APPENDIX H

Modeling Protocol Addendum: Technical Details

Addendum Modeling Protocol: Technical Details

Kirk Baker

October 12, 2006

Lake Michigan Air Directors Consortium
Midwest Regional Planning Organization

Rosemont, Illinois

1. INTRODUCTION

The purpose of this addendum is to provide technical details related to the photochemical transport modeling done to support State Implementation Plans (SIPs) for ozone, particulate matter less than 2.5 microns (PM2.5), and regional haze. This document supplements the June 16, 2004 Modeling Protocol document available at www.ladco.org. 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.

Modeling Platform

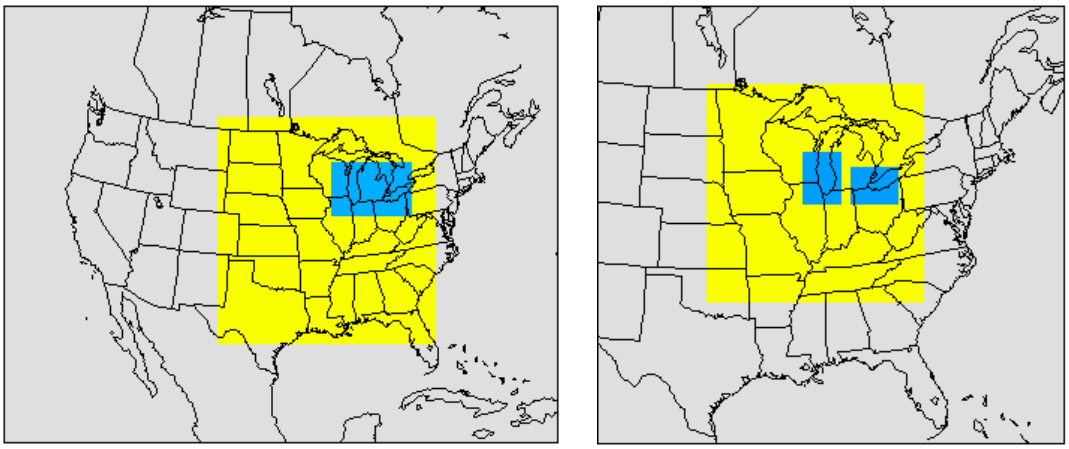
The computing platforms are Intel-based PCs running variations of the Linux operating system. The Portland Group (PGI) Fortran compiler is used to create all executables.

2. METHODOLOGY

Grid Projection and Domains

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.

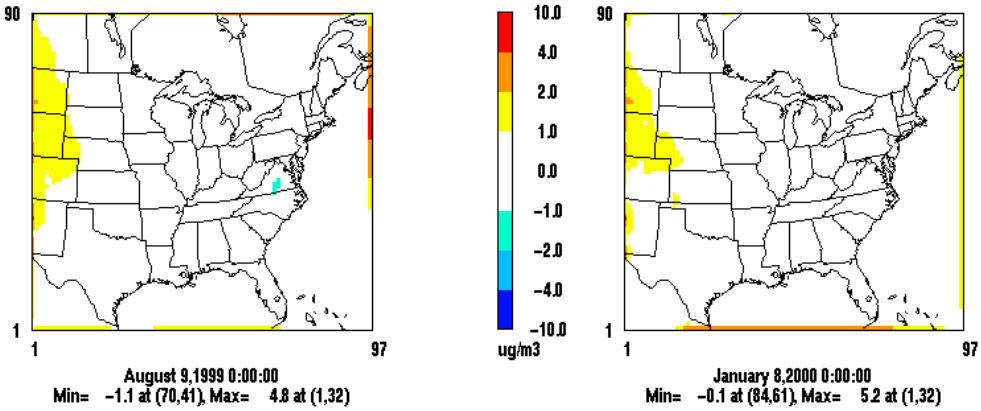
CAMx4 is applied with the vertical atmosphere resolved with 16 layers up to approximately 15 kilometers above ground level.

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 (chimil)	4 km	(680., 176.)	56, 83
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



