APPENDIX I-1

LADCO Modeling Protocol

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Modeling Protocol:
2005 Basecase Technical Details

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1. INTRODUCTION

The purpose of this document is to provide technical details relating to photochemical modeling done to support State Implementation Plans for ozone, PM2.5, and regional haze using the 2005 base year. Information relevant for the 2005 basecase is presented in this document. Documents that relate to a conceptual description of ozone, PM2.5, and regional haze in the Upper Midwest are available on the organization website: www.ladco.org.

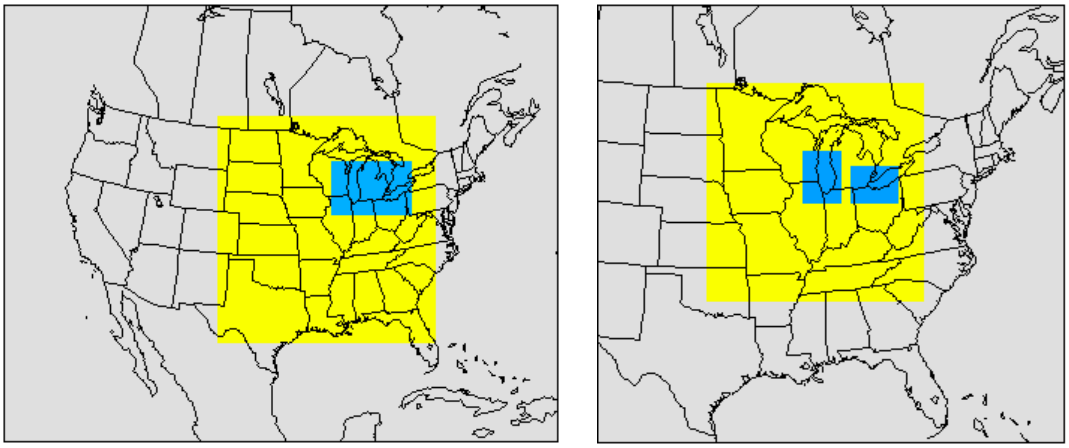
The computing platforms are Intel-based PCs running variations of the Linux operating system. The Portland Group (PGI) Fortran compiler is used to create all executables.

2. METHODOLOGY

Grid Projection and Domains (same as 2002 protocol)

All models are applied with a Lambert projection centered at (-97, 40) and true latitudes at 33 and 45. The 36 km photochemical modeling domain consists of 97 cells in the X direction and 90 cells in the Y direction covering the central and eastern United States with 36 km grid cells (Figure 2.1; Table 2.1). The 2-way nested 12 km photochemical domain covers most of the upper Midwest region. A 2-way nested 4 km photochemical domain is situated over the lower portion of Lake Michigan and over Detroit-Toledo-Cleveland.

Figure 2.1 Modeling Domains: Meteorological (left), photochemical (right)



The 36 km meteorological modeling domain covers the entire continental United States (Figure 2.1; Table 2.1). The 12 km meteorological domain covers most of the central and eastern United States and the 4 km domain covers the lower portion of the Great Lakes. CAMx4 is applied with the vertical atmosphere resolved with 16 layers up to approximately 15 kilometers above ground level.

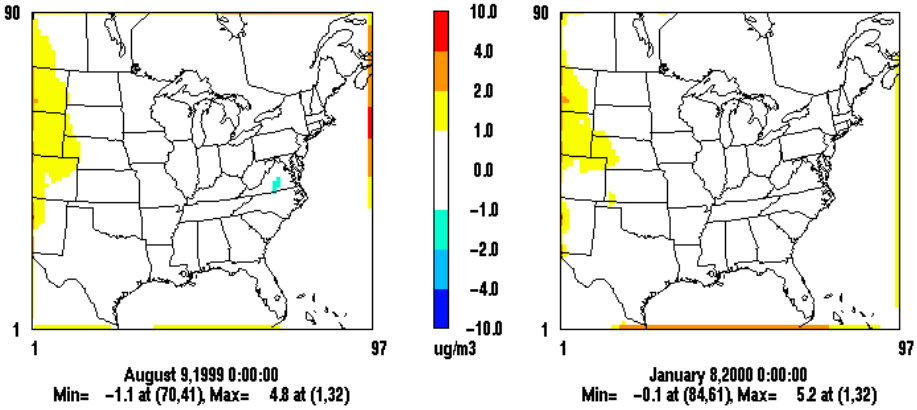
Table 2.1 Modeling Domains

Grid	Cell Size	XY Origin (km)	NX, NY
Emissions	36 km	(-2628., -1980.)	147, 111
Meteorological	4 km	(576., 108.)	214, 142
Meteorological	12 km	(-648., -1260.)	193, 199
Meteorological	36 km	(-2952., -2304.)	165, 129
Photochemical	36 km	(-900., -1620.)	97, 90
Photochemical (lm)	4 km	(608., 140.)	83, 128
Photochemical (detcle)	4 km	(1040., 176.)	74, 56
Photochemical/Emissions	12 km	(-48., -552.)	131,131

The photochemical model is not being applied to the entire 36 km Continental U.S. domain to maximize resources. A sensitivity study was conducted to compare winter and summer episode averaged PM2.5 concentrations between a Continental U.S. domain and Central/Eastern U.S. domain using clean boundary conditions released with the CMAQ model. The episode average differences in PM2.5 were less than 1 ug/m3 in the Midwest RPO States and neighboring States (Figure 2.2).

Figure 2.2 Continental Domain – Central/Eastern U.S. Domain Episode Average

PM2.5 Difference Plots for Summer (left) and Winter (right) episodes



Meteorological Inputs

The meteorological input data for 2005 modeling are developed with the National Center for Atmospheric Research (NCAR) 5th generation Mesoscale Model (MM5) version 3.6 (Dudhia, 1993; Grell et al, 1994) by Alpine Geophysics, LLC under contract from the Midwest Ozone Group. MM5 physics options and configurations for the 2005 simulations are the same as used for 2002 simulations (McNally and Schewe, 2006; Baker et al, 2007c). Important MM5 parameterizations and physics options include mixed phase (Reisner 1) microphysics, Kain-Fritsch 2 cumulus scheme, Rapid Radiative Transfer Model, Pleim-Chang planetary boundary layer (PBL), and the Pleim-Xiu land surface module. Analysis nudging for temperature and moisture is only applied above the boundary layer. Analysis nudging of the wind field is applied above and below the boundary layer.

MM5 performance for 2005 was evaluated by Alpine Geophysics for the Midwest Ozone Group and independently by Lake Michigan Air Directors Consortium. Performance for 2005 is considered comparable to 2002 performance and appropriate for regulatory modeling (Baker et al, 2007).

