emissions plots for major species and each of the grids;
- Diurnal plots of total emissions by major species; and
- Summary tables of emissions for major species for each grid and by major source category.

This QA information will be examined against the original point and area source data and summarized in an overall QA/QC assessment.

Scripts to perform the emissions merging of the appropriate biogenic, on-road, non-road, area and point source emission files will be written to generate the CMAQ-ready three-dimensional day-specific hourly speciated gridded emission inputs. CAMx-ready emissions will be converted from the merged CMAQ inputs as described in the previous section. The resultant CMAQ and CAMx model-ready emissions will be subjected to a final QA using spatial maps, vertical plots and diurnal plots to assure that: (1) the emissions were merged properly; (2) CMAQ and CAMx inputs contain the same total emissions; and (3) to provide additional QA/QC information.

5.2.9 Products of the Emissions Inventory Development Process

In addition to the CMAQ and CAMx model-ready input files generated for each hour of all days modeled in the June-September 2007 modeling period, a number of quality assurance (QA) files will be prepared and used to check for gross errors in the emissions inputs. Importing the model-ready emissions into PAVE and looking at both the spatial and temporal distribution of the emission provides insight into the quality and accuracy of the emissions inputs.

- Visualizing the model-ready emissions with the scale of the plots set to a very low value, we can determine whether there are areas omitted from the raw inventory or if emissions sources are erroneously located in water cells.
- Spot-check the holiday emissions files to confirm that they are temporally allocated like Sundays.
- Producing pie charts emission summaries that highlight the contribution of each emissions source component (e.g. nonroad mobile).
- Normalizing the emissions by population for each state will illustrate where the inventories may be deficient and provide a reality check of the inventories.

State inventory summaries prepared prior to the emissions processing will be used to compare against SMOKE output report totals generated after each major step of the emissions generation process. To check the chemical speciation of the emissions to CB05 species as well as air toxics, we will compare reports generated with SMOKE reports to target these specific areas of the processing. For speciation, the inventory import state totals will be compared against the same state totals with the speciation matrix applied.

The quantitative QA analyses often reveal significant deficiencies in the input data or the model setup. It may become necessary to tailor these procedures to track down the source of each major problem. As such, one can only outline the basic quantitative QA steps that we will perform in an attempt to reveal the underlying problems with the inventories or processing. Following are some of the reports that may be generated to review the processed emissions:

- State and county inventory totals for each source category
- State and county totals after spatial allocation for each source category
- State and county totals by day after temporal allocation for each source category for representative days
- State and county totals by model species after chemical speciation for each source category
- State and county model-ready totals (after spatial allocation, temporal allocation, and chemical speciation) for each source category and for all source categories combined
- If elevated source selection is chosen by user, the report indicating which sources have been selected as elevated and plume-in-grid will be included
- Totals by source category code (SCC) from the inventory for area, mobile, and point sources
- Totals by state and SCC from the inventory for area, mobile, and point sources
- Totals by county and SCC from the inventory for area, mobile, and point sources

- Totals by SCC and spatial surrogates code for area and mobile sources
- Totals by speciation profile code for area, mobile, and point sources
- Totals by speciation profile code and SCC for area, mobile, and point sources
- Totals by monthly temporal profile code for area, mobile, and point sources
- Totals by monthly temporal profile code and SCC for area, mobile, and point sources
- Totals by weekly temporal profile code for area, mobile, and point sources
- Totals by weekly temporal profile code and SCC for area, mobile, and point sources
- Totals by diurnal temporal profile code for area, mobile, and point sources
- Totals by diurnal temporal profile code and SCC for area, mobile, and point sources
- PAVE plots of gridded inventory pollutants for all pollutants for area, mobile, and point sources

5.3 Photochemical Modeling Inputs

5.3.1 CMAQ Science Configuration and Input Preparation

The CMAQ (v4.7.1) model configuration and science options to be used in the St. Louis ozone, $PM_{2.5}$ and air toxics are summarized in Table 5-3. The horizontal and vertical grid structures are defined in the previous section (Tables 4-2 and 4-3). Each of the 36/12/4/1.333 km grids will be modeled sequentially using one-way nesting, and the IC/BC inputs for a nested grid will be extracted from its parent grid modeling output. The CB05 gas-phase chemistry mechanism with AERO5 aerosol option (CB05CL_AE5_AQ) will be used for ozone and PM modeling. Multi-pollutant modeling (CB05CLTX_AE5_AQ) for air toxics will be separately performed so that the ozone and $PM_{2.5}$ SIP modeling schedule won't be affected by issues that may arise with air toxics modeling. Horizontal and vertical advection will be solved by the global mass-conserving scheme developed by Dr. Yamartino which uses the Piecewise Parabolic Method (PPM) scheme for horizontal advection and derives vertical velocity components from the mass continuity equation. Multi-scale Smagorinsky (1963) approach and Asymmetric Convective Model version 2 (ACM2; Pleim, 2007) are used for horizontal and vertical eddy diffusion, respectively.

Meteorological Inputs: The WRF-derived meteorological fields will be prepared for the CMAQ model using the MCIP processor.

Initial/Boundary Conditions: CMAQ's default ICs will be used to initialize the 36 km simulation, and the BCs will be based on results from a 2007 MOZART-4 global model simulation. The IC/BC inputs for the nested grids will be derived from their parent grid simulation outputs.

Photolysis Rates: Several chemical reactions in the atmosphere are initiated by the photo-dissociation of various trace gases. To accurately represent the complex chemical transformations in the atmosphere, accurate estimates of these photo-dissociation rates must be made. The Models-3 CMAQ system includes the JPROC processor, which calculates a table of clear-sky photolysis rates (or J-values) for a specific date. JPROC uses default values for total aerosol loading and provides the option to use default ozone column data or to use the Total Ozone Mapping Spectrometer (TOMS) data for total column ozone. We will download the 2007 TOMS data from the TOMS website[2] and

[2] http://toms.gsfc.nasa.gov/ozone/ozone_v8.html

process JPROC to generate the photolysis rate input file for each simulation day. If the 2007 TOMS data has any missing day, we will use data of previous or next day instead.

Landuse: MCIP processing of the WRF output will provide the landuse data, which is the standard CMAQ approach of deriving landuse.

Spin-Up Initialization: The 36 km simulation will use a 15-day spin up period to eliminate any significant influence of the ICs. ICs for the nested grids will be extracted from their parent grid simulations with a shorter spin up period (at least 5 days for the 12 km; 3 days for the 4 km; 1 day for the 1.333 km).

5.3.2 CAMx Science Configuration and Input Configuration

This section describes the model configuration and science options to be used in the St. Louis ozone, $PM_{2.5}$ and air toxics modeling study. Table 5-4 summarizes the proposed configuration for the CAMx simulations.

As indicated in the CAMx model setup defined in Table 5-4, four modeling grids will be employed. The 36/12/4 km grids will be run using two-way interactive grid nesting. Although the 36 and 12 km grids are only required for ozone, PM will be modeled as well to provide initial and boundary conditions for the 4/1.333 km PM modeling which will also utilize the two-way nesting. Air toxics will be modeled using CAMx Reactive Tracer (RTRAC) tool (ENVIRON, 2010), which will be performed separately so that the ozone and $PM_{2.5}$ SIP modeling schedule won't be affected by issues that may arise with air toxics modeling. The PPM advection solver will be used along with the spatially varying (Smagorinsky) horizontal diffusion approach. K-theory scheme is the default option for vertical diffusion in CAMx, but ACM2 scheme is also available. It should be noted, however, that the ACM2 scheme lengthens CAMx run times and is currently not compatible with certain CAMx diagnostic tools (IPR and DDM). The CB05 chemical mechanism will be used in order to be consistent with CMAQ. However, CAMx also includes the CB6 chemical mechanism that should be considered.

Meteorological Inputs: The WRF-derived meteorological fields will be prepared for CAMx using WRFCAMx.

Initial/Boundary Conditions: The initial and boundary conditions will be converted from the CMAQ inputs using CMAQ2CAMx.

Photolysis Rates: ENVIRON will prepare the photolysis inputs as well as albedo/haze/ozone/snow inputs for CAMx based on TOMS data. For CAMx the TUV processor will be used. If there are periods of more than a couple of days where daily TOMS data are unavailable, monthly average TOMS data will be used.

Landuse: ENVIRON will generate landuse fields for the Zhang dry deposition scheme which uses extended (26) landuse categories.

Spin-Up Initialization: For the 36/12/4 km modeling, 15 days of spin up (May 17-31, 2007) will be used before the first day of the modeling period (June 1, 2007). For the 4/1.333 km modeling, 3 days of spin up will be used.

Table 5-1. Configuration options used in 2007 IDNR 36/12 km WRF simulations.

WRF Treatment	Option Selected	Notes
Microphysics	Morrison 2-moment	Double-moment ice, snow, rain and graupel for cloud-resolving simulations.
Longwave Radiation	RRTMG	Rapid Radiative Transfer Model for GCMs includes random cloud overlap and improved efficiency over RRTM.
Shortwave Radiation	RRTMG	Same as above, but for shortwave radiation.
LSM	Pleim-Xiu	Two-layer scheme with vegetation and sub-grid tiling.
PBL Scheme	ACM2	Assymetric Convective Model with non-local upward mixing and local downward mixing.
Cumulus Parameterization	Kain-Fritsch (new Eta)	Kain-Fritsch is a deep and shallow convection sub-grid scheme. Cumulus paramterization is recommended for grid resolution > 10 km.
Analysis Nudging	Nudging applied to winds, temperature and moisture	Temperature and moisture nudged above PBL only

Table 5-2. Emissions model configurations.

Emissions Component	Configuration	Notes
Model Code	SMOKE version 2.7 MOVES2010a	http://www.smoke-model.org/index.cfm http://www.epa.gov/otaq/models/moves/
Horizontal Grid Mesh	36/12/4/1.333 km	
36 km grid	148×112 cells	
12 km grid	239×239 cells	
4 km grid	173×137 cells	
1.333 km grid	38×38 cells	
Point Source Emissions	SMOKE version 2.7	ERG/AQMP Technical Workgroup
Area Source Emissions	SMOKE version 2.7	ERG/AQMP Technical Workgroup
Nonroad Mobile Source Emissions	SMOKE version 2.7	ERG/AQMP Technical Workgroup
On-Road Mobile Source Emissions	MOVES2010a SMOKE-MOVES	ENVIRON
Emissions Data Sources	2007 CENRAP Point Source Inventory	Being developed
	2007 MRPO Draft Base C Inventory	Nearing completion
	2007 SEMAP Base Inventory	Nearing completion; utilized SMOKE-MOVES
	2007 MARAMA/MANE-VU Inventory	Completed except for on-road mobile
	2008 NEI Version 1	Released April 2011; point (incomplete)/on-road/nonroad only
	2008 NEI Version 1.5	To be released May 2011; area
	2007 EPA CAMD emission database	EGUs
	2006 Canada Inventory	Completed
	2008 Mexico Inventory	Completed
	2005 EPA Transport Rule Modeling Inventory	MOVES-based inventory; to be interpolated for 2007
Biogenic Source Emissions	BEIS3 within SMOKE version 2.7	ENVIRON/AQMP Technical Workgroup
Temporal Adjustments	Seasonal, day, hour	Based on latest collected information
Chemical Speciation	Revised CB05 Speciation with Air Toxics	ENVIRON
Gridding	EPA Spatial Surrogates	
Growth and Controls		ENVIRON/ERG; future year to be specified by MDNR
Quality Assurance	QA Tools in SMOKE	

Table 5-3. CMAQ (version 4.7.1) model configuration.