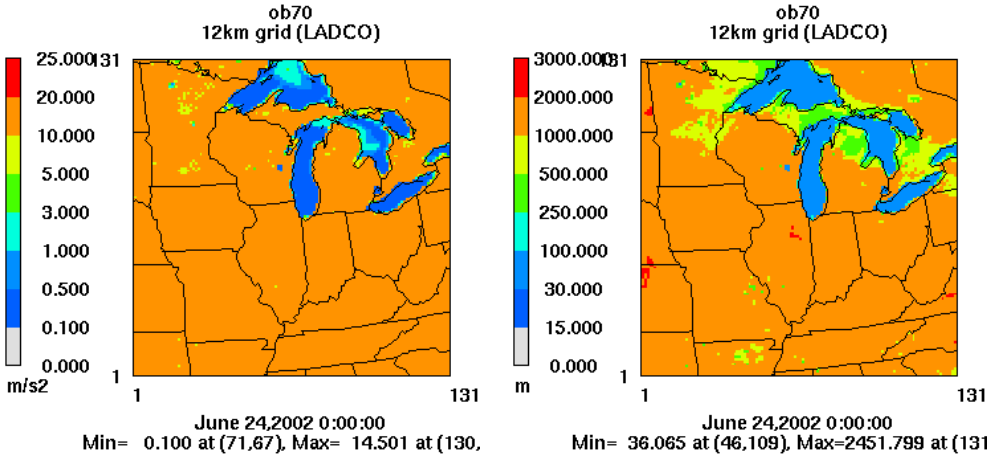
Meteorological Inputs

Meteorological input data for the photochemical modeling runs are processed using the National Center for Atmospheric Research (NCAR) 5th generation Mesoscale Model (MM5) version 3.6.1 (Dudhia, 1993; Grell et al, 1994). 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. These parameters and options are selected as an optimal configuration for the central United States based on multiple MM5 simulations using a variety of physics and configuration options (Johnson, 2003; Baker 2004a).

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

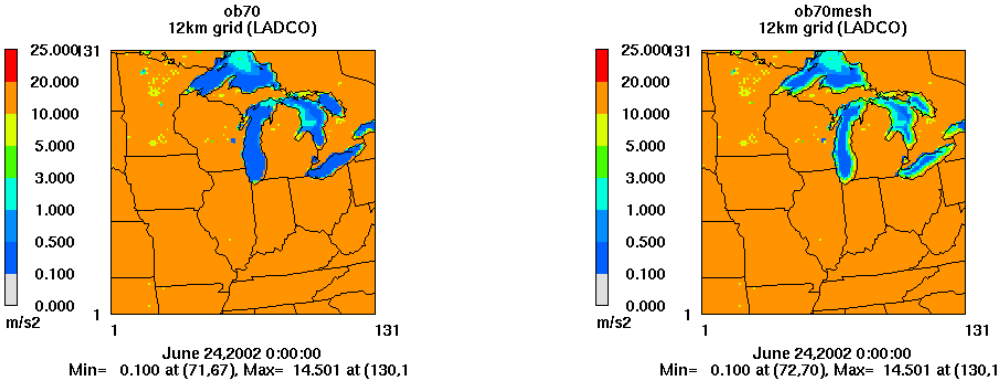
explicitly output by MM5. The MM5CAMx version 4.4 utility is used to translate MM5 output to CAMx input. The vertical diffusivity coefficients are based on the O'Brien 1970 vertical diffusivity algorithm. This scheme takes the PBL height output by MM5 and creates a well-mixed atmosphere inside the PBL. 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). This is done to better represent the greater mechanical mixing overnight in urban areas. An additional adjustment to vertical diffusivity coefficients creates a transitional gradient in values from shore to large water bodies. Figure 2.4 shows maximum vertical diffusivity coefficients and PBL height for a typical model episode day.

Figure 2.4 Peak Kv (m/s^2) values and peak PBL (m) values



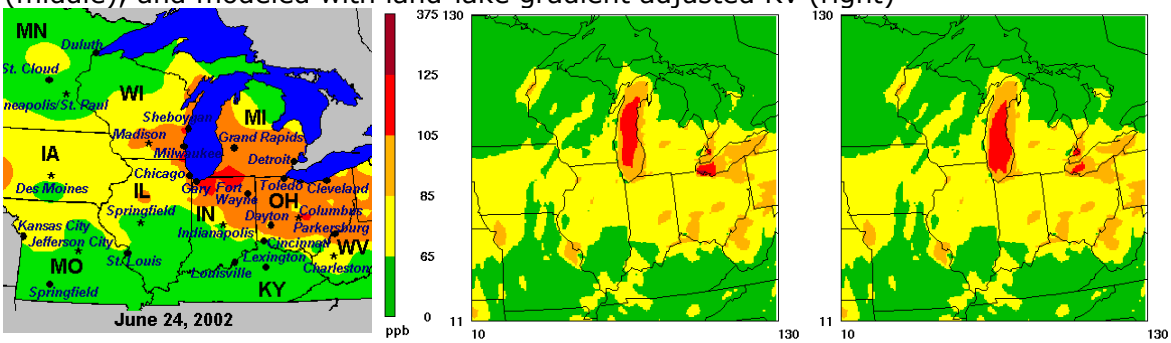
The gradient from land to lake vertical diffusivity coefficients extends over an order of magnitude during mid-day peak photochemical activity. PBL heights at a land cell are typically over 1000 meters and the adjacent cell over one of the Great Lakes is 30 meters. Air over the Great Lakes is typically stable and has low mixing, but the model does not have any transition from land to lake. An adjustment scheme is employed when cells having greater than 75% water have a vertical diffusivity coefficient equal to the average of the 5 x 5 group of cells centered on that particular grid cell.

Figure 2.5. Vertical diffusivity coefficients (m/s^2) using standard MM5 output (left) and land-lake gradient adjustment (right)



The land-lake vertical diffusivity adjustments are shown for an episode day in Figure 2.5. These adjustments result in minimal change to model performance (Figure 2.6) and a reduction in extreme NOX disbenefit response in grid cells near the lake-shore.