The meteorological fields output by MM5 are prepared for use by the photochemical model with processing utilities. These programs translate certain meteorological parameters from the MM5 grid to the photochemical grid. Additionally, these processors estimate parameters such as vertical diffusivity coefficients that are not explicitly output by MM5. The MM5CAMx version 4.4 utility is used to translate MM5 output to CAMx input. The vertical diffusivity coefficients are based on the O'Brien 1970 vertical diffusivity algorithm. This scheme takes the PBL height output by MM5 and creates a well-mixed atmosphere inside the PBL. The minimum vertical diffusivity coefficient is 0.1 m^2/s. A landuse-weighted vertical diffusivity coefficient (maximum of 1.0 m^2/s in a completely urban grid cell) is assigned to all grid cells up to approximately 150 meters above ground (model layer 3).

The vertical resolution used in MM5 consists of 34 sigma layers that represent the terrain following atmosphere up to 100 millibars. Figure 2.7 displays each vertical layer in terms of sigma level, pressure (millibars), height above ground level (meters) and layer thickness (meters). The relationship to the layer structure used in the photochemical models is also shown. The photochemical model layer structure avoids layer collapsing in the lower boundary layer to better resolve the mixing depth.

Figure 2.7 Vertical Layer Structure

k(MM5)	sigma	p(mb)	depth(m)	k(PCM)	depth(m)
34	0.000	100	1841	16	5597
33	0.050	145	1466		
32	0.100	190	1228		
31	0.150	235	1062		
30	0.200	280	939	15	2549
29	0.250	325	843		
28	0.300	370	767		
27	0.350	415	704	14	2533
26	0.400	460	652		
25	0.450	505	607		
24	0.500	550	569		
23	0.550	595	536	13	1522
22	0.600	640	506		
21	0.650	685	480		
20	0.700	730	367	12	634
19	0.740	766	266		
18	0.770	793	259	11	428
17	0.800	820	169		
16	0.820	838	166	10	329
15	0.840	856	163		
14	0.860	874	160	9	318
13	0.880	892	158		
12	0.900	910	78	8	155
11	0.910	919	77		
10	0.920	928	77	7	153
9	0.930	937	76		
8	0.940	946	76	6	151
7	0.950	955	75		
6	0.960	964	74	5	148
5	0.970	973	74		
4	0.980	982	37	4	37
3	0.985	987	37	3	37
2	0.990	991	36	2	36
1	0.995	996	36	1	36
--SURF--	1	1000	0	--SURF--	--SURF--

A compromise in the upper troposphere is met by employing layer collapsing to reduce computational effort and still maintain some upper troposphere resolution for long-range transport. The layer structure chosen for a modeling application should be capable of adequately resolving the diurnal variations in the boundary layer growth and mixing, long-range transport processes, wind shear, as well as transport to and from the free troposphere.

Emissions Inputs

Emissions developed for the 2005 basecase and future year inventories projected from 2005 are discussed in the "Base M/Round 5 Emissions Report" (LADCO, 2007). Anthropogenic emissions are developed for a weekday, Saturday, and Sunday for each month of 2005. On-road motor vehicle emissions were developed for a January and July weekday, Saturday, and Sunday. On-road motor vehicle emissions for other months are interpolated between the January and July estimates. On-road and biogenic volatile organic carbon (VOC) emissions are speciated for the CB05 chemical speciation profile (Environ CB05 report). All other sectors of the inventory are speciated for the CB-IV chemical speciation profile (Carter, 1996). CB-IV emissions are useable with CB05 chemistry (Environ CB05 report).

The Model of Emissions of Gases and Aerosols from Nature (MEGAN) was recently developed as the next generation emission model for biogenic emissions of gases and aerosols (Guenther and Wiedinmyer, 2006). MEGAN has been implemented into the CONsolidated Community Emissions Processing Tool (CONCEPT) emissions modeling framework (Wilkinson, 2006). Biogenic emissions are estimated for each day of the simulation using the MEGAN model as implemented in CONCEPT (Baker, 2007d). MEGAN explicitly outputs import biogenic secondary organic aerosol pre-cursor species including monoterpenes and sesquiterpenes that are used by the CAMx SOA chemistry module.

MEGAN groups plants and area coverages by plant functional type (PFT) rather than treating plant species explicitly as in the BIOME (and BEIS) models. Total emissions are the sum of emissions estimated for each PFT in a given grid cell. PFTs include broadleaf trees, fine leaf evergreen trees, fine leaf deciduous trees, shrubs, grass, and crops. Plant functional type data has been gridded to a scale of 30 seconds by 30 seconds and made available with the MEGAN model (Guenther et al, 2006). Soil wilting point data and leaf area index are also gridded to the same scale and used as input to MEGAN.

Volatile organic compounds are speciated to the Carbon Bond 2005 chemical speciation profile. Inputs to the biogenic model include hourly satellite photosynthetically activated radiation (PAR) and 15 m (above ground level) temperature data output from MM5 (Pinker and Laszlo, 1992). Other inputs to MEGAN include plant functional type (PFT) emission factors, PFT area coverage, soil wilting point data, leaf area index, and additional meteorological variables including soil moisture. Soil moisture estimated by MM5 for the 1 m soil depth is used as input to MEGAN because it represents the plant root layer.

Landuse (same as 2002 protocol)

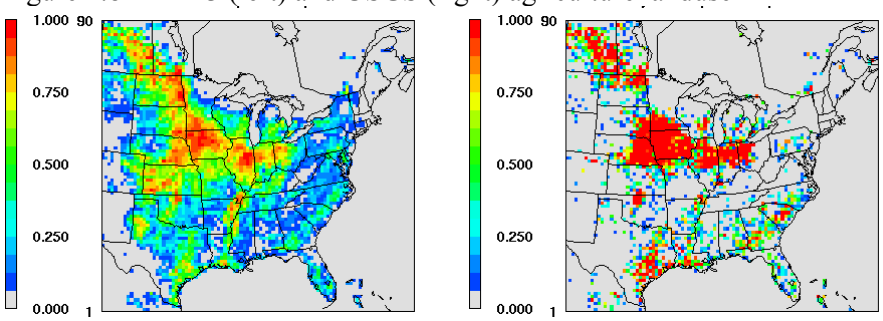
The photochemical model uses 11 land use categories to describe the surface. The land use file is based on BELD3 1 km data (US EPA, 2006; Kinnee et al. 1997; Kinnee et al. *in press*). The 1 km data was aggregated to the appropriate grid resolution for photochemical modeling. Surface roughness varies by season and land use category and are taken from EPA's AERMET User's Guide (EPA, 2004; ENVIRON, 2007).

Table 2.3 Landuse categories

Category	Landuse
1	Urban
2	Agricultural
3	Rangeland
4	Deciduous forest
5	Coniferous forest
6	Mixed forest
7	Water
8	Mixed agriculture/forest
9	Non-forested wetlands
10	Mixed agriculture/range
11	Rocky with low shrubs

USGS data was previously used for landuse information. The BELD3 was chosen because it incorporates the USGS data with other sources of information such as satellite data. A spatial comparison of the agriculture (category 2) landuse fractions are shown below.

Figure 2.8 BELD3 (left) and USGS (right) agriculture landuse



Drought Stress and Snow Cover (same as 2002 protocol)

The Palmer Drought Severity Index (PDSI) is an indicator of unusual excess or deficient moisture. The PDSI is calculated for 350 climatic divisions in the United States and Puerto Rico. PDSI data is available for each week of a calendar year and is obtained from the National Weather Service Climate Prediction Center (National Weather Service, 2005). The dry deposition calculations for non-water landuse categories are impacted by vegetative response to drought stress (ENVIRON, 2007).