Science Options	Configuration	Notes
Model Code	CMAQ version 4.7.1	www.cmascenter.org
Horizontal Grid Mesh	36/12/4/1.333 km	
36 km grid	148×112 cells	
12 km grid	239×239 cells	
4 km grid	173×137 cells	
1.333 km grid	38×38 cells	
Vertical Grid Mesh	24 vertical layers	Layer 1 thickness ~ 20 m
Grid Interaction	One-way nesting	
Initial Conditions	CMAQ default profile	
Boundary Conditions	2007 MOZART-4	
Emissions		
Baseline Emissions	SMOKE version 2.7	
Sub-grid-scale Plumes	No Plume-in-Grid (PinG)	CMAQ no longer supports PinG
Chemistry		
Gas Phase Chemistry	CB05	Yarwood et al. (2005); multi-pollutant mechanism (CB05CLTX_AE5_AQ) for air toxics modeling
Inorganic Aerosol Chemistry	AE5/ISORROPIA	Nenes et al. (1998)
Secondary Organic Aerosols	AE5/SORGAM	Schell et al. (2001); additional SOA formation pathways
Aqueous (Cloud) Chemistry	AE5/RADM	Chang et al. (1987); includes sub-grid cloud processes
Meteorological Processor	MCIP version 3.6	
Horizontal Transport		
Eddy Diffusivity Scheme	Spatially varying	K-theory with Kh grid size dependence
Vertical Transport		
Eddy Diffusivity Scheme	Asymmetric Convective Model version 2 (ACM2)	Pleim (2007)
Diffusivity Lower Limit	0.5-2.0	Based on the percentage of urban area (PURB)
Deposition Schemes		
Dry Deposition	M3dry	Directly linked to Pleim-Xiu LSM parameters
Wet Deposition	RADM	
Numerics		
Gas Phase Chemistry Solver	Euler Backward Iterative (EBI) solver	Hertel et al. (1993)
Vertical Advection Scheme	Piecewise Parabolic Method (PPM) scheme with Yamartino correction scheme	
Horizontal Advection Scheme	PPM with Yamartino correction scheme	

Table 5-4. CAMx (version 5.3) model configuration.

Science Options	Configuration	Notes
Model Code	CAMx version 5.3	www.camx.com
Horizontal Grid Mesh	36/12/4/1.333 km	
36 km grid	148×112 cells	
12 km grid	239×239 cells	
4 km grid	173×137 cells	
1.333 km grid	38×38 cells	
Vertical Grid Mesh	24 vertical layers	Layer 1 thickness ~ 20 m
Grid Interaction	Two-way nesting	36/12/4 km for ozone; 4/1.333 km for PM and air toxics
Initial Conditions	CMAQ default profile	
Boundary Conditions	2007 MOZART-4	
Emissions		
Baseline Emissions	SMOKE version 2.7	
Sub-grid-scale Plumes	No Plume-in-Grid (PiG)	
Chemistry		
Gas Phase Chemistry	CB05	Yarwood et al. (2005); RTRAC for air toxics modeling; Consider sensitivity tests using CB6.
Inorganic Aerosol Chemistry	ISOROPIA	Nenes et al. (1998)
Secondary Organic Aerosols	SOAP	Strader et al. (1999); additional SOA formation pathways
Aqueous (Cloud) Chemistry	RADM	Chang et al. (1987)
Meteorological Processor	WRFCAMx	
Horizontal Transport		
Eddy Diffusivity Scheme	Spatially varying	K-theory with Kh grid size dependence
Vertical Transport		
Eddy Diffusivity Scheme	K-theory	ACM2 is available
Diffusivity Lower Limit	Kvpatch (0.1-1.0)	Based on the urban landuse fraction
Deposition Schemes		
Dry Deposition	Zhang03 scheme	Zhang et al. (2001; 2003)
Wet Deposition	CAMx rainout and washout	
Numerics		
Gas Phase Chemistry Solver	EBI solver	Hertel et al. (1993)
Vertical Advection Scheme	PPM scheme	Colella and Woodward (1984)
Horizontal Advection Scheme	PPM scheme	

6.0 OZONE MODEL PERFORMANCE EVALUATION

This chapter describes the model performance evaluation from which to establish reliable CMAQ and CAMx 8-hour ozone modeling for the St. Louis area. In general terms, this process consists of the following cycle:

- Exercise the modeling system for the base case, attempting to replicate the time and space behavior of the observed 1-hour and 8-hour ozone concentration fields as well as concentrations of precursor and product species:
- Evaluate the model's fidelity in simulating ozone and precursor/product species using a two-step process consisting of: (a) an initial "screening model performance evaluation" (SMPE) process, and if the modeling results pass the screening analysis, (b) a "refined model performance evaluation" (RMPE) consisting of progressively more stressful testing procedures involving multi-species, multi-scale surface and aloft model performance evaluation (MPE);
- Identify sources of error and/or compensating biases, through evaluation of preprocessor models (WRF, SMOKE), air quality model inputs, concentrations aloft, mass budgets and conservation, process analysis, etc;
- Through a documented process of diagnostic and sensitivity investigation, pinpoint and correct the performance problems via model refinement, additional data collection and/or analysis, or theoretical considerations;
- Re-run the model for the base case and re-evaluate performance until adequate, justifiable performance is achieved, or the modeling period is declared unsuited for further use based on documented performance problems.

To an extent, some or all of these steps will be taken by the ENVIRON team for the June-September 2007 period ideally culminating in a modeling database demonstrated to exhibit sufficiently minimal bias and error that they may be used reliably to evaluation 8-hour ozone control strategies and to perform an 8-hour ozone attainment demonstration. In the following subsection, we briefly identify the steps that will be taken by the ENVIRON team in constructing and evaluating the CMAQ and CAMx base cases for 8-hour ozone SIP development in St. Louis.

6.1 Establishing Base Case CMAQ and CAMx Simulations for St. Louis

6.1.1 Setting Up and Exercising CMAQ and CAMx Base Cases

The ENVIRON team will assist the AQMP Technical Workgroup in selecting the final model configurations for the CMAQ and CAMx base case simulations for June-September 2007 (see Chapter 5). The final model configurations will be determined based on results from the initial recommended configuration runs (see Tables 5-1 through 5-4) and a series of model sensitivity tests. The optimum model configurations will be identified based on the following factors:

- Model performance obtained using the initial model configurations and input data;
- Model performance for base case sensitivity tests;
- The ENVIRON team's knowledge of the CMAQ and CAMx model configurations and associated attributes;

- Experience performing sensitivity tests and model performance evaluation for CENRAP, VISTAS, MRPO, WRAP and numerous other studies including previous St. Louis ozone and PM SIP studies; and
- Comments from the AQMP Technical Workgroup, EPA, Stakeholders and other participants.

The objective in identifying optimum model configurations is to obtain the best performance for the right reasons consistent with sound science and EPA guidance. Sometimes, decisions must be made that trade off better/poorer model performance for one pollutant against another. These factors will be considered and potential issues discussed in the recommendations provided to the AQMP Technical Workgroup for the selection of final ozone model configurations.

6.1.2 Use of Sensitivity, Source Apportionment, and Related Diagnostic Probing Tools

The St. Louis modeling study may utilize several diagnostic and probing tools to further test and understand the CAMx and CMAQ base case ozone simulations. The use of these tools is discussed below.

Traditional Sensitivity Testing: Traditional sensitivity testing may be performed with both models. Once each model is operating properly for each base case, sensitivity runs may be performed to explore response to emissions changes as well as changes in key input parameters. These sensitivity runs serve two purposes: (a) They aid in helping to define appropriate emissions control scenarios, and (b) they provide episode-specific model uncertainty information that will be used later in "Weight of Evidence" analyses in support of the 8-hour ozone attainment demonstration.

Ozone Source Apportionment: With CAMx, focused use of ozone source apportionment technology (OSAT) for selected episodes may be employed to better understand model response and to aid in the design of control strategies. The value of source apportionment modeling for subsequent stages of the St. Louis modeling study is that these calculations will help to: (a) assess the contribution of sources in the Missouri/Illinois region and surrounding states to ozone concentrations at key receptor locations and (b) identify the particular source categories that may contribute the most to elevated 8-hour ozone concentrations in the St. Louis nonattainment area. The Anthropogenic Precursor Culpability Assessment (APCA) version of OSAT that can distinguish between controllable and uncontrollable (e.g., biogenic) emissions has proved particularly valuable and was a cornerstone to EPA's CAIR and NOx SIP Call Rules.

DDM Sensitivity Modeling: Another type of sensitivity modeling that may be performed entails the use of the Decoupled Direct Method (DDM) technology in CAMx and CMAQ. DDM may be set up and exercised to produce a numerically intensive, direct sensitivity/uncertainty analysis. The higher-order DDM (HDDM) can provide the first- and second-order sensitivity coefficients of ozone to model inputs (e.g., IC, BC, specific emissions, reaction rate constants). Note that not all model configurations are compatible with DDM (e.g., ACM2 vertical diffusion scheme is not compatible with DDM). ENVIRON will assist the AQMP Technical Workgroup in this diagnostic exploration as time and resources allow.

Process Analysis: Process Analysis (PA) is a tool in CAMx to extract additional information about the various physical and chemical processes in the model that produced the ozone concentrations. Information on VOC-limited versus NOx-limited ozone formation, importance of local production versus entrainment of ozone aloft and identification of the contributions of individual VOC species to ozone formation are the types of information that can be obtained with PA. It can be a powerful tool for diagnosing the causes of poor model performance. Of particular importance to the St. Louis modeling, PA can also improve model diagnosis and performance evaluation efforts by identifying processes that are "out of balance" (Tesche and Jeffries, 2002), by identifying situations for which the model formulation and/or implementation should not be expected to apply, and by suggesting how ambient data can be used to evaluate model accuracy for key terms in the chemical processing of VOC and NOx (e.g., Imre et al., 1998). CMAQ provides a similar process analysis tool (PROCAN) although with limited capability.

For the 2007 base case modeling and model performance evaluation, only traditional sensitivity tests will be utilized to help improve model performance due to resource and time constraints. Source apportionment modeling may be used with the future year modeling to assist in control strategy development.

6.2 Evaluation of CMAQ and CAMx Base Cases for the St. Louis Region

This section describes the procedures for evaluating the performance of the meteorological and photochemical models using the available aerometric data sets for the St. Louis ozone episode.

6.2.1 Overview

Model performance evaluation (MPE) is the process of testing a model's ability to accurately estimate observed atmospheric properties over a range of synoptic and geophysical conditions. When conducted thoughtfully and thoroughly, the process focuses and directs the continuing cycle of model development, data collection, model testing, diagnostic analysis, refinement, and re-testing. Below we summarize the philosophy and objectives that will govern the evaluation of the WRF, CAMx, and CMAQ models for the St. Louis 8-hour ozone application. Specific evaluation methods are identified that will be employed to judge the suitability of the meteorological and air quality models for regulatory applications, using common statistical measures and graphical procedures to elucidate model performance. This evaluation plan conforms to the procedures recommended by the EPA (1991; 1999; 2005; 2007) for 1-hour and 8-hour ozone attainment demonstration modeling.

We begin by establishing a framework for assessing whether the SMOKE/WRF/CAMx and SMOKE/WRF/CMAQ modeling systems (i.e., the emissions, meteorological and dispersion models and their supporting data sets) perform with sufficient reliability to justify one or both models' use in developing 8-hour ozone control strategies for the St. Louis nonattainment area. The models' reliability will be assessed given consideration to the following principals:

The Model Should be Viewed as a System: When we refer to evaluating a "model", we mean this in the broad sense. This includes not only the CAMx and CMAQ photochemical models, but its various components: companion preprocessor models (i.e., the SMOKE emissions and the WRF meteorological models), the supporting aerometric and emissions data base, and any other related analytical and numerical procedures used to produce modeling results. A principal emphasis in the model testing process is to identify and correct flawed model components;

Model Acceptance is a Continuing Process of Non-Rejection: Over-reliance on explicit or implied model "acceptance" criteria should be avoided for the reasons identified by Roth et al. (2005). This includes EPA's ozone performance goals (EPA, 1991). Models should be accepted gradually as a consequence of successive non-rejections. Over time, confidence in a model builds as it is exercised in a number of different applications (hopefully involving stressful performance testing) without encountering major or fatal flaws that cause the model to be rejected;

Criteria for Judging Model Performance Must Remain Flexible: The criteria for judging the acceptability of model performance should remain flexible, recognizing the challenging requirement of simulating air quality in the St. Louis region; and

Previous Experience Used as a Guide: Previous photochemical modeling experience serves as a primary guide for judging model acceptability. Interpretation of the CAMx and CMAQ modeling results for each episode, against the backdrop of previous modeling experience, will aid in identifying potential performance problems and suggest whether the model should be tested further or rejected.

A rigorous ozone model evaluation in typical regulatory applications consists of two components. The *operational evaluation* entails an assessment of the model's ability to estimate correctly surface meteorological or air quality variables largely independent of whether the actual process descriptions in the model are accurate. The operational evaluation essentially tests whether the predicted surface meteorological and air quality fields are reasonable, consistent and agree adequately with routinely available observations. In this study, the operational evaluations focus on the various model's reliability in reproducing hourly-average surface wind speed, wind direction, temperature, mixing ratio and ozone and precursor concentrations within and nearby St. Louis urban area.

