

1. INTRODUCTION

The purpose of this document is to provide technical details relating to photochemical modeling done to support State Implementation Plans for ozone, PM_{2.5}, 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, PM_{2.5}, and regional haze in the Upper Midwest are available on the organization website: www.ladco.org.

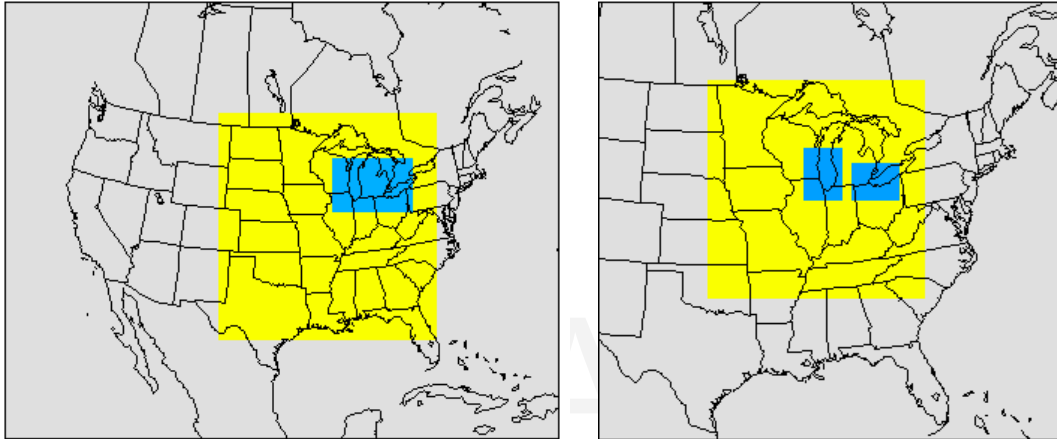
The computing platforms are Intel-based PCs running variations of the Linux operating system. The Portland Group (PGI) Fortran compiler is used to create all executables.

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)



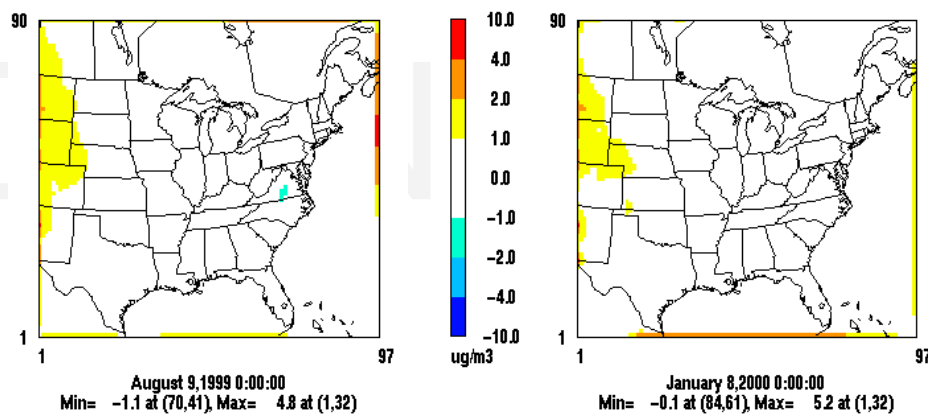
The 36 km meteorological modeling domain covers the entire continental United States (Figure 2.1; Table 2.1). The 12 km meteorological domain covers most of the central and eastern United States and the 4 km domain covers the lower portion of the Great Lakes. CAMx4 is applied with the vertical atmosphere 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 (chimil)	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 PM_{2.5} 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 PM_{2.5} 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 PM_{2.5} 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, 2007). 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 m²/s. A landuse-weighted vertical diffusivity coefficient (maximum of 1.0 m²/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
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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, 2007). 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)

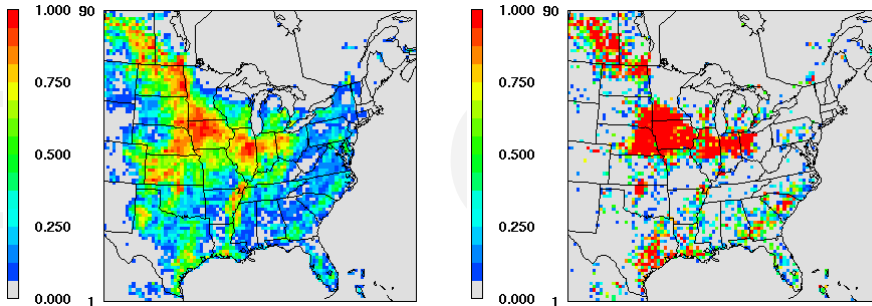
The photochemical model uses 11 land use categories to describe the surface. The land use file is based on BELD3 1 km data (US EPA, 2006; Kinnee et al. 1997; Kinnee et al. *in press*). The 1 km data was aggregated to the appropriate grid resolution for photochemical modeling. Surface roughness varies 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 $\mu\text{g}/\text{m}^3$. 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 protocol)

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 PM_{2.5} sulfate ion, nitrate ion, and ammonium ion contributions from initial concentrations fall below 0.05 $\mu\text{g}/\text{m}^3$ by the seventh day of the episode. PM_{2.5} elemental carbon, PM_{2.5} 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.