Snow cover is also input to CAMx4 for the deposition scheme. Three-hourly snow cover data for each grid cell is extracted from MM5 output files. If snow exists in a grid cell, the deposition characteristics of the landuse are switched from “winter” to “winter with snow.” This switch has an impact on surface resistances for dry deposition, surface roughness, and chemistry due to the ultraviolet albedo being changed to the maximum class (ENVIRON, 2007).

Photolysis Rates (same as 2002 protocol)

Many chemical reactions in the atmosphere are started by the photolysis of certain trace gases. Photochemical models require these rates be input to accurately estimate these reactions. CAMx4 is applied with day specific photolysis rate look-up tables.

The Tropospheric Ultraviolet-Visible (TUV) radiation model is used to calculate photolysis rates based on solar zenith angle, height above ground, ultraviolet albedo of the ground, atmospheric turbidity, and total ozone column density. The TUV generates rates for each day as a function of 11 heights, 10 solar zenith angles, 5 ozone column values, 5 albedo values, and 3 turbidity values (ENVIRON, 2007; NCAR, 2006).

The ozone column data is derived from daily TOMS satellite observations (NASA, 2006). The albedo data varies by month and is based on over 10 years of TOMS satellite reflectivity observations. Actinic flux is estimated using the discrete ordinate algorithm. The two-stream delta-Eddington method is also available in the TUV model, but was not selected because the discrete ordinate approach is more accurate.

A sensitivity application with CMAQ using TOMS derived photolysis rates and rates based on seasonal average ozone column showed differences in ozone up to 3 ppb and differences in sulfate ion up to 1.5 ug/m^3. These differences suggest day specific ozone column data from satellites should be used rather than seasonal averages and that accurate photolysis rates are important for ozone and particulate matter applications.

For those days that do not have TOMS ozone column data, the data from the previous day is used instead. This option is more realistic than defaulting to a seasonal average, which may create a rather large discontinuity between the missing day and adjoining simulation days.

Initial and Boundary Conditions (same as 2002 protcol)

Boundary conditions represent pollution inflow into the model from the lateral edges of the grid and initial conditions provide an estimation of pollution that already exists. In the past a spin-up period of two to three days was used to eliminate initial condition effects for ozone modeling.

CAMx4 source apportionment runs show ozone attributed to initial concentrations does not exceed 5 ppb anywhere in the domain by the 7th day of the episode; ozone modeling episodes will be spun up with 11 days. The monitors used in model performance evaluation are far enough away from the boundaries that boundary influence is considered minimal.

CAMx4 particulate source apportionment (PSAT) runs show PM2.5 sulfate ion, nitrate ion, and ammonium ion contributions from initial concentrations fall below 0.05 µg/m^3 by the seventh day of the episode. PM2.5 elemental carbon, PM2.5 soil, and coarse mass have less than 1 ng/m^3 contribution from initial concentrations on the first day of the model episode everywhere in the modeling domain. Since gas phase chemistry is coupled with particulate formation, the annual simulations have two weeks of spin-up to minimize initial condition influence.

The initial and boundary conditions are based on monthly averaged species output from an annual (calendar year 2002) application of the GEOS-CHEM global chemical transport model (Jacob et al, 2005; Bey et al, 2001). Boundary conditions vary by month and in the horizontal and vertical direction. Where an initial or boundary concentration is not specified for a pollutant the model will default to a near-zero concentration.

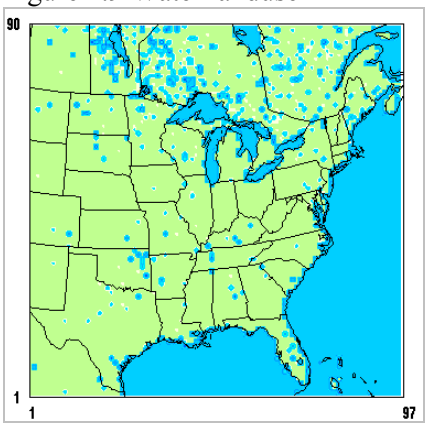
A study applying CMAQ with monthly averaged and 3-hr GEOS-CHEM initial and boundary conditions showed almost no change in model performance for any PM2.5 species. The error for total PM2.5 and each of the chemical species differed by less than 0.04 ug/m^3 at IMPROVE and EPA STN monitor sites (Morris et al, 2004b). Considering the need to model multiple annual simulations and potential issues related with inconsistencies between in-flows and out-flows between the GEOS-CHEM meteorology and the MM5 simulation used for regional modeling, the monthly averaged concentrations are used to support photochemical modeling applications.

Quality Assurance of Model Inputs (same as 2002 protocol)

The model input files are checked for reasonableness to ensure they accurately represent the underlying data used to create the files. The checks described in this document are steps that are in addition to the extensive QA done in the emission inventory compilation process, EMS emissions modeling, and MM5 modeling process.

The landuse files are converted to a CAMx4 output file format and directly viewed in PAVE over a political map. An example of the water landuse category is shown in the figure in this section.

Figure 2.9 Water landuse



The initial and boundary conditions processor outputs an ASCII file showing the specie concentration at each vertical layer. This is visualized in EXCEL to make sure the data is correctly mapped in the vertical direction. The initial and boundary concentration files themselves are also directly viewed in PAVE and the spatial representation is checked. The ozone column, albedo, and turbidity data are kept in ASCII files. Each file is checked to ensure the data looks spatially reasonable and that bad data did not get included in the file.

The emissions inputs are extensively checked for appropriateness. The steps taken in manipulating EMS-2003 output files to CAMx4 input files and the quality assurance of those files are detailed in “Emissions Processing and QA” (Baker, 2004b). Each emission file is checked for spatial and temporal agreement with EMS-2003 and for reasonableness. Additionally, the mass for each species is totaled by State and over the entire modeling domain and compared to EMS-2003 QA reports.

The MM5 output used to support the photochemical modeling is extensively evaluated from a meteorological perspective. An additional layer of quality assurance is done by evaluating model performance of the air quality model input meteorological data at several monitor locations. This is done for temperature, relative humidity, wind speed, and wind direction.

Photochemical model simulations also provide a level of quality assurance since deficiencies in emissions and meteorological inputs will be apparent in the photochemical model performance.

Photochemical Model Configuration

The Comprehensive Air Quality Model with Extensions (CAMx) version 4.50 uses state of the science routines to model particulate matter formation and removal processes over a large modeling domain (Nobel et al. 2002; Tanaka et al. 2003; Chen et al. 2003; Morris, Mansell, Tai, 2004). The model is applied with ISORROPIA inorganic chemistry, SOAP organic chemistry, regional acid deposition model (RADM) aqueous phase chemistry, and the carbon-bond 2005 (CB05) gas phase chemistry module (ENVIRON, 2007; Nenes et al, 1998; ENVIRON, 2007). CAMx4 is applied using the PPM horizontal transport scheme and an implicit vertical transport scheme with the fast CMC chemistry solver (ENVIRON, 2007). The chemical mechanism 6 is selected for the 2005 simulations, which includes additional PM2.5 secondary organic aerosol formation (ENVIRON, 2006; ENVIRON 2007). An updated dry deposition scheme that is based on AEROMOD is chosen for the 2005 simulations. This scheme uses gridded monthly leaf area index to adjust dry deposition velocities (Kemball-Cook et al, 2007).