The *scientific evaluation* addresses the realism of the meteorological and air quality processes simulated by the models through testing the model as an entire system (i.e., not merely focusing on surface wind, temperature or ozone predictions) as well as its component parts. The scientific evaluation seeks to determine whether the model's behavior, in the aggregate and in its component modules, is consistent with prevailing theory, knowledge of physical processes, and observations. The main objective is to reveal the presence of bias and internal (compensating) errors in the model that, unless discovered and rectified or at least quantified, may lead to erroneous or fundamentally incorrect decisions based on model usage. Ideally, the scientific evaluation consists of a series of diagnostic and mechanistic tests aimed at: (a) examining the existence of compensatory errors, (b) determining the causes of failure of a flawed model, (c) stressing a model to ensure failure if indeed the model is flawed, and (d) providing additional insight into model performance beyond that supplied through routine, operational evaluation procedures.

Practically, a rigorous scientific evaluation is seldom feasible due to the absence of the specific measurements needed to test the process modules (e.g., soil moisture, Reynold's stress measurements, PBL heights, trace gas species, and so on). Accordingly, the overall model performance evaluation in this study is constrained mainly to operational testing of the WRF models' primary meteorological outputs (i.e., wind speed, wind direction, temperature, and moisture) and the CAMx and CMAQ models' predictions of ozone, NOx, and potentially VOC. However, some components of the scientific evaluation of the air quality models are possible through examination of ground-level and aloft primary and product species and species ratios. In addition, corroborative analyses involving joint analysis of emissions inventory estimates, air quality model predictions and ambient measurements adds to the scientific evaluation.

6.2.2 Meteorological Model Evaluation Methodology

Meteorological inputs required by CAMx and CMAQ include hourly estimates of the three-dimensional distribution of winds, temperatures, mixing ratio, pressure, clouds, and precipitation, and other physical parameters or diagnosed quantities such as turbulent mixing rates (i.e., eddy diffusivities) and planetary boundary layer (PBL) heights. Accordingly, the objective of the WRF performance evaluation is to assess the adequacy of the surface and aloft meteorological fields for the St. Louis modeling episodes.

Components of the St. Louis WRF Evaluation: The WRF modeling system has been used widely in regional air quality model applications and under continuous development, improvement, testing and open peer-review for more than 10 years. Given that the WRF model code and algorithms have already undergone significant peer review, performance testing of the WRF model in this study will be focused on an operational evaluation. Typically, the scope of the scientific evaluation is limited by the availability of special meteorological observations (radar profiler winds, turbulence measurements, PBL heights, precipitation and radiation measurements, inert tracer diffusion experiments, and so on). Unfortunately, since none of these measurements were available over the St. Louis region during the modeling episodes, a meaningful scientific evaluation of the WRF was not possible in this study. However, if the operational evaluation presented in subsequent chapters is performed thoroughly, they are expected to be sufficient to serve as the basis for judging whether the model is operating with sufficient reliability over the St. Louis domain to be used in the photochemical modeling portion of this study.

Data Supporting Model Evaluation: Hourly surface observations will be obtained from the National Center for Atmospheric Research (NCAR) and other sources to support the evaluation of WRF near-surface temperature, water vapor, and wind speed fields. The specific NCAR data set used for this purpose is DS472.0 which is the hourly airways surface data. The primary data set available for comparing model performance aloft is the NOAA Forecast Systems Lab and National Climatic Data Center's Radiosonde Data of North America. These data sets will be collected in performing the St. Louis WRF model evaluation. For precipitation the Advanced Hydrologic Prediction Service (AHPS)[1] daily observations will be used.

Evaluation Tools: The primary tool used for evaluating the WRF meteorological model in air quality modeling study is the METSTAT program developed by ENVIRON. METSTAT calculates a suite of model performance statistics using surface wind speed, wind direction, temperature and water vapor mixing ratio for user-specified sub-domains. Tables 6-1 and 6-2 list some of the model performance evaluation metrics to be used in evaluating the WRF

[1] http://water.weather.gov/ahps/

model. Additional comparisons of the spatial patterns of precipitation and clouds may also be made using satellite and radar-based data.

6.2.3 Photochemical Model Evaluation Methodology

The CMAQ/CAMx performance evaluations will follow the procedures recommended in the EPA photochemical modeling guidance documents (EPA, 1991; 1999; 2005a; 2007). The evaluation will be carried out in two sequential phases, beginning with the simplest comparisons of modeled and observed ground-level ozone concentrations, progressing to potentially more illuminating analyses if necessary (e.g., examination of precursor and product species, comparisons of pollutant ratios and groupings). That is, the specific two-step ozone evaluation process is:

- An initial “screening model performance evaluation” (SMPE) process, and if the modeling results pass the screening analysis;
- A “refined model performance evaluation” (RMPE) consisting of progressively more stressful testing procedure involving multi-species, multi-scale surface and aloft MPE;

Below, we describe how this evaluation will be conducted. The formal procedures outlined in EPA recent 8-hour modeling guidance (EPA, 2007) will be used to evaluated CMAQ and CAMx for the St. Louis modeling episodes. The ENVIRON team will consider all six means for assessing photochemical model performance as specified in the guidance:

- Use of computer generated graphics;
- Use of ozone metrics in statistical comparisons;
- Comparison of predicted and observed precursor emissions or species concentrations;
- Comparison of observed and predicted ratios of indicator species;
- Comparison of predicted source category contribution factors with estimates obtained using observational models as available; and
- Use of retrospective analyses in which air quality differences predicted by the model are compared with observed trends.

Obviously, a comprehensive measurement database for ozone and precursors from an extensive monitoring network is needed to fully support all six of these analyses. This may not be possible with the current air quality data collected in the St. Louis area, particularly in regards to precursor measurements, since limited measurements were conducted in this area during the proposed modeling year. Therefore, the evaluation approach will consist of a blend of those points above and the steps outlined below. To the extent possible, each of the performance procedures described by EPA’s 8-hour guidance will be addressed, and at a minimum, an explanation of why certain components cannot be fulfilled will be provided.

Initial screening of the CMAQ and CAMx base case ozone predictions (i.e., the SMPE) will be performed for the initial base case in an attempt to identify obviously flawed model simulations and to implement and identify improvements to the model input files in a logical, defensible manner. The screening SMPE will employ some of the more appropriate ozone performance statistics and plots listed in Table 6-3. Examples of the types of graphical displays that may be helpful in the SMPE include the following:

- Spatial mean ozone time series plots;
- Ozone time series plots;
- Ground-level ozone isopleths;
- Ozone concentration scatter plots;
- Bias and error stratified by concentration; and
- Bias and error stratified by time.

Experience in photochemical modeling is the best basis upon which to identify obviously flawed simulation results. Efforts to improve photochemical model performance, where necessary and warranted (i.e., to reduce the discrepancies between model estimates and observations), should be based on sound scientific principles. A “curve-fitting” or “tuning” activity is to be avoided.

The following principals will govern the model performance improvement process (to the fullest extent possible given the project schedule):

- Any significant changes to the model or its inputs must be documented and discussed with key participants (e.g., MDNR, IEPA);
- Any significant changes to the model or its inputs must be supported by scientific evidence, analysis of new data, or by re-analysis of the existing data where errors or misjudgments may have occurred; and
- All significant changes to the model or its inputs should be reviewed by the project sponsors and/or other advisory group(s).

If the initial screening of the CAMx and/or CMAQ ozone results does not reveal obvious flaws, the refined model performance evaluation will be carried out. If significant performance issues are uncovered in the SMPE, further model diagnosis and quality assurance of the input files and related model performance improvement analyses will be performed. That is, the full refined model performance evaluation will not be carried out on obviously flawed model simulations as it would be wasteful of project resources and schedule.

Assuming the SMPE is satisfactory, the formal operational evaluation in the RMPE will commence. First, the graphical displays utilized previously for ozone may be generated for NOx, VOC, and key product species (e.g., HNOx, PAN) as available. Note that model performance for VOC and many product species may be limited since there are little relevant ambient measurements collected in the St. Louis region. But even so, the graphical displays for ozone precursor and product species will be examined for obvious flaws that may be readily apparent even in the absence of measurements. Should these be detected, the model diagnosis and performance improvement efforts may be needed to fully identify, correct (if possible) and document the noted problems. Table 6-4 lists performance evaluation techniques for a RMPE.

Second, diagnostic analysis and testing, including a limited number of model sensitivity and/or uncertainty simulations may be performed to help elucidate model performance and response to changes in key inputs. Sensitivity analysis, often an important component of the evaluation process, may be performed to aid in understanding the air quality model’s response to key input parameter uncertainties. They provide evidence that the model is responding as expected relative to local understanding of the conditions leading to high ozone (i.e., conceptual models). The extent to which sensitivity simulations with CMAQ and/or CAMx will be needed can only be assessed after the initial model evaluations are performed. With the advent more sophisticated one-atmosphere models, certain sensitivity runs historically carried out older models (e.g., UAM family) are no longer feasible, needed, or appropriate (e.g., zero IC/BC or zero-emissions runs). Other, more insightful and physically meaningful experiments are used (e.g., NOx and VOC emission changes, vertical eddy diffusivity and grid changes, alternative chemistry mechanisms, alternative meteorological realizations, etc.). Emission sensitivity tests are particularly relevant as they provide: (1) a reality check that the model is responding as expected; (2) information on which emission source components are important; and (3) initial quantification of potential impacts of controls.

Sensitivity experiments will be conduced as part of the CMAQ/CAMx model performance evaluation analysis to assist in identifying the optimal model configurations for simulating ozone formation in the St. Louis area. The potential need for and nature of these simulations would be discussed with the AQMP Technical Workgroup after the operational evaluation results have been reviewed.

6.2.4 Available Aerometric Data for the Evaluations

Limited concentration measurements and meteorological parameters are available for the St. Louis area. These will be used to the fullest extent possible in the evaluation of the WRF, CMAQ and CAMx models. Table 4-4 presented previously discusses the availability of gaseous and particle air quality measurements from routine monitoring networks operating in the US. Examples of available air quality data for the evaluation include:

Aerometric Information Retrieval System (AIRS): Data files containing hourly-averaged concentration measurements at a wide variety of state and EPA monitoring networks are available in the AIRS database. These data sets will be reformatted for use in the model evaluation software. Typical surface measurements at the ground level routine AIRS monitoring stations include ozone, NO_2, NOx and CO.

Southeastern Aerosol Research and Characterization (SEARCH): 4 urban-rural pairs of stations in the southeastern US conduct continuous measurement of O_3, NO, NO_2, NOy, HNO_3, SO_2, and CO.

Photochemical Assessment Monitoring Stations (PAMS): Measurements at the PAMS sites include O_3, NOx, and a list of VOCs on either an hourly or 3-hour basis.

Table 6-1. Statistical measures and graphical displays used in the WRF operational evaluation.

Statistical Measure	Graphical Display
Surface Winds (m/s)	
Vector mean observed wind speed	Vector mean modeled and observed wind speeds as a function of time
Vector mean predicted wind speed	Scalar mean modeled and observed wind speeds as a function of time
Scalar mean observed wind speed	Modeled and observed mean wind directions as a function of time
Scalar mean predicted wind speed	Modeled and observed standard deviations in wind speed as a function of time
Mean observed wind direction	RMSE, $RMSE_s$, and $RMSE_u$ errors as a function of time
Mean predicted wind direction	Index of Agreement as a function of time
Standard deviation of observed wind speeds	Surface wind vector plots of modeled and observed winds every 3-hrs
Standard deviation of predicted wind speeds	Upper level wind vector plots every 3-hrs
Standard deviation of observed wind directions	
Standard deviation of predicted wind directions	
Total RMSE error in wind speeds	
Systematic RMSE error in wind speeds	
Unsystematic RMSE error in wind speeds	
Index of Agreement (I) in wind speeds	
$SKILL_E$ skill scores for surface wind speeds	
SKILLvar skill scores for surface wind speeds	
Surface Temperatures (Deg-C)	
Maximum region-wide observed surface temperature	Normalized bias in surface temperature estimates as a function of time
Maximum region-wide predicted surface temperature	Normalized error in surface temperature estimates as a function of time
Normalized bias in hourly surface temperature	Scatter plot of hourly observed and modeled surface temperatures
Mean bias in hourly surface temperature	Scatter plot of daily maximum observed and modeled surface temperatures
Normalized gross error in hourly surface temperature	Standard deviation of modeled and observed surface temperatures as a function of time
Mean gross error in hourly surface temperature	Spatial mean of hourly modeled and observed surface temperatures as a function of time
Average accuracy of daily maximum temperature estimates over all stations	Isopleths of hourly ground level temperatures every 3-hr
Variance in hourly temperature estimates	Time series of modeled and observed hourly temperatures as selected stations
Surface Mixing Ratio (G/kg)	
Maximum region-wide observed mixing ratio	Normalized bias in surface mixing ratio estimates as a function of time

Statistical Measure	Graphical Display
Maximum region-wide predicted mixing ratio	Normalized error in surface mixing ratio estimates as a function of time
Normalized bias in hourly mixing ratio	Scatter plot of hourly observed and modeled surface mixing ratios
Mean bias in hourly mixing ratio	Scatter plot of daily maximum observed and modeled surface mixing ratios
Normalized gross error in hourly mixing ratio	Standard deviation of modeled and observed surface mixing ratios as a function of time
Mean gross error in hourly mixing ratio	Spatial mean of hourly modeled and observed surface mixing ratios as a function of time
Average accuracy of daily maximum mixing ratio	Isopleths of hourly ground level mixing ratios every 3-hr
Variance in hourly mixing ratio estimates	Time series of modeled and observed hourly mixing ratios at selected stations

Table 6-2. Statistical measures and graphical displays used in the WRF scientific evaluation (measures and displays developed for each simulation day).