Figure 2.6. Peak 8-hr O3 (ppb) observations (left), modeled with standard Kv (middle), and modeled with land-lake gradient adjusted Kv (right)



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 data is processed using EMS-2003. The EMS-2003 model is selected for its ability to efficiently process the large requirements of regional and daily emissions processing. In addition to extensive quality assurance and control capabilities, EMS-2003 also performs basic emissions processes such as chemical speciation, spatial allocation, temporal allocation, and control of area, point, and mobile source emissions (Janssen, 1998; Wilkinson et al, 1994). Outputs from EMS-2003 include a coordinate-based elevated point source file and gridded emissions estimates for low-point, area, mobile, and biogenics sources. Anthropogenic emission estimates are made for a weekday, Saturday, and Sunday for each month. The biogenic emissions are day-specific. Volatile organic compounds are speciated to the Carbon Bond IV (CB4) chemical speciation profile (Carter, 1996).

Table 2.2 CAMx Emissions Species

SPECIE	DESCRIPTION
ALD2	Aldehydes
ETH	Ethylene
FORM	Formaldehyde
ISOP	Isoprene
OLE	Olefins - Anthropogenic
OLE2	Olefins - Biogenic (OVOC)
PAR	Paraffins
TOL	Toluene
XYL	Xylene
NH3	Ammonia
CO	Carbon monoxide
NO2	Nitrogen dioxide
NO	Nitrogen oxide
SULF	Sulfur
SO2	Sulfur dioxide
PEC	Primary PM-fine elemental carbon
PNO3	Primary PM-fine nitrate
POA	Primary PM-fine organic aerosol
PSO4	Primary PM-fine sulfate
CCRS	Primary PM-coarse crustal
FCRS	Primary PM-fine crustal
CPRM	Primary PM-coarse "other"
FPRM	Primary PM-fine "other"

The point and area source inventories are based on the State Consolidated Emissions Reporting Rule (CERR) submittals, other RPOs, and the 2002 National Emission Inventory (EPA, 2005). Continuous emissions monitoring data were used to develop temporal profiles for electrical generating units. These new profiles account for month of year and day of week variations and are unit specific.

On-road emissions are estimated using MOBILE6.2 emission factors and VMT from the 2002 NEI. The MOBILE6 inputs were supplied by the MRPO States, Iowa, and

Minnesota and from the 2002 NEI for all other States. Updated on-road temporal data is based on an analysis of traffic count data in Michigan, Wisconsin, and Minnesota. Default temporal tables are modified to represent a more complex distribution of vehicle miles traveled for the weekend.

Off-road emissions are estimated with the NONROAD2004 and NMIM models using data from the State CERR submittals, EPA's 2002 NEI, and local data for agricultural equipment for the MRPO States plus Iowa and Minnesota. Contractor supplied emissions estimates are used for commercial marine and locomotive non-road categories. NMIM was run with fuel parameter inputs consistent with the on-road emissions modeling. These emissions do not include permeation effects.

Biogenic emissions are estimated with EMS-2003 using the BEIS3 model (Guenther et al, 2000). The BELD3 land use dataset is input to the biogenic model for fractional land-use and vegetative speciation information (US EPA, 2006; Kinnee et al. 1997; Kinnee et al. *in press*). Other inputs to the biogenic emissions model include hourly satellite photosynthetically activated radiation (PAR) and 15 m (above ground level) temperature data output from MM5 (Pinker and Laszlo, 1992).

Ammonia emissions are based on the July 2004 version (v3.6) of Carnegie Mellon University's (CMU) ammonia model using 2002 census of agriculture data (Strader et al. 2005; Pinder et al., 2004; Goebes et al., 2003). CMU ammonia emissions estimates are not used from the following categories: humans, dogs, cats, and deer. These omissions are based on the low likelihood that ammonia emissions from these sources would make it out of domestic dwellings in the case of humans, cats, and dogs and forested areas in the case of deer. Ammonia emissions are removed from other RPO's point source inventory to eliminate double-counting confined animal operations with CMU model estimates. Updated monthly and diurnal profiles were developed using the new process based ammonia model. The new profile represents beef, hogs, and dairy. Hog farms are assumed to represent poultry since the new process based ammonia model did not have a fully functional poultry housing model.

Currently, there are no anthropogenic Mexican emissions in the emissions input files. Canadian emissions are based on a 2000 inventory made available by Environment Canada to the Environmental Protection Agency.

The speciation profiles used by EMS are obtained from the latest version of EPA's SPECIATE database. MRPO contracted improved speciation profiles for certain emission categories. Details of this project are available in "Improving Modeling Inventory Data: Speciation Profiles – February 17, 2005" and available by request.

The development of the future year and even the base year emissions are continually being updated. The best place to find the most recent explanation of the base and future year scenarios is at the LADCO website (LADCO, 2006).