CAMx4 models PM particles in the fine and coarse size fraction. There is no mechanism in the model to transfer mass between these 2 size sections. The particle density and diameter does not change from specie specific input values during a model simulation for either particle size bin.

The photochemical model is initiated at midnight Eastern Standard Time and run for 24 hours for each episode day. The summer 2005 simulation is initiated on June 2 and run through September 15. The annual simulation is run separately by calendar quarter and is initiated 2 weeks prior to each quarter: December 17 (2004), March 15, June 15, and September 15. The base and future year scenarios submitted as support for the annual PM2.5 standard will be using a horizontal grid resolution of 12 km. The modeling to support the 8-hr Ozone NAAQS will be at 12 km horizontal resolution over the entire upper Midwest with optional 2-way nested 4 km grids over the lower portion of Lake Michigan and over the Detroit-Toledo-Cleveland region.

Future year simulations will be applied with the same model configuration as for the base case simulation. All inputs except for emissions will be the same in the future year and base year simulations to assess changes in ozone, visibility, and PM2.5 due to control strategies and future growth. The terms base case and base line emissions inventories are one in the same, both referring to day specific biogenics and monthly weekday, Saturday, Sunday anthropogenic emissions.

Plume-in-Grid and Nesting

The GREASD sub-grid plume treatment option is being applied in CAMx4 for the summer season 12 km ozone simulations. This option is selected to improve the model treatment of large NOx plumes being released near Lake Michigan and Lake Erie. Sources included for the plume-in-grid treatment include any source near the Great Lakes with NOx emissions greater than 12 tons per day for any day of the summer in 2005 and 6 tons per day in future year scenarios.

At high grid resolutions of 4 km or finer, sub-grid scale treatment of plumes should not be applied since the fine grid appropriately captures the small scale physical and chemical processes.

Nested grids are useful to keep computational and data management resources acceptable while addressing important model application issues such as complex terrain, land-sea or land-lake breezes, and spatial emission gradients. They may also be useful to keep large point source plumes in smaller grid cells in lieu of having explicit sub-grid scale plume treatments.

CAMx4 allows for the inclusion of a fine grid within the coarse grid in a 2-way nesting mode. The 2-way nesting mode allows for interaction between the larger coarse grid with the smaller fine grid. This improves pollutant transport around the boundaries of the fine grid since a parcel of air may move from the fine grid, out to the coarse grid, and back into the fine grid depending on the shifting wind fields. This re-circulation is impossible in 1-way nesting applications.

Probing Tools

Probing tools are valuable from a scientific and regulatory perspective for one-atmosphere modeling. Use of source apportionment is more desirable for regulatory applications than the use of the "zero-out" approach to determine geographic and emissions sector culpability for long-term modeling simulations. Zeroing out emissions for large regions such as entire States fundamentally changes the atmospheric chemistry and makes interpretation of the results difficult.

An option in CAMx is employed to force elevated point sources into particular regions rather than placement based on coordinates and the 12 km geographic region map. This ensures that elevated emissions are placed in the appropriate geographic region and not incorrectly grouped with another region when a grid cell contains the boundary for more than one region. A good example of this is the Ohio River Valley where many large stationary point sources exist along State boundaries and could be grouped into the wrong region based on the 12 km grid cell source region map. This option improves the confidence in the source apportionment results for stationary point sources.

Ozone

CAMx is a state of the science photochemical model that contains a variety of ozone source apportionment tools, including the original ozone source apportionment tool (OSAT) and the anthropogenic pre-cursor culpability assessment (APCA) tool. The APCA tool assesses regional and emission sector contribution to ozone formation and provides information that is most policy relevant. When ozone is formed under VOC limited conditions due to biogenic VOC + anthropogenic NOx then OSAT attributes it to the biogenic VOC sources. When ozone is formed under NOx-limited conditions due to biogenic VOC + anthropogenic NOx then OSAT attributes it to the anthropogenic NOx sources. APCA is designed to provide more control strategy relevant information and recognizes that there are source categories such as biogenics that can not be controlled so the model only attributes ozone to biogenics when it is due to the interaction of biogenic VOC + biogenic NOx. In the case where ozone formed to biogenic VOC + anthropogenic NOx under VOC-limited conditions, OSAT attributes it to biogenic VOC, but APCA redirects the attribution to anthropogenic NOx. In NOx-limited conditions both OSAT and APCA attribute the ozone to anthropogenic NOx (ENVIRON, 2007). The APCA tool is chosen to track ozone contribution for this modeling study.

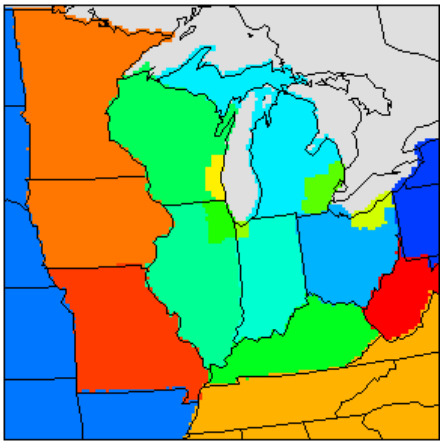
The source apportionment data is the average contribution over all modeled hours where predicted ozone at the monitor is greater than a threshold concentration value. Two different thresholds are used to examine different distributions of high modeled 8-hour ozone: 75 and 85 ppb (Baker, 2007). The geographic regions tracked for ozone contribution are listed in Table 2.4

and shown graphically in Figure 2.10 over the 12 km modeling domain. The contribution from the lateral and top boundaries of the model is also tracked for each receptor location.

Table 2.4 Complete list of source regions tracked for ozone contribution

Canada	Illinois Chicago non-attainment (NA) Counties
Northeast States (MANE-VU)	Detroit NA Counties
Central/Western States (CENRAP+ WRAP)	Indiana Chicago NA Counties
Ohio	Cleveland NA Counties
Michigan	Milwaukee NA Counties
Indiana	Southeast States (VISTAS)
Illinois	Minnesota+Iowa
Wisconsin	Missouri
Kentucky	West Virginia

Figure 2.10 Source regions tracked in the 12 km grid domain



Six emissions source sectors are tracked for contribution to ozone: onroad mobile, offroad mobile, area, electrical generating units, non-electrical generating units, and biogenics. Offroad mobile emissions include sources such as construction equipment, locomotives, commercial marine vessels, and airports. Two distinct groups of stationary point sources are tracked for contribution to ozone: electrical generating units and non-electrical generating units.