Statistical Measure	Graphical Display
Aloft Winds (m/s)	
Vertically averaged mean observed and predicted wind speed aloft for each sounding	Vertical profiles of modeled and observed horizontal winds at each NWS sounding location and at each NOAA continuous upper-air profiler location in the 36, 12, and 4-km grids.
Vertically averaged mean observed and predicted wind direction aloft for each sounding	
Aloft Temperatures (Deg-C)	
Vertically averaged mean temperature observations aloft for each sounding	Vertical profiles of modeled and observed temperatures at each sounding location
Vertically averaged mean temperature predictions aloft for each sounding	

Table 6-3. Statistical measures and graphical displays for 1-hour and 8-hour ozone concentrations to be used in the screening model performance evaluation (SMPE) of CAMx/CMAQ surface ozone concentrations.

Statistical Measure on 36/12/4 km grids	Graphical Display on all grids
Maximum observed concentration	Modeled and observed spatial mean concentrations as a function of time
Maximum modeled concentration	Measures of peak estimation accuracy (A_{TS}, A_T, A_S, A_U, A)
Maximum modeled concentration at a monitoring station	Normalized bias as a function of time
Ratio of maximum modeled to observed concentrations	Normalized gross error as a function of time

Statistical Measure on 36/12/4 km grids	Graphical Display on all grids
Accuracy of peak estimation (paired in time and space)	Normalized bias as a function of concentration level
Accuracy of peak estimation (unpaired in time and space)	Normalized gross error as a function of concentration level
Average accuracy over all stations	Scatter plot of hourly concentration pairs
Normalized bias in hourly concentrations	Scatter plot of daily maximum concentration pairs
Mean bias in hourly concentrations	Quartile plots of hourly species concentrations
Normalized gross error in hourly concentrations	Daily maximum ground-level concentration isopleths
Mean gross error in hourly concentrations	
Variance in hourly concentrations	

Table 6-4. Statistical measures and graphical displays for 1-hour and 8-hour ozone, VOCs, NOx, and indicator species and indicator species ratios to be used in the refined model performance evaluation (RMPE) involving multi-species, multi-scale evaluation of CAMx/CMAQ surface and aloft concentrations.

Statistical Measure on 36/12/4 km grids	Graphical Display on all grids
Maximum observed concentration	Modeled and observed spatial mean concentrations as a function of time
Maximum modeled concentration	Measures of peak estimation accuracy (A_{TS}, A_T, A_S, A_U, A)
Maximum modeled concentration at a monitoring station	Normalized bias as a function of time
Ratio of maximum modeled to observed concentrations	Normalized gross error as a function of time
Accuracy of peak estimation (paired in time and space)	Normalized bias as a function of concentration level
Accuracy of peak estimation (unpaired in time and space)	Normalized gross error as a function of concentration level
Average accuracy over all stations	Scatter plot of hourly concentration pairs
Normalized bias in hourly concentrations	Scatter plot of daily maximum concentration pairs
Mean bias in hourly concentrations	Quartile plots of hourly species concentrations
Normalized gross error in hourly concentrations	Daily maximum ground-level concentration isopleths
Mean gross error in hourly concentrations	
Variance in hourly concentrations	
Mean, maximum, minimum, standard deviation, bias and error of observed and modeled aloft concentrations (e.g., ozone, NO_x) along individual aircraft paths	Modeled and observed time series of ozone and NO_x concentrations along individual aircraft flight paths

7.0 $PM_{2.5}$ AND AIR TOXICS MODEL PERFORMANCE EVALUATION

This section describes the procedures to be used to evaluate the CMAQ and CAMx base case modeling of the St. Louis area for fine particulate matter ($PM_{2.5}$) and air toxics.

7.1 Overview

This section lays out the "roadmap" for achieving an adequately tested modeling system for regulatory use. This does not mean that every analysis identified in this chapter will be carried out or is indeed even possible given the St. Louis modeling study schedule and resources, the existing aerometric data bases, and present technology constraints. Hence, this chapter describes a range of model testing methodologies *potentially* available to the St. Louis modeling study team in its efforts to adequately evaluate the performance of the CMAQ and CAMx air quality modeling systems for the 2007 modeling period. We identify the core operational evaluation procedures, recommended in EPA (2007) modeling guidance that will be performed in the model performance evaluation. We also describe a broad range of additional performance testing methods that may be worth considering, if deemed necessary as long as resources and time are available.

At a minimum, the evaluation of the CMAQ and CAMx modeling systems for the St. Louis base case simulations will be consistent with EPA's modeling guidance, which essentially calls for an operational evaluation of the model focusing on a specific set of gas-phase and aerosol chemical species and a suite of statistical metrics for quantifying model response over the annual cycle. The emphasis is on assessing: (a) How accurately the model predicts observed concentrations; and (b) how accurately the model predicts responses of predicted air quality to changes in inputs. States are encouraged to utilize the evaluation procedures set forth in the modeling guidance document (EPA, 2007). Thus, in carrying out the initial operational evaluation and the subsequent final evaluation, we will implement the suggested EPA performance testing methodologies for the key gas phase and aerosol species.

We again emphasize that most important goal of the St. Louis CMAQ and CAMx PM evaluation is to determine whether the aggregate modeling systems (model codes plus input data sets and observational data for testing) offers sufficiently reliable and accurate results that public decision-makers may have reasonable confidence in using the model to help choose between alternative $PM_{2.5}$ reduction scenarios for the St. Louis area. If the CMAQ and CAMx model evaluation, as outlined in this chapter, provides sufficient evidence that the modeling systems are operating reliably and in conformance with measurements and scientific expectations, then specific justifications explaining why the model is acceptable for developing $PM_{2.5}$ reduction strategies will be offered in the Final Modeling Report. Conversely, should the evaluation determine that the modeling systems suffers from important flaws or errors that undermine its reliability or use, these findings will also be documented, together with recommendations regarding the use of alternate methods, steps to improve the model and/or data base, or other approaches.

While we will focus on $PM_{2.5}$, the model performance for air toxics will also be performed to the extent possible. One of the goals of the St. Louis AQMP3 (MDNR and IEPA, 2010) is "the inclusion of air toxics exposure as an important metric for consideration of alternative control requirements for all NAAQS." Therefore, the models' ability to adequately represent these air toxics should also be assessed. The evaluation procedure for air toxics will generally follow that for $PM_{2.5}$ as described below while mostly focusing on the operational evaluation.

7.1.1 Context for the St. Louis Model Performance Evaluation

When designing a model performance evaluation, it is important to understand how the modeling results will ultimately be used. EPA has published the final guidance document that encompasses ozone, fine particulate, and regional haze/visibility modeling (EPA, 2007). That document not only provides a framework for the St. Louis model performance evaluation approach, but just as importantly describes the methodology by which to project base-year pollutant levels to target years. A key concept in EPA's guidance is that the modeling projections are used in a relative sense to scale or roll back the observed individual PM species concentrations. The model-derived ratios of future-year to current-year concentrations are called relative reduction factors (RRFs). Since the model is used to project future year $PM_{2.5}$ species components rather than total $PM_{2.5}$ mass, then the model performance for each of the components is actually more important than for total $PM_{2.5}$ mass for which the standard was written. These components are:

- Sulfate (SO4);
- Nitrate (NO3);
- Ammonium (NH4);
- Organic Carbon (OC);
- Elemental Carbon (EC); and
- Other Inorganic fine Particulate (IP or Soil).

Therefore, the St. Louis CMAQ and CAMx base case model testing will concentrate on an operational evaluation of those model predictions for those PM components listed above. Where feasible and supported by sufficient measurement data, we will also evaluate the modeling system for its ability to accurately estimate coarse PM mass (CM) and other gas-phase precursor, product and indicator species. The correct simulation of gas-phase oxidant species is needed for PM since correct, unbiased simulation of gas-phase photochemistry is a necessary element of reliable secondary PM predictions. This evaluation will be carried focusing on the St. Louis area for the entire modeling period (June through September 2007) and also on a month-by-month to daily basis to help build confidence that the modeling system is operating correctly. With this context in mind, we next turn to the philosophy of the model evaluation process.

7.1.2 Multi-Layered Model Testing Process

EPA's final modeling guidance document (EPA, 2007) affirms the recommendations of numerous modeling scientists over the past decade (see, for example, Dennis et al., 1990; Tesche et al., 1990, 1994; Seigneur et al., 2000; Russell and Dennis, 2000; Arnold et al., 2003; Boylan et al., 2003; Tonnesen, 2003) that a comprehensive, multi-layered approach to model performance testing should be performed, consisting of the four components: operational, diagnostic, mechanistic (or scientific) and probabilistic. As applied to $PM_{2.5}$ modeling, this multi-layered framework may be viewed conceptually as follows:

Operational Evaluation: Tests the ability of the model to estimate total and component PM concentrations. This evaluation examines whether the measurements are properly represented by the model predictions but does not necessarily ensure that the model is getting "the right answer for the right reason";

<u>Diagnostic Evaluation</u>: Tests the ability of the model to predict PM chemical composition including PM precursors (e.g., SOx, NOx, and NH_3) and associated oxidants (e.g., ozone and nitric acid); PM size distribution; temporal variation; spatial variation; and mass fluxes;

<u>Mechanistic Evaluation</u>: Tests the ability of the model to predict the response of PM to changes in variables such as emissions and meteorology; and

<u>Probabilistic Evaluation</u>: Takes into account the uncertainties associated with the model predictions and observations of PM.

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

7.2 Development of Consistent Evaluation Data Sets

Before discussing the types of testing procedures available for the evaluation components listed above, we first identify the surface data sets that are available to support these comparisons. Unfortunately, we are not aware of any aloft data for the 2007 modeling period in the St. Louis area.

The ground-level model evaluation database will be developed using several routine and research-grade databases. The first is the routine gas-phase concentration measurements for ozone, NO, NO_2 and CO archived in EPA's Aerometric Information Retrieval System/Air Quality System (AIRS/AQS) database. Other sources of information come from the various PM monitoring networks in the US. These include the: (a) Interagency Monitoring of Protected Visual Environments (IMPROVE), (b) Clean Air Status and Trends Network (CASTNET), (c) Southeastern Aerosol Research and Characterization (SEARCH), (d) EPA $PM_{2.5}$ and PM_{10} Mass Networks (EPA-FRM), (e) EPA Chemical Speciation Network (CSN); and (f) National Acid Deposition Network (NADP). Typically, these networks provide ozone, other gas phase precursors and product species, PM, and visibility measurements. Of key importance for the St. Louis PM modeling will be the FRM $PM_{2.5}$ mass and CSN speciated $PM_{2.5}$ measurements.