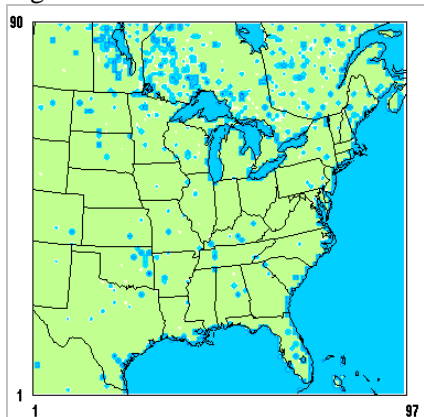
The initial and boundary conditions are based on monthly averaged species output from an annual (calendar year 2002) application of the GEOS-CHEM global chemical transport model (Jacob et al, 2005; Bey et al, 2001). Boundary conditions vary by month and in the horizontal and vertical direction. Where 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 (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, 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

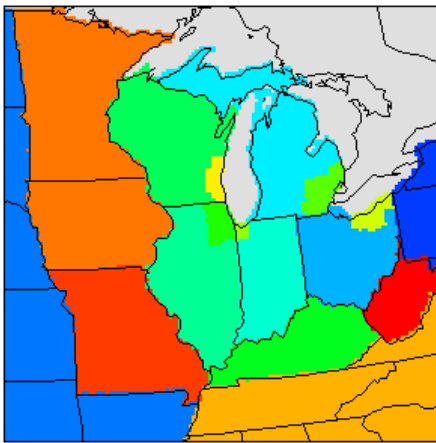
CAMx is a state of the science photochemical model that contains a variety of ozone source apportionment tools, including the original ozone source apportionment tool (OSAT) and the anthropogenic pre-cursor culpability assessment (APCA) tool. The APCA tool assesses regional and emission sector contribution to ozone formation and provides information that is most policy relevant. When ozone is formed under VOC limited conditions due to biogenic VOC + anthropogenic NO_x then OSAT attributes it to the biogenic VOC sources. When ozone is formed under NO_x-limited conditions due to biogenic VOC + anthropogenic NO_x then OSAT attributes it to the anthropogenic NO_x 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 NO_x. In the case where ozone formed to biogenic VOC + anthropogenic NO_x under VOC-limited conditions, OSAT attributes it to biogenic VOC, but APCA redirects the attribution to anthropogenic NO_x. In NO_x-limited conditions both OSAT and APCA attribute the ozone to anthropogenic NO_x.¹ 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, 2006). The geographic regions tracked for ozone contribution are listed in Table 2 and shown graphically in Figure 2 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. 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. 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 1 and shown graphically in Figure 1. The contribution from the lateral and top boundaries of the model is also tracked for each receptor location.

Figure 1. Model domain and source regions tracked with PSAT

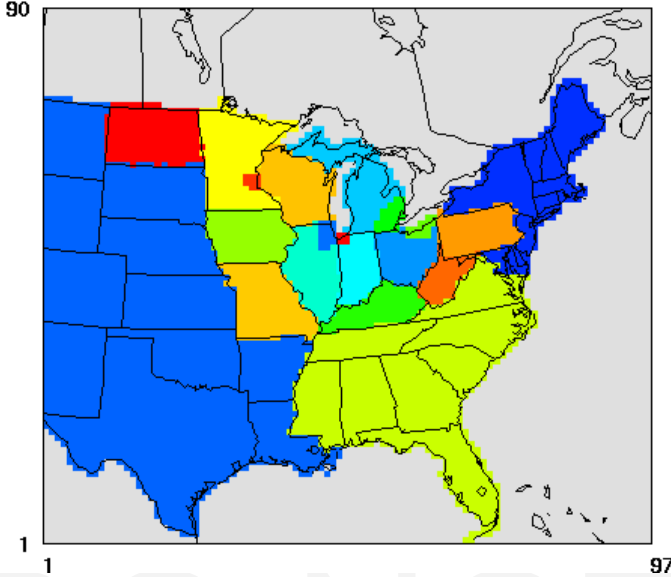


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Canada	Illinois Chicago non-attainment (NA) Counties
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Central/Western States (CENRAP+ WRAP)	Indiana Chicago NA Counties
Ohio	Cleveland NA Counties
Michigan	Milwaukee NA Counties
Indiana	Southeast 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.

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