Particulate Matter and Visibility

The Particulate Source Apportionment Tool (PSAT) tracks contributions of PM2.5 sulfate ion, nitrate ion, ammonium ion, elemental carbon, and primary emissions of organic aerosol, soil, and coarse mass. Secondary organic aerosol tracking is also part of the tool but not employed for this study due to resource constraints. Secondary organic aerosol contributions from biogenic and anthropogenic sources are part of the standard CAMx output and included in the analysis.

Source apportionment results will be estimated on an annual average basis and on a daily 24-hr basis to be relevant to the annual and 24-hr PM2.5 NAAQS. The 24-hr average source apportionment results for the 20% worst and 20% best days at the Class I area receptors will be converted to light extinction then averaged together using the latest IMPROVE Steering Committee recommended equation (IMPROVE, 2006). Contributions from initial conditions are quantified to determine an optimal amount of spin-up time required to minimize the impacts from initial concentrations.

The geographic regions tracked for contribution are listed in Table 2.5 and shown graphically in Figure 2.11. The contribution from the lateral and top boundaries of the model is also tracked for each receptor location.

Figure 2.11 Model domain and source regions tracked with PSAT

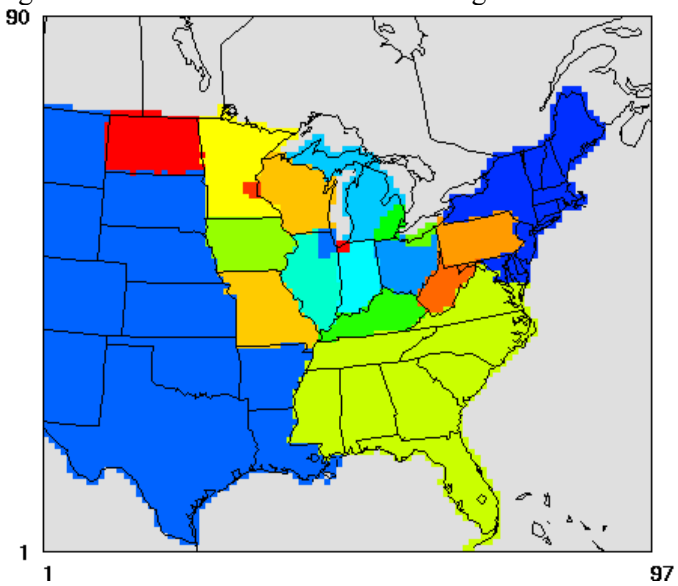


Table 2.5 Complete list of source regions tracked for contribution

Canada	Illinois Chicago non-attainment (NA) Counties
Northeast States (MANE-VU)	Detroit NA Counties
Central/Western States (CENRAP+ WRAP)	Indiana Chicago NA Counties
Ohio	Cleveland NA Counties
Michigan	Milwaukee NA Counties
Indiana	Southeast States (VISTAS)
Illinois	Minnesota
Wisconsin	Minneapolis-St. Paul
Kentucky	West Virginia
Iowa	North Dakota
Missouri	

Seven emissions source sectors are tracked for contribution to particulate matter: onroad mobile, offroad mobile, area, electrical generating units, non-electrical generating units, agricultural ammonia, and biogenics.

3. Model Performance Evaluation (same as 2002 protocol)

State Implementation Plans will include modeling the impacts of emission control scenarios with 3-D Eulerian photochemical transport models. Model performance is typically evaluated on an operational basis and rarely to support a diagnostic (dynamic) assessment. Operational evaluations for ozone modeling purposes include matching model estimates with observation data for ozone, nitrogen oxides (NO_X), and total volatile organic compounds (VOC). Operational evaluations for PM2.5 and visibility modeling purposes include matching model estimates with observation data for chemically speciated PM2.5 and important pre-cursor species including sulfur dioxide, nitric acid, and ammonia.

A diagnostic evaluation assesses how appropriately the modeling system responds to emissions adjustments. Since the modeled attainment demonstration includes modeling current and future year emissions it is important to have confidence that the model will predict concentrations appropriately when emissions change (US EPA, 2007). This type of evaluation includes modeling two different ozone episodes that are separated by enough years that large emissions differences exist. The diagnostic evaluation is an important assessment to make in addition to an operational evaluation because it is directly linked to the end use of the model, which is modeling the change in ozone concentrations after emissions adjustments.

A comparison between observed and estimated ozone for the summers of 2002 and 2005 is useful for a diagnostic assessment because high quality emission inventories were developed for each year and a large NO_X emissions reduction occurred between these years due in part to NO_X SIP Call compliance. Modeling two full summer seasons provides an opportunity to make another diagnostic evaluation which assesses model performance for high ozone by day of the week (Baker, 2007b). Emissions change substantially from weekday to weekend and having two full summers provides enough days with high ozone on each day of the week to make this type of evaluation useful.

The photochemical modeling applications are designed to support the development of regional control strategies for PM2.5 and Regional Haze. EPA guidance states that an attainment test for either standard will require the use of chemically speciated PM relative reduction factors (US EPA, 2007). Additionally, the model will be used to assess improvements in PM2.5 concentrations and visibility as a result of changes in emissions. These prominent end-uses of the modeling applications make comprehensive evaluations important. Clearly, reliance on model performance for PM2.5 total mass would be misleading since it is likely that the model and ambient data could estimate the same total mass but very different chemical composition. This scenario would compromise the development and interpretation of potential regulatory control strategies (Baker, 2004d).

The species to be compared to monitor concentrations include ozone, total VOC, NOX, SO2, NH3, HNO3, and speciated PM2.5 (see Table 3.1). Initially, scatter-plots of point-to-point relationships for all monitors in the domain for all episode days will be used for analysis for PM. This will allow for identification of gross model over or under-prediction by specie. Gas and aerosol data are taken from a variety of monitor networks for comparison to modeled estimates: IMPROVE, EPA Speciation Trends (STN), AIRS, and PAMS. The data is obtained directly from the VIEWS website and from the AFS database; a comparison of the monitor species to model species is shown below. PM2.5 ammonium ion is only measured at EPA Speciation Trends locations so the model performance for this chemical specie is dominated by, but not limited to, urban measurement locations.