An important consideration in evaluating PM models is that each monitoring network employs a unique measurement approach that "measures" a different amount of a given species. For example, the IMPROVE network only speciates $PM_{2.5}$, so any sulfate or nitrate in the coarse mode ($PM_{2.5\text{-}10}$) is included in the coarse mass (CM) "measurement". Thus, the CMAQ and CAMx models will be evaluated separately for each monitoring network. Additionally, there is often ambiguity in the mapping of modeled PM species to measurements. For example, PM monitors measure only the carbon component of OC, whereas in the model the entire mass of organics (OMC) is simulated, which includes carbon and the other elements attached to the carbon (e.g., hydrogen and oxygen). Thus, a factor is assumed to adjust the measured OC to OMC. In the past an OMC/OC factor of 1.4 has been used based on urban scale measurements of fresh OC emissions, and this has been the factor used in the IMPROVE reconstructed mass equation (Malm et al., 2000). However, this OMC/OC factor is likely too low, especially for aged OC compounds where ratios of 1.4 to 2.2 have been observed (Turpin and Lim, 2001); currently an average OMC/OC ratio value of 1.8 has been adopted for revised IMPROVE reconstructed mass equation. Alternatively, the OMC/OC factors can be applied in the opposite direction to convert the modeled OMC to OC. Advantage of using this approach is that because the models normally distinguish secondary biogenic, secondary anthropogenic, and primary organic PM, different OMC/OC factor can be applied for each of these components. However, there still exist significant uncertainties in these factors.

Evaluation for air toxics will be focused on the model results within and near the St. Louis urban area. Available measurement data for air toxics identified in the AQMP3 (lead, acetaldehyde, arsenic compounds, benzene, chromium compounds, formaldehyde and diesel particulate matter) will be compiled from the AQS and NATTS databases and may be supplemented with trace element data from IMPROVE and SEARCH. Initial screening shows that measurement data for lead, acetaldehyde, arsenic compounds, benzene, chromium compounds and formaldehyde are available for the modeling period (June to September 2007) at some of the NATTS monitoring sites within Missouri and Illinois. The AQS HAP database includes some measurements for acetaldehyde, benzene and formaldehyde during the modeling period. Diesel PM is evaluated using elemental carbon as a surrogate, which is regularly monitored at PM monitoring networks such as IMPROVE, CSN, and SEARCH.

7.3 Model Evaluation Tools

This section introduces the various statistical measures, graphical presentations, and related analytical procedures that have proven useful over the years in evaluating grid-based chemical transport models. Many of the methodologies mentioned below have been utilized in the CENRAP, WRAP, MRPO, VISTAS and other studies. While we plan on calculating a rich variety of statistical performance metrics, only a very limited subset of these measures will actually be relied upon to form judgments concerning model acceptability.

7.3.1 Statistical Performance Metrics

The EPA modeling guidance document (EPA, 2007) focuses more on a holistic model evaluation approach compared to the original 1-hour ozone and draft PM guidance (EPA, 1991; 2001). Not only should we assess how well the model matches the observation, but we also need to determine whether the model is correctly simulating the processes that produce the elevated concentrations, which includes comparing against a conceptual model. Table 7-1 lists a standard set of statistical performance measures that can be used to evaluate fine particulate models. From past regional PM model evaluations we have found the fractional bias and fractional error to be the most useful summary measures for PM model evaluation since it accounts for the range of PM species concentrations and we will focus mainly upon them in the St. Louis modeling, but not to the exclusion of others that are found to yield discriminating power. For ozone and other gas phase species (NO, NO_2, SO_2) we will include use the traditional statistical measures as described in Chapter 6.

Typically, the statistical metrics are calculated at each monitoring site across the full computational domain for all simulation days. In the St. Louis CMAQ/CAMx evaluation, we will stratify the performance statistics across relevant space and time scales, in particular for a subdomain of the St. Louis metropolitan statistical area (MSA). As part of the operational evaluation, the gas-phase and aerosol statistical measures shown in Table 7-1 will be computed for each of the 4 and 1.333 km domains and for urban vs. rural monitoring sites. Temporally, we will compute the statistical measures for the appropriate averaging times following the monitoring network's sampling or reporting frequency. Should it become necessary as part of model performance diagnosis, we will consider aggregating the statistics in various ways, e.g., (a) day vs. night, (b) weekday vs. weekend, (c) precipitation vs. non-precipitation days, (d) month of the year, and (e) exceedance events, in order to help elucidate model performance problems. The amount of these supplemental time/space analyses would depend on schedule and available resources.

7.3.2 Graphical Representations

The St. Louis CMAQ and CAMx operational air quality model evaluation will utilize numerous graphical displays to facilitate quantitative and qualitative comparisons between CMAQ/CAMx predictions and measurements. Together with the statistical metrics listed in Table 7-1, the graphical procedures are intended to help: (a) identify obviously flawed model simulations, (b) guide the implementation of performance improvements in the base case model input files in a logical, defensible manner, and (c) elucidate the similarities and differences between the alternative CMAQ/CAMx simulations. These graphical presentations are intended to depict the model's ability to predict the observed fine particulate and gaseous species concentrations.

The core graphical displays to be considered for use include the following:

- Scatter plots of predicted and observed concentrations;
- Time series plots at monitoring locations;
- Ground-level gas-phase and particulate concentration maps (i.e., tile plots);
- Bias and error stratified by concentration;
- Bias and error stratified by time; and
- Separate displays of above by monitoring network, subregions and time.

These graphical displays will be generated, were appropriate for the full moeling period as well as for monthly periods.

7.3.3 Probing Tools and Allied Methods

Ideally, the operational evaluation described above will confirm that the modeling systems are performing consistent with its scientific formulation, technical implementation, and at a level that is at least as reliable as other current state-of-science methods. Should unforeseen model performance problems arise in the 2007 base case model simulations, it may be necessary to draw into the evaluation supplemental diagnostic tools to aid in model testing. These diagnostic techniques are loosely referred to as "probing tools". The actual need for their use, if any, can only be determined once the initial 2007 CMAQ/CAMx operational evaluation is completed. Should such diagnostic methods actually be needed, their usage would require additional resources. Below, we identify the types of probing tools that could be brought to bear under should their use become necessary.

Current "one-atmosphere" models, such as CMAQ and CAMx have been outfitted with a number of "probing tools" that have proven to be very useful in testing and improving model performance and in evaluating emission control strategies. Among the probing tools available in one or both models are: (a) ozone and particulate source apportionment technology (OSAT and PSAT), (b) process analysis (PA), and (c) the decoupled direct method (DDM) of sensitivity analysis. These tools for ozone modeling have been described in Chapter 6. PSAT is a PM counterpart of OSAT and implemented and fully tested in CAMx. The Tagged Species Source Apportionment (TSSA), which is similar to PSAT, has been implemented in a previous version of CMAQ, but not available in the current CMAQ version (v4.7.1). DDM has also been implemented for PM in both CAMx and CMAQ, but limited to the first-order sensitivities.

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

7.4 Model Evaluation Procedures

EPA modeling guidance (EPA, 2007) suggests that the performance evaluation focus on two aspects:

- How well is the model able to replicate observed concentrations of total and components $PM_{2.5}$ mass?
- How accurately does the model characterize the sensitivity of changes in component concentrations to changes in emissions?

Recognizing that the former is much easier to accomplish than the latter, EPA goes on to declare that testing of a model's reliability in estimating the actual effects of emissions changes is the more important. Over the past 20 years, a substantial body of information and analytical techniques has been developed to address the first aspect. Unfortunately, even today there are little rigorous methods available for quantifying the accuracy and precision of a model's predicted concentration changes as the result of emissions changes. In this section we explain how the St. Louis PM model testing will address the first aspect of the performance evaluation, i.e., how does the model compare against observed data. In section 7.4.5 we consider the second performance consideration.

7.4.1 Assessment of Ground-Level Concentrations

Given that the $PM_{2.5}$ attainment demonstration test involves the separate projection of each PM component, the model should be evaluated separately for each. Current EPA guidance suggests that the model should also be evaluated for several key gas-phase species that are important for $PM_{2.5}$ modeling. The *particulate species* include SO_4 and/or S, mass associated with SO_4, NH_4, NO_3, mass associated with NO_3, EC, OC, IP, mass of individual constituents of IP, and CM. The *gaseous species* include O_3, HNO_3, NO_2, PAN, NH_3, NOy, SO_2, CO, and H_2O_2. As noted previously, the modeling guidance includes model performance goals, but further stresses additional confirmatory and corroborative techniques and process-based evaluation to assure that the model is getting the right answer for the right reason, in addition to demonstrating that the model exhibits skill in predicting the $PM_{2.5}$ concentrations.

As part of the CMAQ/CAMx operational evaluation, model outputs will be compared statistically and graphically to observational data obtained from the AIRS/AQS, IMPROVE, SEARCH, CASTNET, FRM, CSN, and other monitoring networks. These comparisons will likely include:

- Daily or monthly averages for SO_2, SO_4, NO_3, EC, OC, $PM_{2.5}$, and PM_{10}, taking care to exclude periods of sampling interference in the observational data. We will look for systematic biases between the model results and observations, and if biases are found, identify possible sources of error in the model inputs.
- Hourly, high resolution PM species and gaseous species concentrations at sites where available (e.g., AIRS/AQS, SEARCH).
- For ozone, comparisons against observed hourly and 8-hour ozone concentrations in nonattainment areas (this will be done in the ozone MPE).

The types of analysis that could be performed as part of the diagnostic model evaluations are:

- Evaluate seasonal trends in observations of organic and inorganic aerosol precursors and their effects on PM composition, and evaluate the ability of the model to capture these seasonal trends.
- Evaluate how well the model simulates various physico-chemical processes by: (a) examining observed and modeled correlations between various species pairs, and (b) comparing model-predicted ratios of various species (individual or families) with observations to evaluate gas/particle partitioning (e.g., nitrate/total nitrate, SO_4/SO_x).
- Investigate the performance of the model at selected observational sites characterized by different chemical regimes that may be encountered either spatially or during different seasons to help identify any inadequacies in the model and to provide a better understanding of conditions under which model inferences may be weak.
- Create scatter plots of modeled vs. observed data and hourly and 24-hour averages by site and sub-region to help identify any site-specific biases.
- Create time series plots of predicted and observed concentrations stratified by key variables as appropriate.
- Evaluate for total sulfur (SO_2 + SO_4), nitrate (HNO_3 + NO_3) and ammonium (NH_3 + NH_4).
- Compare observed versus modeled mass fractions of PM constituents at various sites that are characterized by their proximity or remoteness relative to sources, or by specific meteorological conditions (e.g., frontal passage, stagnation, precipitation); these will enable identification of trends in the model of over- or under-prediction of specific PM constituents under these conditions.
- Calculate the measured and predicted relative abundance of key PM components and compare with EPA guideline recommendations and emergent alternative science recommendations (e.g., removing the soil component from the calculations, use of alternative relative importance equations (Boylan, 2004)).
- Evaluate for ozone precursors and key indicator species and ratios (e.g., HNO_3/H_2O_2) as well as product species.

The suite of statistical metrics and graphical displays identified in the previous section for the core operational evaluation efforts would also be used to diagnose performance problems with the CMAQ/CAMx simulations should they exist and to highlight differences between model runs. Experience in ozone/PM modeling is the best basis upon which to identify obviously flawed simulation results. Efforts to improve the CMAQ/CAMx base case performance will be made, where necessary, warranted (i.e., to reduce the discrepancies between model estimates and observations), and consistent with the project resources and schedule; however, these model performance improvements efforts must be based on sound scientific principles. "Curve-fitting" exercises will be avoided.

7.4.2 Performance Goals and Criteria

Establishment of performance goals and criteria for regulatory modeling is a necessary but difficult activity, and has been an area of ongoing research and debate (Morris et al., 2005). Here, performance *goals* refer to targets that we believe a good performing model should achieve, whereas less stringent performance *criteria* represent a minimal level of model performance that a model should achieve for use in regulatory modeling. Performance goals are necessary in order to provide consistency in model applications and expectations across the country, while criteria provide standardization in how much weight may be accorded modeling study results in the decision-making process. It is a problematic activity, though, because many areas present unique challenges and no one set of performance goals is likely to fit all needs. Equally concerning is the very real danger that modeling studies will be truncated when the "statistics look right" before full assessment of the model's reliability is made. This has the potential for breeding built-in compensating errors (Reynolds et al., 1996) as modelers strive to get good statistics as opposed to searching for the explanations for poor performance and then rectifying them. A NARSTO review of more than two-dozen urban-scale ozone SIP applications found this tendency to be all too prevalent in the regulatory modeling of the 1990s (Roth et al, 1997).