Landuse

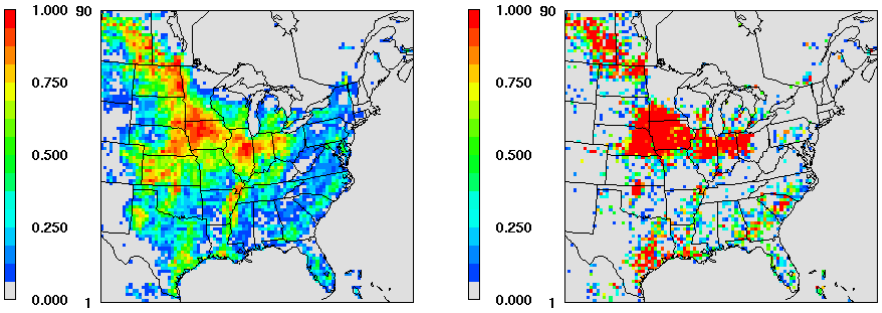
The photochemical model uses 11 land use categories to describe the surface. The land use file is based on BELD3 1 km data (US EPA, 2006; Kinnee et al. 1997; Kinnee et al. *in press*). The 1 km data was aggregated to the appropriate grid resolution for photochemical modeling. Surface roughness varies by season and land use category and are taken from EPA's AERMET User's Guide (EPA, 2004; ENVIRON, 2005).

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

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, 2005).

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, 2005).

Photolysis Rates

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, 2005; 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

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

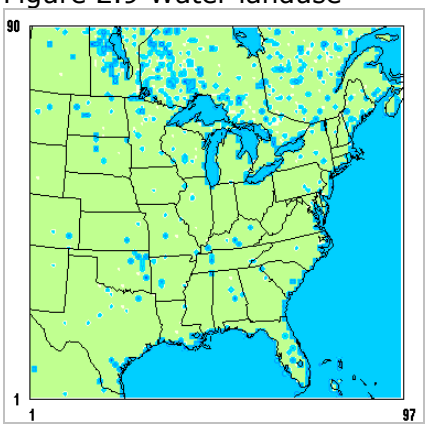
transport model (Jacob et al, 2005; Bey et al, 2001). Boundary conditions vary by month and in the horizontal and vertical direction. Where an initial or boundary concentration is not specified for a pollutant the model will default to a near-zero concentration.

Quality Assurance of Model Inputs

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 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 4.30 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 an updated carbon-bond IV (CB4) gas phase chemistry module (ENVIRON, 2005; Nenes et al, 1998; Carter, 1996). CAMx4 is applied using the PPM horizontal transport scheme and an implicit vertical transport scheme with the fast CMC chemistry solver (ENVIRON, 2005).

The photochemical model is initiated at midnight Eastern Standard Time and run for 24 hours for each episode day. The summer 2002 simulation is initiated on June 2 and run through August 31. The annual simulation is run separately by calendar quarter and is initiated 2 weeks prior to each quarter: December 17, 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 and 2-way nested grids over the lower portion of Lake Michigan and over the Detroit-Toledo-Cleveland region.

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.

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.

Gas Phase Chemistry

CB4 was originally developed for application to high NOx conditions, such as those that exist in urban areas (Tonnesen et al, 2001). RADM and SAPRC were developed specifically for low NOx conditions, such as those that exist in rural areas. The United States Environmental Protection Agency ran CMAQ with CB4 and RADM gas-phase chemistry and found the ozone predictions to be very comparable. However, the run times associated with RADM were twice as long as those with CB4 (Timin, 2002). SAPRC chemistry also typically has run times much longer than CB4, usually at least twice as long.

Starting in version 4.20, CAMx4 contains 17 new inorganic reactions that improve the science in the model without being inconsistent with the evaluation of CB4 against smog chamber data. The new reactions have little impact on predicted PM2.5, but increase ozone concentrations regionally. This regional increase in ozone

improves model performance in the Midwest United States and is due to reactions that recycle NOX. These reactions include the photolysis of organic nitrates and nitric acid and are included in other mechanisms including SAPRC99 and CBM-Z (ENVIRON, 2005; Carter, 2000; Zaveri and Peters, 1999).

Deposition

Deposition processes are an important factor in pollution and visibility estimation. Wet and dry removal play an even more important role in regional modeling as the spatial and temporal scope of application increase. The wet deposition routine in CAMx4 has been upgraded to improve cloud and rainfall estimation (Kemball-Cook et al, 2004). The dry deposition routine is based on the equations developed by Wesley (ENVIRON, 2005; Wesley, 1989). The dry deposition equation is modified to adjust for special properties of certain chemical species such as nitric acid (very sticky) and ammonia (very reactive, fairly sticky, and shows a high degree of near-field deposition).

The ammonia RSCALE factor in the chemistry parameters input file to CAMx4 is set to 0.0, which is the same as nitric acid to account for the chemical characteristics of ammonia and physical processes (near-field deposition) not in the deposition model. A field study at a Colorado alpine tundra location showed that ammonia and nitric acid deposition velocities were very similar: both 1.3 ± 0.6 cm/s (Rattray et al., 2001). The photochemical landuse model annual mean ammonia deposition velocity for all sites is 3.0 cm/s and the annual mean estimated nitric acid deposition velocity is 2.5 cm/s. The modeled ammonia and nitric acid deposition velocities agree within the uncertainty provided for in the Colorado alpine tundra field study.