Table 3.1 Species mapping between modeled and observed species (observed species from the VIEWS website)

	IMPROVE	STN	CAMx4 species
Sulfate aerosol	SO4f	SO4f	PSO4
Nitrate aerosol	NO3f	NO3f	PNO3
Ammonium aerosol		NH4f	PNH4
Organic aerosol	OCf*FACTOR FACTOR = 1.6 rural 2.1 urban	OCf*FACTOR FACTOR = 1.6 rural 2.1 urban	SOA1+SOA2+ SOA3+SOA4+ SOA5+POA
Elemental carbon	ECf	ECf	PEC
Soil/Crustal	SOILf	SOIL = 2.2*ALf + 2.49*SIf+1.63*CAf+ 2.42*FEf+1.94*TIf	FCRS
PM2.5 other	MF-RCFM	MF-(RCFM)	FPRM
Coarse mass	CM_calculated		CPRM+CCRS
PM2.5	MF	MF	PSO4+PNO3+PNH4+POA+ SOA1+SOA2+SOA3+SOA4+ SOA5+PEC+NA+PCL+ FPRM+FCRS
Re-constructed fine mass	RCFM	RCFM = SO4f+NO3f+ NH4f+OCf*FACTOR+ ECf+(SOIL)	1.375*PSO4+1.29*PNO3+ POA+SOA1+SOA2+SOA3+ SOA4+SOA5+PEC+NA+ PCL+FPRM+FCRS
Re-constructed bext	aerosol_bext		fRH*[4.125*PSO4+ 3.87*PNO3]+4*(SOA1+SOA2+ SOA3+SOA4+SOA5+POA)+ 10*PEC+NA+PCL+FPRM+FCRS+ 0.6*(CPRM+CCRS)

Model performance evaluation plots and metrics will be based on matching predictions and observations in time and space. There will not be any averaging over multiple-cell regions to match with an observation value. Qualitative evaluation will be done largely through graphical comparison of predictions and observations using spatial plots, time series plots, and scatter plots. The US EPA modeling guidance recommends against using any bright-line evaluation of performance metrics to determine whether the modeling is satisfactory (US EPA, 2007).

3.1 Particulate Matter and Regional Haze

The components of the visibility equation match up very closely to the prominent chemical forms of PM2.5: nitrate ion, sulfate ion, ammonium ion, organic carbon, elemental carbon, and soil (US EPA, 2007). Since these modeling applications will support PM2.5/Haze rules, model performance will be most rigorous for each of these PM2.5 species and coarse mass.

One of the problems related to PM model performance evaluation involves matching inconsistent monitor methodologies and model specie definition. Additionally, speciated measurements rarely add up to measurements of total fine mass. This unexplained fraction is usually attributed to the retention of water on the weighed samples (Timin, 2002). Other problems with comparing speciation samples and FRM measurements include volatilization of nitrate and positive and negative organic carbon artifacts (Timin, 2002).

Organic material is typically estimated from organic carbon using a 1.4 factor, which is based on the assumption that carbon accounts for 70% of the organic mass. Recent literature recommends a factor of 1.6 ± 0.2 for urban aerosol and 2.1 ± 0.2 for non-urban areas that would see more aged aerosol (Turpin and Lim, 2001; IMPROVE, 2006). These factors are applied to the observation data based on landuse type before being compared to model output. These factors may also be used to reduce modeled estimates of organic material to organic carbon.

Performance metrics used to describe model performance for PM2.5 species include mean bias, gross error, fractional bias, and fractional error (Table 3.2) (US EPA, 2007; Boylan et al, 2006). The bias and error metrics are used to describe performance in terms of the measured concentration units (μg/m^3). Even though the distribution of PM2.5 is log-normal, the data is not transformed for this analysis. The model attainment tests outlined by EPA for the PM2.5 NAAQS and Regional Haze rule require relative reduction factors to be applied to actual concentrations and not transformed concentrations. No minimum value is used to eliminate data points for the purposes of this analysis.

Table 3.2. Model Performance Metrics.

Mean Bias	$= \frac{1}{N \times M} \sum_{i=1}^{N} \sum_{j=1}^{M} (P_i^j - O_i^j)$
Gross Error	$= \frac{1}{N \times M} \sum_{i=1}^{N} \sum_{j=1}^{M} \lvert P_i^j - O_i^j \rvert$
Fractional Bias	$= \frac{1}{N \times M} \sum_{i=1}^{N} \sum_{j=1}^{M} \left(2 \times \frac{P_i^j - O_i^j}{P_i^j + O_i^j} \right)$
Fractional Gross Error	$= \frac{1}{N \times M} \sum_{i=1}^{N} \sum_{j=1}^{M} \left\lvert 2 \times \frac{P_i^j - O_i^j}{P_i^j + O_i^j} \right\rvert$

*P=model prediction; O=observation; N=number of days; M=number of monitors

Fractional bias and fractional error metrics are useful for comparison of model performance between species that tend to have large concentrations and those with small concentrations. It also helps compare performance of the same specie if concentrations are very large in some seasons and very small in others. The fractional metrics are best when close to 0 and worst when close to 2.

3.2 Ozone

Hourly running 8-hour averaged surface ozone observations from EPA's AIRS database are matched to hourly running 8-hour averaged layer 1 (30 m height) model estimates for evaluation. Only monitors in the 12 km modeling domain are included in the analysis. Model performance evaluation plots and metrics are based on matching predictions and observations in time and space. EPA has suggested several statistical metrics to describe model performance and include mean normalized bias error (MNBE) and mean normalized gross error (MNGE) (see Table 3.3) (US EPA, 2007).

This modeling system is used to support regulatory applications, so the model performance analysis reflects this end-use of the modeling results. It is well known that ozone data tends to follow a log-normal distribution and for the purposes of scientific evaluations the data is often log-transformed before evaluation (Hogrefe et al, 2003). Observations and predictions used in the

attainment test may not be transformed, so the data used for model performance evaluation will likewise not be transformed.

Table 3.3 Model Performance Metric Definitions.

Metric	Equation
Mean Normalized Bias Error (MNBE)	$=\frac{1}{N \times M}\sum_{i=1}^{N}\sum_{j=1}^{M}\left(\frac{P^j - O_i^j}{O_i^j}\right)$
Mean Normalized Gross Error (MNGE)	$=\frac{1}{N \times M}\sum_{i=1}^{N}\sum_{j=1}^{M}\left\lvert\frac{P_i^j - O_i^j}{O_i^j}\right\rvert$

**P=model prediction; O=observation; N=number of days; M=number of monitors*

These metrics have traditionally been calculated when the observation value exceeds a certain minimum value, often 60 ppb for 1-hour ozone evaluation (Hogrefe et al, 2003). The MNBE and MNGE will be estimated using 3 different minimum 8-hour ozone thresholds: 20, 40, and 60 ppb. The 60 ppb minimum threshold level excludes prediction-observation pairs that are not of direct regulatory importance since the 8-hour ozone attainment test only applies to days with high ambient concentrations (US EPA, 2007). The 20 and 40 ppb minimum thresholds are included in the evaluation to get a better idea about how well the model is performing at predicting diurnal formation and removal processes and for days between high ozone episodes.

The metrics are estimated for all stations in the 12 km modeling domain for each day of the summer episode. The episode average metrics are estimated from the daily metrics.

3.3 Deposition

Wet deposition is measured at several monitoring networks and is also output by the photochemical model. The National Trends Network (NTN) and the Atmospheric Integrated Research Monitoring Network (AIRMoN) make up the National Atmospheric Deposition Program (NADP). NTN sites collect weekly measurements of wet deposition fluxes of sulfate and nitrate anions and the ammonium cation. NADP network stations measure wet deposition as mass per volume (mg/L) and the model outputs mass per area (g/ha or mole/ha). CAMx4 wet deposition output is matched to NTN/NADP measurement data in units of kg/km^2 according to the details outlined below.