Decades ago, EPA (1991) established performance goals for 1-hour ozone centered on the use of normalized bias (<15%) and error (<35%). However, when these evaluation metrics and goals were later adapted to PM and its components, difficulties arose because performance statistics that divide by low concentration observations (such as nitrate, which is often zero) become practically meaningless. In time, this has led to the introduction of the fractional and normalized mean bias and error metrics in addition to the mean normalized metrics and related performance expectations based on these alternative measures. EPA modeling guidance notes that PM models may not be able to achieve goals similar to those of ozone, and that better performance should be achieved for those PM components that make up the major fraction of total PM mass than those that are minor contributors. In fact, differences in measurement techniques for some PM species likely exceed the more stringent ozone performance goals. For example, comparisons of PM measurements using the IMPROVE and STN technologies found differences of ~20% for sulfate and ~50% for elemental carbon (Solomon et al., 2004).

As with ozone in the 1980s, actual experience with PM models has led to the development of the current performance expectations for these models. For example, PM_{10} SIP model performance goals for mean normalized gross error of 30% and 50% have been used for southern California (SCAQMD, 1997; 2003) and Phoenix (ENVIRON, 1998), respectively. Boylan and Russell (2006) have proposed fractional bias and error goals of 30% and 50%, and fractional bias and error criteria of 60% and 75%, respectively. Furthermore, they proposed that these goals and criteria values vary as a function of concentration, such that below 2 $\mu g/m^3$, they expand exponentially to 200% (the maximum of fractional bias and error) at zero observed concentrations. The following levels of fractional bias (FB) and error (FE) have been adopted as model performance criteria for VISTAS regional visibility modeling using CMAQ:

- FB ≤ ±15% & FE ≤ 35%: Excellent
- FB ≤ ±30% & FE ≤ 50%: Good
- FB ≤ ±60% & FE ≤ 75%: Average, each PM component should meet for regulatory modeling
- FB > ±15% & FE > 35%: Poor, indicating fundamental problems with the modeling system

We regard the above goals and criteria not as a pass/fail test, but rather as a basis of inter-comparing model performance across studies, sensitivity tests and models.

7.4.3 Diagnostic and Sensitivity Testing

Diagnostic sensitivity testing of the PM modeling is an integral component of the model performance evaluation process. In Section 1.5.8, the three levels of sensitivity tests were identified. Depending on the findings of the initial simulations and model performance evaluation the need for and level of diagnostic sensitivity analysis will vary. It is impossible to anticipate the exact diagnostic sensitivity tests that will be needed to improve model performance a priori. Suffice it to say that emissions, meteorological (e.g., mixing), boundary conditions and other perturbations are fairly typical sensitivity tests that are conducted to improve model performance.

7.4.4 Corroborative and Weight of Evidence Modeling Analyses

This section identifies additional modeling analyses that might be worth pursuing to add strength to the core model evaluation efforts already planned as part of the St. Louis modeling study.

7.4.4.1 Corroborative Models

Noteworthy in EPA's new guidance document is the encouragement of the use of alternative modeling methods to corroborate the performance findings and control strategy response of the primary air quality simulation model. This endorsement of the use of corroborative methodologies stems from the common understanding that no single photochemical modeling system can be expected to provide exact predictions of the observed ozone and PM species concentrations in large regions, especially over time scales spanning 1 hour to 1 year. Although the photochemical/PM models identified in EPA's guidance document possess many up-to-date science and computational features, there still can be important differences in modeled gas-phase and aerosol predictions when alternative models are exercised with identical inputs.

Mindful of EPA's endorsement of corroborative modeling methods and the rigorous use of "weight of evidence" investigations, we recommend that the most recent version of CMAQ and CAMx be carried through the study, including the evaluation of emissions control strategies. Among other things, this will permit us to more explicitly identify the expected range of model uncertainty and to corroborate the general effectiveness of the CMAQ and CAMx ozone and PM control strategies.

7.4.4.2 Weight of Evidence Analyses

EPA's guidance recommends three general types of "weight of evidence (WOE)" analyses in support of the attainment demonstration: (a) use of air quality model output, (b) examination of air quality and emissions trends, and (c) the use of corroborative modeling such as observation-based (OBM) or observation-driven (OBD) models. We will consider the use of one or more methods in conducting the CMAQ/CAMx modeling because it could significantly strengthen the credibility and reliability of the modeling available to the states for their subsequent use. The exact details of the "weight of evidence" analyses must wait until the St. Louis modeling study evolves further. It is premature to prescribe which, if any of the WOE analyses would be performed since the model's level of performance with the base case is obviously not known at this time and the time and remaining project resources available to support WOE analyses is unknown as well. Nonetheless, we outline below our thoughts regarding what would likely be considered should the operational CMAQ/CAMx model evaluation need to be bolstered with WOE analyses.

> **<u>Use of Air Quality Models</u>:** Applying the PSAT and DDM tools to develop corroborative information on source-receptor relationships and model sensitivities would strengthen the analyses. These supplemental calculations would be performed for one or more key periods within the base case modeling. The results of this additional modeling would be used directly in the WOE analyses to quantify the degree of modeling uncertainty and to corroborate appropriateness of the subsequent PM emissions reductions scenarios.
>
> **<u>Use of Emissions and Air Quality Trends</u>:** A limited scope emissions and trend analysis could be employed by MDNR and IEPA to support the WOE determinations. With this expectation, we would coordinate our efforts with the state agencies to develop a trends analysis supporting the future year applications of CMAQ/CAMx.
>
> **<u>Use of Corroborative Observational Modeling</u>:** As noted, EPA's guidance now encourages the use of observation-based or observation-driven models (OBMs/ODMs). We will consider the merits of using these techniques as supportive WOE. While the OBD/OBM models cannot predict future year air quality levels, they do provide useful corroborative information on the extent to which specific subregions may be VOC-limited or NOx-limited, for example, or where controls on ammonia or SO_2 emissions might be most influential in reducing $PM_{2.5}$. Information of this type, together with results of DDM and traditional "brute-force" sensitivity simulations, can be extremely helpful in postulating emissions control scenarios since it helps focus on which pollutant(s) to control.

7.4.5 Assessing Model Reliability in Estimating the Effects of Emissions Changes

EPA guidance identifies three methods potentially useful in quantifying a model's reliability in predicting air quality response to changes in model inputs, e.g., emissions. These include:

- Examination of conditions for which substantial changes in (accurately estimated) emissions occur;
- Retrospective modeling, that is, modeling before and after historical significant changes in emissions to assess whether the observed air pollution changes are adequately simulated; and
- Use of predicted and observed ratios of "chemical indicator species."

We also note that in some urban-scale analyses, the use of weekday/weekend information has been helpful in assessing the model's response to emissions changes.

Recent analytical and numerical modeling studies have demonstrated how the use of ambient data and indicator species ratios can be used to corroborate the future year control strategy estimates of Eulerian air quality models. With respect to secondary aerosol PM, the recent CMAQ evaluation by Arnold et al. (2003) clearly demonstrated how the use of indicator species analysis could be use to develop insight into the expected reliability and adequacy of a photochemical/PM model for simulating the effects of emissions control scenarios. These researchers used three indicator ratios (or diagnostic "probes") to quantify the model's response to input changes:

- The ozone response surface probe (O_3/NOx);
- The chemical aging probe (NOz/NOy); and
- The ozone production efficiency probe [O_3/NOz].

By closely examining the model's response to key input changes, properly focused in time and spatial location, Arnold et al. (2003) were able to conclude that the photochemical processing in CMAQ was substantially similar to that in the atmosphere.

The extension of these techniques to address CMAQ and CAMx predictions for secondary aerosols will doubtless be quite challenging, but the use of indicator species (e.g., ammonia or HNO_3 limitation for nitrate particle formation) and species ratios appears to offer, at this time, the only real opportunity to quantify the expected reliability of the air quality model to correctly simulate the effects of emissions changes. In the St. Louis CMAQ and CAMx model evaluation, we will remain alert to opportunities to extend the indicator species ratio analyses to the problem of fine particulates. This is one area where technical collaboration between the ENVIRON team and the AQMP Technical Workgroup can be especially fruitful in terms of identifying and testing emergent methods for challenging the model's ability to correctly simulate the effects of future year emissions changes. Finally, we note that this is truly a current research area and as such falls outside the scope of the current modeling effort. However, given its importance, we will remain alert to opportunities to utilize newly available methods should this prove feasible within resources and schedule**.**

Table 7-1. Core statistical measures to be used in the St. Louis air quality model evaluation with ground-level data (see ENVIRON, 2003b,c for details).

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

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

8.0 FUTURE YEAR MODELING

This chapter discusses the future year modeling procedures to be performed by the ENVIRON/ERG team and AQMP Technical Workgroup for the St. Louis ozone, $PM_{2.5}$ and air toxics modeling study.

8.1 Future Year to be Simulated

The specific future year has not been determined, but will be specified by the State Air Agencies (MDNR and IEPA) after U.S. EPA's promulgation of the final 8-hour ozone standard which was originally scheduled to occur by the end of 2010, but postponed. According to the current schedule, the new 8-hour ozone standard will be finalized and set by the end of July, 2011. The future year for the ozone attainment demonstration modeling is expected to be no later than 2019.

8.2 Development of Future Year Emissions and QA

In addition to the 2007 base year emissions, the ENVIRON/ERG team will also develop relevant future year emissions inputs (i.e., growth and control factors) based upon the future year to be identified by MDNR/IEPA. The ENVIRON/ERG team will develop and compile SMOKE-ready area, point and non-road source emission inputs and SMOKE-MOVES ready future year Vehicle Miles Travelled (VMT) estimates for the 36/12/4/1.333 km modeling domains and June-September 2007 modeling period. The AQMP Technical Workgroup will then run SMOKE and SMOKE-MOVES to generate CMAQ model-ready emission inputs (CAMx model-ready emission inputs will be converted from those of CMAQ using the CMAQ2CAMx processor).

8.2.1 Development of Control and Growth Factors

The first step will be to identify any future year inventories that have previously been developed by other inventory and modeling efforts that could be potentially utilized. For instance, the SEMAP project is developing future year inventories for 2013, 2017, and 2020. The RPOs also developed 2018 future year inventories in support of regional haze- and visibility-related modeling activities. Finally, 2012, 2018, and 2030 future year projections were also developed for the Mexico National Emissions Inventory.

The future year growth and control factors from these inventories will not be automatically used. The ENVIRON/ERG team will carefully examine the inventory documentation to determine the extent that these future year inventories represent that conditions desired for the future year base case emissions. It is possible that these future year growth and control factors could be used directly. However, it is more likely that some adjustments might be needed (e.g., different future years, additional federal or state rules, etc.) before the future year inventories could be used. Also, it may be necessary to develop the future year growth and control factors without relying on previously developed future year inventories. Regardless of the specific future year ultimately selected, the future year base case emissions will be affected by two factors relative to the 2007 base year: controls and growth.

> **<u>Develop Control Factors</u>:** The first step in developing control factors is to identify any existing and "on the books" control measures due to existing federal and state (i.e.,

Missouri and Illinois) rules in effect or expected to be in effect through the future year that reduce emissions which contribute to ozone and $PM_{2.5}$ (the "on the books" control measures identified in the final AQMP3 are listed in Sections 1.4.2 and 1.4.3). These control measures will not have been accounted for in the 2007 base year emissions inventory. In addition, only those control measures that will be implemented with a high degree of certainty will be considered for the future year base case. Control measures that are hypothetical or have a low probability of implementation will not be included.

Develop Growth Factors: Future year growth is driven by population growth within the inventory domain for many area source categories, as well as changes in industrial activity for point sources and some area source categories. Demographic data from the U.S. Census Bureau and state demographers will be appropriate for some types of area source categories. In addition, sector-specific fuel use projections from the Energy Information Administration's *Annual Energy Outlook (AEO)* will be appropriate for other area source categories. Previously, U.S. EPA assumed in its guidance for projections development, particularly for point sources, that economic growth (typically expressed as economic output) is an appropriate surrogate for emissions growth. However, U.S. EPA is currently conducting research examining the validity of this assumption through detailed analysis of energy or combustion emissions versus non-energy or process emissions for 10 key industries (i.e., petroleum refining, pulp and paper, iron and steel, cement, primary aluminum, secondary aluminum, black carbon, copper, sulfuric acid, and glass). These latest findings will be considered in the development of the future year base case emissions.