Nesting

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

Several modeling applications have shown minimal benefit to PM2.5 model performance from the inclusion of a nested 12 km grid (Baker, 2004c; Morris, Koo et al, 2004). The EPA modeling guidance recommends that modeling to support the annual PM2.5 NAAQS be applied at a 12 km horizontal grid resolution so that grid resolution will be used to support the SIP. A 2-way nested 4 km grid will be applied over the lower portion of Lake Michigan and over the Cleveland-Toledo-Detroit area to better resolve the complex interaction between high density urban emissions and land-Lake meteorology.

Plume-in-Grid

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 2002 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.

Probing Tools (Source Apportionment)

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 annual modeling simulations. Zeroing out emissions for large regions such as entire States fundamentally changes the atmospheric chemistry and makes interpretation of the results difficult.

Particulate Source Apportionment Technology (PSAT) will be applied with CAMx4. The model will be run separately to track source region and emissions group contributions to the following: PM2.5 sulfate, PM2.5 nitrate, PM2.5 ammonium, and PM2.5 primary emissions (PEC, POA, FCRS, FPRM, CCRS, CPRM).

CAMx4 contains a variety of ozone source apportionment tools, which includes the standard ozone source apportionment tool (OSAT). The anthropogenic pre-cursor culpability assessment (APCA) tool assesses regional and emission sector contribution to ozone formation and provides information that is most policy relevant. The APCA tool is chosen over the other options, including the standard OSAT option.

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 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. There is a similar situation with biogenic NOx + anthropogenic VOC but this rarely happens in the eastern United States (ENVIRON, 2005).

Probing Tools (Other)

Currently, none of the PM models include process analysis for inorganic, secondary organic aerosol, or aqueous phase chemistry. A limited amount of information regarding nitric acid formation is available as process analysis implementation is

limited to gas phase chemistry reactions. Process analysis will not be emphasized until further development makes it useful beyond gas phase chemistry.

3. Model Performance Evaluation

An evaluation of model performance should be considered for modeling to be used in support of an attainment demonstration. Model performance evaluation is typically categorized into 4 separate categories: operational, diagnostic, mechanistic, and probabilistic (Seigneur et al., 2000, Tonnesson et al., 2001).

Operational evaluation describes the model's skill in estimating chemically speciated particulate matter in the fine and coarse mode. The diagnostic evaluation is more rigorous and tests the model's skill in estimating PM precursors, associated oxidants, deposition, temporal variation, and spatial variation. Mechanistic evaluation examines the skill of the model in making appropriate responses of PM concentrations to changes in emissions and meteorology. Probabilistic evaluation includes the examination of uncertainties in both model predictions and ambient measurements of PM2.5 and visibility (Tonnessen et al., 2001). A probabilistic evaluation is out of the scope of the current modeling effort. Information available regarding uncertainties in the measurement of the chemically speciated PM will be used in assessing the reasonableness of model estimates.

Operational and diagnostic evaluation will be done by comparing model predictions to ambient measurements of chemically speciated PM2.5 and precursor species including SO2, NOx, and ammonia. Additionally, species that participate in reactions that form particulate matter such as ozone and nitric acid will also be used for performance evaluation. Operational evaluation for ozone modeling purposes will include evaluating model estimates against observation data including ozone, nitrogen species, and total VOC.

A rigorous mechanistic evaluation would entail modeling a historic episode and comparing that to a current episode with similar meteorology. An evaluation of ozone performance for an episode in 2002 and an episode in 1991 could potentially help determine the appropriateness of ozone response to emissions changes. This type of evaluation is problematic for PM2.5 since very little historical chemically speciated PM2.5 data exists. Other serious problems with this type of evaluation include differences in emission inventory compilation and differences in the meteorological analysis data used as input to MM5. Analysis of the model's skill in estimating speciated PM in different seasons and for weekends and weekdays is another way to assess whether the model accurately responds to different emissions and meteorology (US EPA, 2006c).

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, 2006c). 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)

Initial model performance evaluation plots and metrics will be based on matching predictions and observations in time and space. Alternatively, the closest prediction in the 5 x 5 grid of cells around the monitor location will be compared to the observation value to assess model performance "near" the monitor. 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.

Model performance evaluation methodology for PM2.5 and Regional Haze is described in the EPA document "Guidance for Demonstrating Attainment of Air Quality Goals for PM2.5 and Regional Haze" (US EPA, 2006C). The guidelines describing good model performance for chemically speciated PM2.5 are based on a

few early modeling applications that were limited in domain and episode length. For these reasons, the suggested guidelines for model performance to support regulatory applications are not included in this document. The newer 8-hr ozone modeling guidance recommends against using any bright-line evaluation of performance metrics to determine whether the modeling is satisfactory (US EPA, 2005).

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 (EPA, 2006C). 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 Steering Committee, 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, 2006C). The bias and error metrics are used to describe performance in terms of the measured concentration units ($\mu g/m^3$). 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, 2005).