The calculations used to convert CAMx wet deposition output to compare to NTN/NADP network data:

SPECIE_WD (g/ha) * (1 ha / 2.5 acres) * (1 acre / 0.0040469 km^2) * (1 kg / 1000 g)

The calculations used to convert NTN/NADP data to compare with CAMx output data:

SPECIES (mg/L) * (1 L / 1,000,000 mm^3) * precipitation in mm * (1 mm^2 / 0.000000000001 km^2) * (1 g / 1000 mg) * (1 kg / 1000 g)

The table below outlines the matching of observed species to CAMx output species.

Table 3.4 Observed and Modeled Wet Deposition		
	NADP/NTN	CAMx4
Sulfate	SO4	PSO4_WD + SULF_WD
Nitrate	NO3	PNO3_WD + HNO3_WD
Ammonium	NH4	PNH4_WD + NH3_WD
Crustal	Ca + Cl + Mg +K + Na	FCRS_WD + FPRM_WD

4. Attainment Tests

Visibility

Visibility may be estimated by two similar methods that relate light extinction to ambient PM2.5 concentrations (FLAG, 2000; US EPA, 2007). Visibility will be estimated using the new equation recommended by the IMPROVE steering committee (IMPROVE, 2006). The new and old equations produce very similar estimates of light extinction in the upper Midwest. The new equation will be emphasized for the SIP modeling demonstration due to its more up to date science.

The equation shown below relates PM2.5 specie concentrations to light extinction. Additional factors of f(RH) are included that change the light scattering of sulfate and nitrate based on climatologically averaged relative humidity.

β_{ext} = 2.2*f_SRH*[small sulfate] + 2.4*f_S(RH)*[small nitrate] + 4.8*f_LRH*[large sulfate] + 5.1*f_L(RH)*[large nitrate]+ 2.8*[small OCM] + 6.1*[large OCM] + 10*EC + 1*SOIL + 0.6*CM + 1.7*f_{SS}(RH)*SS + $\beta_{rayleigh}$

Bext	Estimated extinction coefficient (Mm-1)
Sulfate	Sulfate associated with ammonium (SO4*1.375)
Nitrate	Nitrate associated with ammonium (NO3*1.29)
OCM	Organic carbon Mass
EC	Elemental carbon
SOIL	Inorganic primary PM2.5 (soil, crustal, other)
CM	Coarse fraction particulate matter
SS	Sea salt
$\beta_{rayleigh}$	Light scattering due to Rayleigh scattering (site specific)
fRH	Relative humidity adjustment factor

The apportionment of sulfate, nitrate, and organic carbon mass into small and large size fractions is shown below using 'X' as a placeholder for these species.

Large X = ([Total X] / [20 ug/m3]) * [Total X], where [Total X] < 20 ug/m3

Large X = [Total X], where [Total X] ≥ 20 ug/m3

Small X = [Total X] – [Large X]

The fRH values are long-term averages that are site and month specific (US EPA, 2003a; US EPA 2003b; FLAG, 2000). The light scattering due to Rayleigh is site specific (IMPROVE, 2006). The NO_2 component to the light extinction equation is not included since it is not measured at Class I areas in the upper Midwest. The visibility equation is expressed as an extinction coefficient (β_{ext}) and is converted to deciviews using the equation below.

$$\text{Deciview} = 10\ln(\beta_{ext}/\ \beta_{rayleigh})$$

The reasonable progress test to determine the relationship between current and future year visibility is expressed in deciview units. The changes in deciview between the current and future year strategy is the reasonable progress test and is shown below.

$$\text{Change in Deciview} = 10\ln[(\beta_{ext})_{future} / (\beta_{ext})_{base}]$$

- or -

$$\text{Change in Deciview} = \text{Deciview}_{base} - \text{Deciview}_{future}$$

Visibility will be estimated for key Class I area in the Midwest for the base year and various future year scenarios. The changes in visibility between the base line and future year will be assessed using procedures in U.S. EPA's modeling guidance document (US EPA, 2007).

1. The visibility in deciviews will be ranked from high to low at each Class I area for the calendar years 2000-2004 using the monthly and site specific fRH values and the more recent IMPROVE light extinction equation.
2. The mean deciviews for the 20% days with the best and the 20% days with the worst visibility is estimated for each Class I area for each year of the 2000-04 baseline period.
3. The mean observed extinction coefficient for the days during the modeling period (2005) with the 20% best and 20% worst visibility will be calculated.
4. The mean predicted extinction coefficient for the corresponding 20% best and 20% worst days of the modeling period of the base case and future year strategy will be calculated using monthly site specific fRH values.
5. The relative reduction factor for the 20% best and 20% worst group of days for each site for each of the particulate matter species in the light extinction equation are estimated.
6. The relative reduction factors are multiplied by daily measured PM data during the 2000-04 baseline to estimate future daily values of these species.
7. These future daily PM estimates are used to estimate light extinction for each of the previously identified 20% best and 20% worst days of monitored data. Light extinction is converted to deciviews and the mean value for the best and worst days for each year of the baseline period is estimated.
8. The 5 mean deciview values for the worst and best days (one from each of the 5 years) are averaged together for a mean value for the best and worst days.
9. The future year mean deciview values in step 8 are compared to the observed values from step 2. The differences are compared to established goals for reasonable progress to determine if reasonable progress is demonstrated.

Annual PM2.5 Standard

Progress in meeting the annual PM2.5 standard will be assessed by application of the procedures outlined by the U.S. EPA modeling guidance document (US EPA, 2007). The major steps of this attainment test are outlined below:

1. Chemically speciated IMPROVE and STN PM2.5 data from 2001-2005 is spatially interpolated to match the grid domain and resolution used for the photochemical modeling. Spatial fields are developed for each PM2.5 chemical species for each season using the SAS statistical software package PROC KRIG function (EPA, 2004b).
2. The estimated fractional composition of each species by quarter is multiplied by the 5 year weighted average 2001-2006 FRM quarterly mean concentrations at each FRM monitor, resulting in estimated quarterly mean ambient concentrations of PM2.5

components sulfate, nitrate, ammonium, elemental carbon, organic carbon, particle bound water, and crustal material.

3. Estimate the modeled quarterly mean concentration for each chemical component of PM2.5 in the base year and future scenarios.
4. Calculate quarterly relative reduction factors for sulfate, nitrate, elemental carbon, organic carbon, and crustal material. The RRF is the ratio of the future year to the base year.
5. Quarterly specific RRFs are multiplied by the quarterly average species concentration from step 2 to estimate future case quarterly average concentrations for each of the PM2.5 species.
6. Calculate the quarterly average future scenario concentrations for ammonium and particle bound water using estimated ambient concentrations of sulfate, nitrate, and degree of sulfate neutralization. Particle bound water is estimated with an empirical equation.
7. Sum the quarterly future species concentrations to estimate the future quarterly average PM2.5 concentration.
8. The annual average future scenario concentration is the average of the 4 future year quarterly average PM 2.5 concentrations.
9. Compare value to annual NAAQS standard of 15 ug/m^3. If value is ≤ 15 ug/m^3 then the test is passed.