Typically, the control factor is represented by a number between 0 and 1, where 0 represents no controls/uncontrolled and 1 represents 100 percent control (e.g., complete suppression, source elimination, etc.). The growth factor is represented by a number 0 or greater. A growth factor greater than 1 indicates growth, while a growth factor less than 1 indicates negative growth (i.e., shrinkage). A growth factor of exactly 1 represents no growth or unchanged activity, while a growth factor of exactly 0 represents facility shutdown or elimination of a particular source category.

After developing the relevant growth and control factors for the future year inventory, the ENVIRON/ERG team will efficiently conduct a QA review of the developed growth and control factors. This review will focus on identifying those growth and control factors that appear to be "outliers" (i.e., excessively large or small). For the identified "outliers", the underlying activity data will be examined to determine any possible reasons for the excessively large or small values. If "outliers" are identified, then potential alternative factors will be discussed. Following this QA review, the ENVIRON/ERG team will convert the growth and control factors into a SMOKE-ready format.

8.2.2 Development of Future Year VMT Estimates

ENVIRON will acquire or project future year VMT estimates for counties in the 36/12/4/1.333 km modeling domains and reformat them for the SMOKE-MOVES module. The AQMP Technical Workgroup will perform the future year MOVES modeling to generate MOVES outputs for counties in Missouri and Illinois and the future year.

For counties outside of Missouri and Illinois, ENVIRON will obtain MOVES outputs from the RPOs (e.g., SEMAP and LADCO), EPA or states and provide them to the AQMP Technical Workgroup. Based on potential changes in county vehicle characteristics (e.g., adoption of a vehicle inspection and maintenance (I/M) or fuel program), the representative county cross reference file would be updated. ENVIRON will then provide SMOKE-MOVES set-up for the 2007 base year to the Workgroup and advise them on how to update it for the future year on-road mobile source emissions modeling.

8.2.3 Development of Model-Ready Emissions and QA

The future year point, area and non-road emissions will be processed into the gridded, speciated, hourly three-dimensional emissions inputs for the CMAQ model using SMOKE by the AQMP Technical Workgroup. With ENVIRON's assistance, the Workgroup will apply the SMOKE-MOVES tool using the future year VMT estimates (provided from ENVIRON) and MOVES output files (generated by the Workgroup) as well as the same June-September 2007 meteorological conditions as used for the base year (provided by ENVIRON). The Workgroup would then provide ENVIRON with the resulting CMAQ model-ready on-road mobile source emissions inputs and ENVIRON will QA the on-road emissions by examining the spatial and temporal distributions and by animating the differences with the 2007 base year on-road mobile source emissions to assure the future year on-road mobile source emissions are changing as expected. The future year biogenic emissions will be the same as used in the 2007 base year modeling. This assumes that the same land use and biomass distribution as used in the base case emissions would exist in the future-year emission scenarios.

Similar QA/QC will be performed on the future year model-ready emissions inventories as were utilized in checking the base year datasets described in Chapter 5. Standard inventory assessment methods will be employed to generate the future year emissions data including, but not limited to: (a) visualizing the model-ready emissions graphically, (b) spot-checking the holiday emissions files to confirm that they are temporally allocated like Sundays, (c) producing pie charts emission summaries for each source category, (d) normalizing the emissions by population for each state to reveal where the future year inventories may be suspect and (e) spot-checks of the vertical allocation of point sources using PAVE. The additional QA analyses and reports that we may find particularly useful for the future year emissions files are given in Section 5.2.9.

8.3 Development Future Year Initial and Boundary Conditions

The same initial conditions (ICs) as used in the base year would be used in the future-year modeling. Because a 15-day spin up period is being used on the 36 km grid, ICs should have minimal if any influence on the model estimated concentrations.

Boundary conditions (BCs) for the future year 36 km simulations will be consistent with those developed for the 2007 base case modeling discussed in Chapter 5. The exact definition of the future year BCs for the 36 km domain cannot be specified at this time, but because the relative changes in the modeling results between 2007 and the future year (to be specified by MDNR/IEPA) are used then the BCs for the two years must be consistent.

8.4 Other Future Year Modeling Inputs

All other future year CMAQ/CAMx modeling inputs will be identical to the base year simulation, including meteorology, photolysis rates, landuse, and other inputs. Thus, the only changes between the 2007 and the future year modeling databases will be anthropogenic emissions and possibly BCs. This will allow for the comparison of the changes in 8-hour ozone and annual $PM_{2.5}$ concentrations in the study area from the current to future year due to changes in emissions only. This means that the effects of inter-annual variability, land use variations and climatic variations will not be accounted for in the future year inputs.

8.5 Emissions Sensitivity Experiments

Model sensitivity experiments are a vital and mandatory component of an 8-hour ozone and annual $PM_{2.5}$ SIP attainment demonstration analysis – both for the base case performance assessment (see Chapters 6 and 7) as well as in the future year control strategy assessment and uncertainty analysis.

Turning specifically to the future year assessments, sensitivity analyses are designed to facilitate the emissions control scenario identification and evaluation process. Today, four complimentary "Probing Tools" can be used in the CAMx and/or CMAQ regional photochemical model. These methods include: (a) traditional or "brute force" testing, (b) the decoupled direct method (DDM) sensitivity, (c) Ozone and Particulate Source Apportionment Technology (OSAT and PSAT), and (d) Process Analysis (PA). The AQMP Technical Workgroup may use at least two types of emissions sensitivity testing methods with the CAMx and CMAQ future year simulations.

Traditional Sensitivity Testing: Traditional sensitivity testing may be performed by the Workgroup with both models. Once each model is operating properly for each base case, the Workgroup may perform numerous sensitivity runs to explore response to emissions changes as well as changes in key input parameters. Typically, these sensitivity runs entail scalar reductions to key categories of anthropogenic emissions (e.g., 50% reduction in on-road motor vehicle emissions, 20% reduction in emissions from elevated point sources, 75% reduction in architectural coating VOC emissions). These sensitivity runs serve two purposes. They (a) aid in helping to define more refined emissions control scenarios, and (b) they provide episode-specific model uncertainty information that will be used later in the "Weight of Evidence" analyses in support of the 8-hour ozone and/or $PM_{2.5}$ attainment demonstrations.

DDM Sensitivity Modeling: Another type of sensitivity modeling that the Workgroup may perform entails the use of the sophisticated Decoupled Direct Method (DDM) technology in CAMx and CMAQ. For one or more episodes, the Workgroup may set up and exercise the DDM algorithms to produce a numerically intensive, direct sensitivity/uncertainty analysis. ENVIRON will assist the Workgroup in this diagnostic exploration as time and resources allow. These future year DDM sensitivity simulations are an adjunct to the brute force runs and also help to design future year, realistic ozone and/or PM control strategies, as needed, for the St. Louis region.

Ozone Source Apportionment: With CAMx, focused use of ozone source apportionment technology (OSAT) for selected episodes may be employed to better understand model response and to aid in the design of control strategies. The value of source apportionment modeling for subsequent stages of the St. Louis modeling study is that these calculations will help to: (a) assess the contribution of sources in the

Missouri/Illinois region and surrounding states to ozone concentrations in key receptor areas and (b) identify the particular source categories that may contribute the most to elevated 8-hour ozone concentrations at various nonattainment monitors. ENVIRON will assist the Workgroup define source region maps and job scripts for the source apportionment runs.

Particulate Source Apportionment: CAMx includes fine particulate source apportionment tool (PSAT). Analogous to the OSAT methodology, the PSAT tool may be used to test annual PM, NH_3, VOC, NOx, and/or SO_2 control strategies using the base year episode. Should the Workgroup wish to use this technique to aid in crafting $PM_{2.5}$ control strategies for the St. Louis region, ENVIRON will assist the Workgroup in setting up the PSAT runs.

8.6 Control Strategy Development, Testing and Analysis

The general approach to be followed in assessing whether the St. Louis region is likely to be in attainment of the 8-hour ozone and annual $PM_{2.5}$ standards or whether and to what extent additional VOC, NOx, SO_2, NH_3, and/or primary particulate emissions reductions will be required to achieve attainment will be consistent with the methodologies stipulated in EPA's final ozone, $PM_{2.5}$ and regional haze guidance (EPA, 2007). The procedures to be followed in performing the ozone and $PM_{2.5}$ attainment demonstrations are discussed in Chapter 9. The main theme of this approach is to use the model in a relative sense through model-derived site-specific relative response factors (RRFs) that are used to scale the current observed Design Values.

The CAMx and CMAQ future-year 8-hour ozone simulations will reveal the extent to which further emissions reductions are needed in the region to provide for attainment of the new NAAQS. Should ozone exceedances be modeled in the region in the future year simulation, the severity, location, and spatial extent of the modeled exceedances will be studied in order to postulate candidate emissions reductions strategies within and upwind of the nonattainment area. That is, should the future year modeling reveal a nonattainment problem, then an attainment demonstration analysis will be performed that will include the 8-hour ozone modeled attainment tests, specific screening analysis and supplemental corroborative analyses set forth in the EPA guidance. These attainment demonstration procedures for ozone and fine particulate are described in detail in the following Chapter 9.

It is difficult when a modeling study protocol is first prepared to specify precisely the nature of the future year St. Louis ozone control scenarios that may be required; indeed, the application of existing and mandated regional and local controls "on the books" and "on the way" will potentially change dramatically the current attainment picture in the region. Expecting that future year control scenario modeling will be required, the MDNR and IEPA will develop specific updates to this protocol defining the nature and extent of the future emissions control scenarios to be examined.

9.0 ATTAINMENT DEMONSTRATION

The ultimate objective of the St. Louis Modeling Study is the development modeling databases that can be used to define emissions control strategies that demonstrate future-year attainment of the 8-hour ozone National Ambient Air Quality Standard (NAAQS). This section describes the procedures for demonstrating future-year attainment of 8-hour ozone (and $PM_{2.5}$ for the sake of completeness) NAAQS.

9.1 Ozone and $PM_{2.5}$ Weight of Evidence Analyses

A central theme of EPA's 8-hour ozone and $PM_{2.5}$ modeling guidance document is the use of supporting corroborate analyses to bolster confidence that the selected control plan will in fact achieve attainment in the future year (EPA, 2007). This corroborative analysis is part of the Weight of Evidence (WOE) used in a State Implementation Plan (SIP) to support the final control plan selection. Details of the WOE and types of corroborative analysis that can be used in an ozone and $PM_{2.5}$ SIP have been discussed earlier in Section 1.5.9.

9.2 8-Hour Ozone Attainment Demonstration Procedures

The procedures for performing a modeled ozone attainment demonstration are outlined in EPA's final modeling guidance (EPA, 2007). These procedures involve the use of the model in a relative sense to scale the observed site-specific 8-hour ozone Design Values (DVs) based on the relative changes in the modeled 8-hour ozone concentration between the current-year and future-year. The model-derived scaling factors are called Relative Response Factors (RRFs) and are based on the relative changes in the modeling results between the 2007 base case and the future-year emission scenarios. Note that EPA's recommended approach for demonstrating attainment of the 8-hour ozone NAAQS were developed for the 1997 0.08 ppm (85 ppb) ozone NAAQS. EPA is in the process of revising their recommended attainment demonstration approach that will address the new (July 2011) ozone NAAQS that is expected to have a lower threshold (0.060-0.070 ppm). We do not expect EPA's basic ozone attainment demonstration procedures to change, however the threshold concentrations used to select modeling days will likely be lowered to reflect the lower ozone NAAQS.

The EPA guidance procedures for performing 8-hour ozone DV projections (EPA, 2007) have been codified in EPA's Modeled Attainment Test Software (MATS) tool. MATS includes ambient ozone air quality data and the user provides modeling results for the current year base case and the future year. MATS performs two types of 8-hour ozone DV projections: (a) projections at monitoring sites with observed 8-hour ozone Design Values; and (b) unmonitored area screening analysis 8-hour ozone projections that interpolates the observed 8-hour ozone DVs across the modeling domain to obtain gridded fields of 8-hour ozone DV projections.