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, 2005). 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 anions (NO3-, Cl-, SO4=) and cations (Ca2+, Mg2+, K+, Na+, NH4+, H+). 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; EPA 2006c). 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.

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

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 "Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze" (EPA, 2006).

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 (2002) 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 document "Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze" (EPA, 2006c; EPA, 2004b). The major steps of this attainment test are outlined below:

1. Chemically speciated IMPROVE and STN PM2.5 data from 2000-2004 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, 2004c).

2. The estimated fractional composition of each species by quarter is multiplied by the 5 year weighted average 2000-2004 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" (EPA, 2006c; EPA, 2005). 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: 2000-2002, 2001-2003, and 2002-2004.
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 2002 that meet the meet the inclusion criteria for the relative reduction factor calculation (EPA, 2005). 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, 2005). 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, 2006c). This analysis uses interpolated spatial fields of ambient concentrations and photochemical model estimated concentrations to develop "model adjusted spatial fields of observations" (US EPA, 2006b). 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 average of the 2000-2002, 2001-2003, and 2002-2004 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, 2006b). 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" (EPA, 2006c). The major steps of this attainment test are outlined below:

1. Chemically speciated IMPROVE and STN PM2.5 data from 2000-2004 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, 2004c). 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

Resource Requirements

Photochemical models have different resource requirements: disk space for inputs and outputs, model run times, and staff time required for application.

The staff time required for CAMx model input set-up and post processing is minimal compared to other photochemical models due to the simple binary file formats, the lack of 3rd party software required for model application and intermediate processing utilities, and the availability of useful and simple pre-processors from the model developers.

The amount of time required to run our annual 36 km simulation is approximately 5 days. The approach is to run 4 seasons concurrently on 4 separate 2.0 GHz processors. A summer season 36/12 km 2-way nested simulation for ozone chemistry only takes about 6-7 days to complete using a single processor.

The input and output disk requirements for an annual simulation are 195 and 54 gigabytes respectively. So an annual simulation for the Eastern and Central United States at 36 km would total 250 gigabytes. Most of this space is taken up by emission inputs (low level and elevated point emissions). Since these files need to be modified for strategy runs, a significant amount of extra disk space should be allocated to store extra emission input files.

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.

6. References

Baker, K. Meteorological Modeling Protocol For Application to PM2.5/Haze/Ozone Modeling Projects, 2004a. http://www.ladco.org/tech/photo/photochemical.html

Baker, K. Processing and Quality Assurance of Emissions Files for Photochemical Model Input, 2004b. http://www.ladco.org/tech/photo/photochemical.html

Baker, K. Fine Grid v. Coarse Grid results, presented at the National Regional Planning Organization Modeling Meeting, Denver, CO, 2004c.

Baker, K. Application of Multiple One-Atmosphere Air Quality Models Emphasizing PM2.5 Performance Evaluation, presented at the Air & Waste Management Association 2004 Annual Meeting, Indianapolis, IN, 2004d. http://www.ladco.org/tech/photo/photochemical.html

Bey, I.; Jacob, D; Yantosca, R.; Logan, J.; Field, B.; Fiore, A.;Li, Q.; Liu, H.; Mickley, L.; Schultz, M. Global modeling of tropospheric chemistry with assimilated meteorology: Model description and evaluation, J. Geophys. Res., 106, 23,073-23,096, 2001.

Carter, W.P.L. (1996) Condensed Atmospheric Photooxidation Mechanisms for Isoprene. Atmos. Environ., 30, 4275-4290.

Carter, W.P.L. 2000. Programs and Files Implementing the SAPRC-99 Mechanism and its Associates Emissions Processing Procedures for Models-3 and Other Regional Models. January 31, 2000. http://pah.cert.ucr.edu/~carter/SAPRC99.htm

Chen, K. S., Y. T. Ho, C. H. Lai and Y.-M. Chou (2003) Photochemical modeling and analysis of meteorological parameters during ozone episodes in Kaohsiung, Taiwan, Atmospheric Environment, 37(13), 1811-1823.

Claeys, M.; Graham, B.; Vas, G.; Wang, W.; Vermeylen, R.; Pashynska, V.; Cafmeyer, J.; Guyon, P.; Andreae, M.O.; Artaxo, P.; Maenhaut, W. Formation of Secondary Organic Aerosols Through Photooxidation of Isoprene. Science, 303, 1173-1176, 2004a.

Dudhia, J. A nonhydrostatic version of the Penn State/NCAR mesoscale model: Validation tests and simulation of an Atlantic cyclone and cold front, Mon. Wea. Rev., 121, 1493-1513, 1993.

ENVIRON International Corporation. 2005. User's Guide Comprehensive Air Quality Model with Extensions (CAMx4) Version 4.20. ENVIRON International Corporation, Novato, California. www.camx.com

FLAG. 2000. Federal Land Manager's Air Quality Related Values Workgroup (FLAG) Phase I Report. http://www2.nature.nps.gov/ard/flagfiee/AL.doc

Gery, M.W.; Whitten, G.Z.; Killus, J.P.; Dodge, M.C. A photochemical kinetics mechanism for urban and regional scale computer modeling. Journal of Geophysical Research, 1989, 94, 12925–12956.