Organic carbon mass is estimated using a mass balance approach (EPA, 2006). The organic carbon spatial fields are only used to supply a minimum value for OCM when OCM estimated by mass balance is less than OC*1.4*0.7. A spatial field of the degree of sulfate neutralization is developed to estimate PM2.5 ammonium. Particle bound water is estimated using an empirical equation with spatially interpolated PM2.5 sulfate ion, FRM equivalent PM2.5 nitrate ion, and FRM equivalent PM2.5 ammonium ion (EPA, 2006).

Ozone

Progress in meeting the 8-hour ozone standard will be assessed in part using the modeled attainment test outlined by the U.S. EPA's "Guidance on the Use of Models and Other Analyses in Attainment Demonstrations for the 8-hour Ozone, PM2.5, and Regional Haze" (US EPA, 2007). The attainment test is only applicable to monitors with design values ≥ 75 ppb. The major steps of the attainment test are described below:

1. Calculate the 8-hour ozone design value at each monitor location; the design value used in the attainment test is the average of 3 consecutive 3 year averaged design values: 2003-2005, 2004-2006, and 2005-2007.
2. Apply the photochemical model to a current year and future year to estimate a monitor specific relative reduction factor.
3. Calculate the future year design value by multiplying the monitor-specific observed design value by the monitor-specific relative reduction factor.
4. If the future year design value is ≤ 84 ppb then the test is passed at that monitor location.

The highest 8 hour daily maximum predicted in the 3x3 (or 7x7 for 4 km modeling) group of cells surrounding and including the cell in which the monitor is located will be used in the attainment test. The attainment test will be applied to all days during the summer of 2005 that meet the meet the inclusion criteria for the relative reduction factor calculation (US EPA, 2007). An episode day must have a peak 8-hr ozone model prediction > 85 ppb at a specific monitor or near the monitor (definition of near mentioned above) to be included in the attainment test. If there are less than 10 days of estimated peak 8-hr ozone at a monitor then the threshold for inclusion to the relative

reduction factor is decreased until the number of days equals 10 or the threshold goes below 70 ppb (US EPA, 2007). If there are less than 4 days in the relative reduction factor calculation then the attainment test is not applied for that monitor.

Unmonitored Area Analysis

An un-monitored area analysis is an additional review to identify areas that might exceed the 8-hr ozone or annual PM2.5 NAAQS if monitors were present (US EPA, 2007). This analysis uses interpolated spatial fields of ambient concentrations and photochemical model estimated concentrations to develop "model adjusted spatial fields of observations" (US EPA, 2007). The model adjusted spatial fields are developed for the base year. Future year concentrations are estimated by applying RRFs to the base year model adjusted spatial field.

8-hr Ozone NAAQS

1. Ambient 8-hr ozone design values are interpolated to create the ambient spatial field. The design values are the 2003-2005 8-hr ozone design values.
2. The ambient spatial field is adjusted using gridded ozone seasonal average base year model output gradients.
3. Gridded RRFs are applied to the adjusted spatial field developed in step 2.
4. If any grid cell exceeds 84 ppb then that grid cell is predicted to exceed the 8-hr ozone NAAQS in the future scenario.

Annual PM2.5 NAAQS

1. Quarterly PM2.5 chemical species are interpolated to create the ambient spatial fields.
2. The ambient spatial field is adjusted using gridded ozone seasonal average base year model output gradients.
3. Quarterly gridded RRFs for each PM2.5 species are applied to the adjusted spatial field developed in step 2.
4. If any grid cell exceeds 15 ug/m3 then that grid cell is predicted to exceed the annual PM2.5 NAAQS in the future scenario.

US EPA intends to provide software that incorporates monitor observation data and CAMx output to generate the gridded future year 8-hr ozone and annual PM2.5 estimates (US EPA, 2007). This software will be used to apply the un-monitored area analysis.

24-hr PM2.5 Standard

Progress in meeting the new 24-hr PM2.5 standard will be assessed by application of the procedures outlined by the U.S. EPA document "Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze" (US EPA, 2007). The major steps of this attainment test are outlined below:

1. Chemically speciated IMPROVE and STN PM2.5 data from 2001-2005 is spatially interpolated to match the grid domain and resolution used for the photochemical modeling. Spatial fields are developed for each PM2.5 chemical species for each season using the SAS statistical software package PROC KRIG function (EPA, 2004b). Rather than interpolating seasonal averages, the top 15% of reconstructed PM2.5 mass samples are used as the basis of the chemically speciated data used for seasonal spatial fields.

2. Estimate the observed 98th percentile value for each year of the 5 year baseline period. Additionally, the next highest concentration in each quarter is identified. This results in data for each year and site which contains one quarter that equals the 98th percentile and 3 quarters which are less than or equal to the 98th percentile.
3. The quarterly maximum daily concentration is multiplied by the fractional composition of PM2.5 species based on the spatial fields.
4. PM2.5 component specific relative reduction factors are estimated at each monitor for each quarter.
5. The component specific RRFs are multiplied by the observed values to estimate future year concentrations.
6. The quarterly components are summed to estimate the quarterly future year 98th percentile value.
7. The 3 consecutive future year 98th percentiles are averaged together to estimate 3 different future year design values. The 3 future year design values are averaged to estimate a single 5-year weighted average 24-hour design value.
8. If this 5 year weighted average 24-hour design value is less than 35 ug/m3 then the test is passed.

The relative reduction factor is only estimated for days with 24-hour average modeled PM2.5 greater than 35 ug/m3. If less than 10 days in a quarter meet this criteria, then the threshold is lowered until the number of days equals 10 or the threshold goes below 20 ug/m3. If there are less than 5 days in the RRF calculation then that quarter is not used for the estimation of the future year design value. If no quarter has more than 5 days included in the RRF calculation then the attainment test is not applied for that monitor.

5.0 Other Issues

Technology Transfer and Modeling Capacity Building

States that are part of the Midwest Regional Planning Organization and cooperating organizations have to opportunity to acquire a turn-key modeling system. This will include all the model inputs, scripts, and support documents to perform model simulations. States participate in an extensive sensitivity projects and preliminary strategy rounds which are designed in part to allow States to develop modeling expertise in-house.

The model input data will be available on an FTP site. The drawback is that transfer times will be long since the files are rather large, but the benefit is that as improvements and updates to input files, model code, and processing utilities become available they will immediately be available to everyone. This approach greatly reduces the resource burden involved with data distribution of media (i.e. hard drives or DLT tapes) via the mail system.

Where very large datasets need to be transferred USB/firewire drives will be sent via the mail system. A general figure where USB drives will be used for transfer instead of FTP would be 50+ gigabytes of data.

States and cooperating organizations will also participate in regular conference calls and face to face meetings to discuss problems, progress, and outline cooperative work objectives.

Ultimately, States that are inclined will be able to use the model inputs developed by the Midwest Regional Planning Organization as the basis for local emphasis modeling projects.

Data Management and Storage

The file storage requirements for annual modeling are large and data backup is an important consideration. Important files including raw emissions and meteorological files will be stored redundantly on multiple hard drives. Additionally, all the model inputs will have a redundant copy at each member State as they will be using them for model simulations as part of the technology transfer and capacity building.

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