The general procedures for projecting 8-hour ozone DVs at a monitoring site given in EPA's guidance are as follows (EPA, 2007):

- The starting point for the 8-hour ozone DV projections is the current year Design Value (DVC) that EPA guidance suggests should be based on the average of three 3-year periods of 8-hour ozone DVs centered on the modeling year. This results in a DVC that is a "5-year DV" that is used as the starting point for the 8-hour ozone DV projections. For the 2007 modeling year, this would mean averaging the 2005-2007, 2006-2008 and 2007-2009 8-hour ozone DVs at each ozone monitoring site in St. Louis;

- Perform 2007 base year modeling on the 36/12/4 km grid for the June-September 2007 episode using the 2007 base case emissions;
- Perform the future-year base case and control strategy modeling on the 36/12/4 km grid for the June-September 2007 meteorological conditions;
- Develop RRFs, defined as the ratio of the average of 8-hour daily maximum ozone concentrations "near" each monitor for the future year emission scenarios to the 2007 base year for all days in which the 2007 base case ozone values are above a "threshold" value:
  - o Here, "near" the monitor is defined as a grid cell size dependent array of cells centered on a monitor, where EPA guidance suggest that the arrays be 1x1 for 36 km, 3x3 for 12 km and 7x7 for 4-km grid cells.
  - o EPA's 8-hour ozone guidance specifies that RRFs should be calculated using all days with base-year ozone concentrations near the monitor greater or equal to 85 ppb, and also recommends that at least 10 modeling days should be included – these two recommendations may be in conflict:
    - ▪ In the event that there are less than 10 modeling days with base year daily maximum 8-hour ozone concentrations near the monitor $\geq$ 85 ppb threshold then:
      - – The threshold is successively reduced by 1 ppb (e.g., 84 ppb, 83 ppb, etc.) until 10 modeling days are obtained; or
      - – A 70 ppb threshold floor is imposed;
      - – *[note we expect EPA's new guidance to lower these threshold]*
    - ▪ If there are still less than 10 days upon reaching the 70 ppb threshold then:
      - – If there are 5 or more days, proceed with the attainment demonstration but the results should be analyzed carefully to be sure no single day is producing unusual model signals; or
      - – If there are less than 5 days the issue will be discussed with the State Air Agencies and EPA;
- Apply the modeled-derived RRFs to the DVC at each ozone monitor to obtain a projected future year 8-hour ozone DV (DVF);
- Truncate the future-year DVF to the nearest ppb;
- Compare the projected 8-hour ozone at each monitor (DVF) with the 8-hour ozone standard, where if all projected 8-hour ozone values are 84 ppb or lower then attainment has been demonstrated;
- Even if the modeled future-year 8-hour ozone DVF is 85 ppb or higher, a WOE attainment demonstration may be possible using supportive, corroborative and additional analysis:
  - o In fact, EPA recommends that the WOE analysis be conducted with projected 8-hour ozone DVFs in the 82 to 87 ppb range;
  - o EPA notes that for projected 8-hour ozone DVFs of 88 ppb or higher no amount of supportive information would likely be convincing for an attainment demonstration.

9.3 $PM_{2.5}$ Attainment Demonstration Procedures

The procedures for demonstrating attainment of the $PM_{2.5}$ NAAQS are given in EPA's final modeling guidance (EPA, 2007). $PM_{2.5}$ attainment is based on $PM_{2.5}$ mass measurements collected at FRM monitoring sites. In order to apply the $PM_{2.5}$ component-specific RRFs, the FRM $PM_{2.5}$ mass measurements must be speciated into the individual components of $PM_{2.5}$. There are two routine $PM_{2.5}$ speciation networks being operated in the U.S.: CSN and IMPROVE networks. Thus, the $PM_{2.5}$ speciation data from these two networks need to be mapped to the FRM $PM_{2.5}$ mass measurements in order to apply the RRFs to project $PM_{2.5}$ DVFs. This results in two main components for using modeling results to project $PM_{2.5}$ DVFs:

Speciation of Measured FRM $PM_{2.5}$ Mass using the SANDWICH Method: The FRM $PM_{2.5}$ mass and CSN/IMPROVE $PM_{2.5}$ speciation measurements have positive and negative artifacts that need to be accounted for when mapping observed $PM_{2.5}$ speciation data to the FRM mass measurements. As $PM_{2.5}$ attainment is based solely on the FRM $PM_{2.5}$ mass measurements, then the CSN/IMPROVE $PM_{2.5}$ speciation measurements must be adjusted to mimic the FRM $PM_{2.5}$ mass measurements. EPA has developed the "**S**ulfate, **A**djusted **N**itrate, **D**erived **W**ater, **I**nferred **C**arbonaceous material balance approac**H** (SANDWICH)" for estimating $PM_{2.5}$ mass composition produced by the FRM $PM_{2.5}$ mass measurements to account for measurements artifacts (Frank, 2006a,b).

Projection of Current-Year $PM_{2.5}$ Components to Future-Year using SMAT: Speciated Modeled Attainment Test (SMAT) (EPA, 2007; Timin, 2007) uses the relative changes in modeled concentrations to project observed $PM_{2.5}$ DVC to the future. EPA has codified the SMAT recommended procedures for projecting future-year annual $PM_{2.5}$ Design Value in MATS (EPA, 2007).

9.3.1 Speciation of FRM $PM_{2.5}$ Mass Measurements

Since the FRM, CSN and IMPROVE networks use different measurement technologies, each exhibits its own measurement artifacts. For example, FRM uses a single Teflon filter to measure total $PM_{2.5}$ mass, and includes water in the measurement (after equilibration at ~35% relative humidity). Particulate nitrate may volatilize off of the FRM Teflon filter. The CSN measurement technology uses Teflon, Nylon and Quartz filters for measuring the speciated PM and does not measure the water component. The CSN Quartz filters are also not blank-corrected which results in inaccurate OC measurements. IMPROVE also uses multiple filters and does not include ammonium in its measurements.

As the FRM is the de-facto regulatory definition of $PM_{2.5}$, EPA has developed procedures for adjusting the CSN and IMPROVE speciated $PM_{2.5}$ measurements to account for the measurement artifacts of the different networks and to make the speciated PM measurements consistent with the FRM $PM_{2.5}$ mass measurements. These adjustments include the following:

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

The resultant fine particle chemical speciation approach has been named the sulfates, adjusted nitrates, derived water, inferred carbonaceous material balance approach, or SANDWICH. Details on the SANDWICH procedures are given in Frank (2006a,b) and in EPA (2007).

9.3.2 Speciated Modeled Attainment Test

EPA's MATS tool automates the combination of CSN and IMPROVE data to speciate the FRM $PM_{2.5}$ mass measurements using SANDWICH and perform the SMAT future-year $PM_{2.5}$ DV projections at both the monitor and unmonitored areas of the domain. The MATS tool currently includes the SMAT procedures applied to the monitoring sites for both the annual and 24-hour $PM_{2.5}$ NAAQS. However, it currently only includes the unmonitored area analysis for the annual $PM_{2.5}$ NAAQS.

9.3.2.1 Annual $PM_{2.5}$ Projection Procedures

Once the FRM $PM_{2.5}$ mass is speciated using SANDWICH, the SMAT procedure for the annual $PM_{2.5}$ NAAQS involves the following steps:

1. Derive quarterly mean average concentrations for each of the major components of $PM_{2.5}$ and a 5-year weighted average of observations from the 2005-2009 baseline period. This is done by applying the fractional contribution of each major component of $PM_{2.5}$ from the SANDWICH $PM_{2.5}$ speciation data to the FRM $PM_{2.5}$ mass after subtracting the blank mass, for the same quarter. Major components are as follows:

   - Sulfate (SO4);
   - Nitrate (NO3);
   - Ammonium (NH4);
   - Elemental Carbon (EC);
   - Organic Mass Carbon (OMC);
   - Final Crustal/Other; and
   - Particle Bound Water (PBW).

2. Use the 2007 and future year model-estimated $PM_{2.5}$ components near each monitor and for each of the four quarters of 2007 to develop monitor-, quarter- and $PM_{2.5}$ component-specific Relative Response Factors (RRFs) using the ratio of the future year to 2007 quarterly average modeling results.

3. Apply the monitor-, quarter- and species-specific RRF to each quarterly average observed $PM_{2.5}$ species concentrations from 2005-2009 to obtain quarterly average $PM_{2.5}$ species concentrations representative of the future year conditions.

4. Recalculate the Particle Bound Water (PRB) component from the future year projected quarterly average sulfate and nitrate concentrations.

5. Sum over the 7 $PM_{2.5}$ components and add the blank mass back to make quarterly mean future year $PM_{2.5}$ concentrations for each quarter.

6. Average the four quarterly mean future year $PM_{2.5}$ concentrations to make an annual average $PM_{2.5}$ at each monitor which is the future year $PM_{2.5}$ DV.

7. Compare the future year $PM_{2.5}$ DV against the NAAQS $PM_{2.5}$ in the attainment test.

There are a few issues that need to be resolved and defined to apply the above $PM_{2.5}$ attainment test:

> **What quarterly average model-estimated $PM_{2.5}$ species components are used "near" the monitor?** As is done for ozone projections, EPA (2007) recommends a grid resolution-dependent array of cells centered on the monitor is used (i.e., 7x7 array for 4-5 km grid, 3x3 for 12-km grid and 1x1 for 36-km grid). However, for the $PM_{2.5}$ projections the average of the estimated $PM_{2.5}$ species across the array of cells is used, rather than the highest value as is used in ozone projections.
>
> **What $PM_{2.5}$ DVs should be used in the projections?** An average of the 2006, 2007 and 2008 $PM_{2.5}$ DVs will be used for the 2007 base year $PM_{2.5}$ DV. As a DV is a three-year average of annual values, then this three year average of $PM_{2.5}$ DVs will weigh the annual average $PM_{2.5}$ concentrations from the years 2005 and 2009 once, 2006 and 2008 twice and 2007 three times.
>
> **When is $PM_{2.5}$ attainment demonstrated?** The SMAT attainment test is passed when the future year projected 3-year average DV is 15.0 µg/m^3 or lower. However, EPA recommends that a WOE attainment demonstration be conducted when the projected $PM_{2.5}$ DV is close to the $PM_{2.5}$ NAAQS. If projected future-year $PM_{2.5}$ DV is lower than 14.5 µg/m^3 then basic supplemental analysis should be performed to support the modeled attainment demonstration. If projected future-year $PM_{2.5}$ DV is 14.5-15.5 µg/m^3 then a WOE attainment demonstration with supplemental and supporting information must be conducted. If projected future-year $PM_{2.5}$ DV is greater than 15.5 µg/m^3 then EPA notes that more qualitative results are less likely to support a conclusion different from the modeled attainment test.

More details on the SMAT procedure are provided in EPA's modeling guidance (EPA, 2007).

9.3.2.2 24-Hour $PM_{2.5}$ Projection Procedures

A modeled attainment test for the 24-hour NAAQS for $PM_{2.5}$ is similar to the previously described test for the annual NAAQS in that it uses model predictions in a relative sense to project the current DV by developing quarterly RRFs. The 24-hour Design Values should be based on the same 5 year weighted average methodology that was used for the annual standard, but calculated from the 98th percentile value for each year. The specific steps for the test are as follows:

1. Compute observed 98th percentile value for each site for each year and next highest concentrations for each of the other quarters.

2. Identify the species composition for each quarter for each site by multiplying the quarterly maximum daily concentrations by the estimated fractional composition of $PM_{2.5}$ species.

3. Using model results, derive component-specific RRFs at each site for each quarter.

4. Apply the component-specific RRFs (from step 3) to the quarterly component concentrations (from step 2).

5. Sum the quarterly components to get quarterly "potential" 98th percentile $PM_{2.5}$ values. Repeat this procedure for each quarter and for each of the 5 years of ambient data. The highest daily value (from the 4 quarterly values) for each year at each site is considered to be the estimated 98th percentile value for that year.

6. Calculate future year 5-year weighted average 24-hour Design Values and compare to the 24-hour $PM_{2.5}$ NAAQS.

More details can be found in the EPA's modeling guidance (EPA, 2007).

9.4 Unmonitored Areas Attainment Test

The MATS tool includes an unmonitored area attainment test to examine for potential 8-hour ozone or $PM_{2.5}$ hotspots away from the monitors. Given the uncertainties in these procedures, EPA guidance is clear that projected 8-hour ozone or $PM_{2.5}$ DVs exceeding the NAAQS away from the monitors do not necessarily imply that the NAAQS would be violated, rather they suggest an unmonitored location where high ozone or $PM_{2.5}$ could be occurring and additional monitoring stations should be deployed to determine whether the location is a potential trouble spot.

The MATS procedures for conducting the unmonitored area attainment test are as follows:

- Interpolate base year ambient data to create a set of spatial fields.
- Adjust the spatial fields using gridded model output gradients (base year values).
- Apply gridded model RRFs to the gradient adjusted spatial fields.
- Determine if any unmonitored areas are predicted to exceed the NAAQS in the future.

Details of this procedure are described in the EPA guidance (EPA, 2007).

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