Grell, G. A.; Dudhia, J.; Stauffer, D. A description of the Fifth Generation Penn State/NCAR Mesoscale Model (MM5), NCAR Tech. Note, NCAR TN-398-STR, 138 pp., 1994.

Goebes MD, Strader R, Davidson CI. 2003. An ammonia emission inventory for fertilizer application in the United States. Atmospheric Environment 37, 2539-2550

Guenther A., C. Geron, T. Pierce, B. Lamb, P. Harley, and R. Fall (2000) Natural emissions of non-methane volatile organic compounds; carbon monoxide, and oxides of nitrogen from North America, Atmos. Environ., 34: 2205-2230.

Hogrefe, C., G. Sistla, E. Zalewsky, W. Hao, and J.-Y. Ku (2003) An assessment of the emissions inventory processing systems EMS-2001 and SMOKE in grid-based air quality models, J. Air & Waste Management Assoc., 53(9): 1121-1129.

IMPROVE Steering Committee. Revised IMPROVE Algorithm for Estimating Light Extinction from Particle Speciation Data. http://vista.cira.colostate.edu/improve/Publications/GrayLit/gray_literature.htm Accessed August 22, 2006.

Kinnee, E., C. Geron, and T. Pierce (2004) Development of a 1-km resolved vegetation database for surface exchange modeling in North America, Ecological Applications, in press.

Kinnee, E., C. Geron, and T. Pierce (1997) United States land use inventory for estimating biogenic ozone precursor emissions. Ecological Applications, 7(1), 46-58.

Jang, M.; Czoschke, N.M.; Lee, S.; Kamens, R.M. Heterogeneous atmospheric aerosol production by acid-catalyzed particle-phase reactions. Science, 298, 814-817, 2002.

Jacob, D.; Park, R.; Logan, J., Documentation and Evaluation Of The Geos-Chem Simulation for 2002 Provided to the Vistas Group. June 24, 2005. djacob@fas.harvard.edu.

Janssen, M.; Hua., C. Emissions Modeling System-95 User's Guide. 1998. http://www.ladco.org/emis/guide/ems95.html

Johnson, M. Meteorological Modeling Protocol: IDNR 2002 Annual MM5 Application, 2003.

Kalberer, M.; Paulsen, D.; Sax, M.; Steinbacher, M.; Dommen, J.; Prevot, A.; Fisseha, R.; Weingartner, E.; Frankevich, V.; Zenobi, R.; Baltensperger, U. Identification of Polymers as Major Components of Atmospheric Organic Aerosols. Science, 303, 1659-1662, 2004.

Kemball-Cook, S., Emery, C, Yarwood, G, Working Draft Report: Improvements to the MM5-CAMx Interface for Wet Deposition and Performance Evaluation for 2002 Annual Simulations, 2004.

LADCO. http://www.ladco.org/tech/photo/photochemical.html (Protocols/Documents section) and http://www.ladco.org/mrpo.html (Emissions section of RPO Projects) Accessed August 22, 2006.

NCAR. National Center for Atmospheric Research. http://cprm.acd.ucar.edu/Models/TUV/ Accessed February 26, 2006.

NASA. Goddard Space Flight Center. http://jwocky.gsfc.nasa.gov/ (accessed January 23, 2006).

National Weather Service. Climate Prediction Center. See http://www.cpc.ncep.noaa.gov/products/analysis_monitoring/cdus/palmer_drought/wpdanote.shtml (accessed October 1, 2005)

Nenes A, Pandis SN, Pilinis C. 1998. ISORROPIA: A new thermodynamic equilibrium model for multiphase multicomponent inorganic aerosols. Aquat.Geoch. 4: 123-152.

Morris, R.E., G. Mansell, and E. Tai. (2004) Air Quality Modeling Analysis for the Denver Early Action Ozone Compact. Prepared for Denver Regional Air Quality Council, Denver, CO.

Morris, R., Koo, B., Lau, S., McNalley, D., Tesche, T., Tonnesen, G., Wang, Z., Chien, C. Initial Phase II 2002 CMAQ Operational Model Performance Evaluation. Presented at the VISTAS TAWG Meeting, September 2004. http://pah.cert.ucr.edu/vistas/vistas2/docs.shtml

Nobel, C. E., E. C. McDonald-Buller, Y. Kimura, K .E. Lumbley, and D. T. Allen (2002) Influence of Population Density and Temporal Variations in Emissions on the Air Quality Benefits of NOx Emission Trading, Environmental Science & Technology, 36, 3465-3473.

Pinder RW, Strader R, Davidson CI, Adams PJ. 2004. A temporally and spatially resolved ammonia emission inventory for dairy cows in the United States. Atmospheric Environment 38, 3747-3756.

Pinker, R.T. and I. Laszlo (1992) Modeling surface solar irradiance for satellite applications on a global scale. J. Appl. Meteor., 31, 194-211.

Rattray, G., Sievering, H.: Dry deposition of ammonia, nitric acid, ammonium, and nitrate to alpine tundra at Niwot Ridge, Colorado. Atmospheric Environment. 35; 1105-1109: 2001.

Seigneur, C.; Pun B.; Pai, P.; Louis, J.; Solomon, P.; Emery, C.; Morris, R.; Zahniser, M.; Worsnop, D.; Koutrakis, P.; White, W.; Tombach, I. 2000. Guidance for the performance evaluation of three-dimensional air quality modeling systems for particulate matter and visibility, J. Air Waste Manage. Assoc., 50, 588-599.

Seinfeld, J.H.; Gao, S.; Ng, S.; Kroll, J.; Surratt, J.; Erdakos, G.; Pankow, J.F.; Flagan, R.C.; Knipping, E.M.; Edgerton E. Secondary Organic Aerosol: Recent Results. 23rd Annual Conference of the American Association for Aerosol Research. Atlanta, GA, October, 2004.

Strader, R, Peckney, NJ, Pinder, RW, Adams, PJ, Goebes, M, Ayers, J, Davidson, CI. 2005. The CMU Ammonia Emission Inventory. Available at http://www.cmu.edu/ammonia

Tanaka, P. L., D. T. Allen, E. C. McDonald-Buller, S. Chang, Y. Kimura, C. B. Mullins, G. Yarwood, and J. D. Neece (2003) Development of a chlorine mechanism for use in the CAMx regional photochemical model, J. Geophys. Res., 108(D4), 4145.

Timin, B., Jang, C., Dolwick, P., Possiel, N., Braverman, T., 2002. Operational Evaluation and Comparison of CMAQ and REMSAD- An Annual Simulation. 1st Annual CMAS Conference, Research Triangle Park, NC.

Tombach, I.; Seigneur, C. 1999. Review of the EPA Draft Document "Guidance For Demonstrating Attainment of Air Quality Goals for PM2.5 and Regional Haze".

Tonnesen, G.; Wang, Z.; Lents. J.; Gemmill, D.; Morris, R. Modeling Protocol and Quality Assurance Plan for the WRAP Visibility Modeling Project, 2001.

Turpin, B.J., and Lim, H.-J., 2001: Contributions to PM2.5 mass concentrations: revisiting common assumptions for estimating organic mass. Aerosol. Sci. Technol., 35, 602-610.

Wilkinson, J.; Loomis, C.; Emigh, R.; McNalley, D.; Tesche, T., 1994. Technical Formulation Document: SARMAP/LMOS Emissions Modeling System (EMS-95). Final Report prepared for Lake Michigan Air Directors Consortium (Des Plaines, IL) and Valley Air Pollution Study Agency (Sacramento, CA).

U. S. Environmental Protection Agency, Appendix E: Speciated Modeled Attainment Test Documentation; Guidance for Demonstrating Attainment of Air Quality Goals for PM2.5 and Regional Haze, 2002.

U. S. Environmental Protection Agency, Guidance for Tracking Progress Under the Regional Haze Rule, EPA-454/B-03-004, Office of Air Quality Planning and Standards, Research Triangle Park, NC, 2003a.

U. S. Environmental Protection Agency, Guidance for Estimating Natural Visibility Conditions Under the Regional Haze Program, EPA-454/B-03-005, Office of Air Quality Planning and Standards, Research Triangle Park, NC, 2003b.

U.S. Environmental Protection Agency, User's Guide for the AERMOD Meteorological Preprocessor (AERMET), EPA-454/B-03-002, Office of Air Quality Planning and Standards, Research Triangle Park, NC, 2004.

U. S. Environmental Protection Agency, Procedures for Estimating Future PM2.5 Values for the CAIR Final Rule by Application of the (Revised) Speciated Modeled Attainment Test (SMAT). November 8, 2004 (2004b).

U. S. Environmental Protection Agency, Developing Spatially Interpolated Surfaces and Estimating Uncertainty, EPA-454/R-04-004, Office of Air and Radiation, Office of Air Quality Planning and Standards, Research Triangle Park, NC, 2004 (2004c).

U. S. Environmental Protection Agency, Guidance on the Use of Models and Other Analyses in Attainment Demonstrations for the 8-hour Ozone NAAQS, EPA-454/R-05-002, Office of Air Quality Planning and Standards, Research Triangle Park, NC, 2005.

U. S. Environmental Protection Agency. See http://www.epa.gov/ttn/chief/net/2002inventory.html (accessed March 2, 2006).

U. S. Environmental Protection Agency. See http://www.epa.gov/ttn/chief/emch/biogenic/ (accessed August 9, 2006).

U. S. Environmental Protection Agency, Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze, Draft 3.2. September 2006 (2006c).

van Loon, G.; Duffy, S. Environmental Chemistry: A Global Perspective; Oxford University Press, 2000.

Wesely, M.L. 1989. Parameterization of Surface Resistances to Gaseous Dry Deposition in Regional-Scale Numerical Models. *Atmos. Environ.*, **23**, 1293-1304.

Zaveri, R.A. and L. K Peters. 1999. A new lumped structure photochemical mechanism for large-scale applications. *J. Geophys. Res.*, **104**, 30: 387-30,415.