Source Apportionment Results for PM2.5 and Regional Haze at Receptors in the Great Lakes Region

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ABSTRACT

Photochemical model source apportionment probing tools are valuable from a scientific and regulatory perspective for tracking source contribution to particulate matter. The use of source apportionment is more desirable than the "zero-out" approach to determine geographic and emissions sector culpability. Zeroing out emissions for large regions such as entire States fundamentally changes the atmospheric chemistry. Source apportionment of 24-hr and annual PM2.5 concentrations at important monitor locations is useful for regulators in developing effective emissions control scenarios for the PM2.5 NAAQS. Contribution to regional haze on the 20% worst and 20% best days at Class I areas provides direction to regulators for emissions control scenarios to meet the uniform rate of progress as detailed in the Regional Haze rule.

The Comprehensive Air-Quality Model with extensions is a state of the science photochemical model containing particulate source apportionment tools. Contributions are tracked for 21 geographic regions and 6 emissions sector categories: EGUs, non-EGU point, on-road, off-road, area, and agricultural ammonia. Projected emissions for 2018 are used for this application to present a better understanding of what is contributing to PM2.5 concentrations when certain emissions controls and sector growth is taken into consideration. Results are given for receptors in counties near the Great Lakes that may not meet the annual or 24-hr PM2.5 NAAQS by 2018 and Class I areas in the region.

The contributions to annual and high daily PM2.5 at the urban receptors is dominated by stationary point sources and other area sources. Stationary point source emissions dominate the contribution to visibility on the 20% worst days followed by contributions from other area sources and agricultural ammonia and boundary conditions dominate visibility on the 20% best days. Initial conditions contribute less than 0.5 $\mu g/m^3$ to every grid cell in the domain by the 9^{th} day of each quarter.

INTRODUCTION

Source apportionment is a valuable scientific and regulatory tool to understand emissions contributions to estimate particulate matter. 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.

CAMx is a state of the science photochemical model that contains an extension that tracks contributions to estimated particulate matter. 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 (SOA) contributions from biogenic and anthropogenic sources are part of the standard CAMx output and included in the analysis. Geographic contribution to controllable (anthropogenic) SOA is not tracked since estimated anthropogenic SOA is very small and tracking geographic contributions to SOA is resource intensive.

Contributions are tracked using the PSAT source apportionment tool for 21 geographic regions and 6 emissions sector categories: electrical generating units (EGUs), non-electrical generating units (non-EGUs), on-road mobile, off-road mobile, area, and agricultural ammonia. A scenario representing emissions in 2018 is used for the source apportionment application to present a better understanding of contributions when certain emission controls and sector growth is taken into consideration. Contribution is shown for monitor locations in the Great Lakes region that may not show attainment of the annual or 24-hr PM2.5 standard in 2018 and at Class I areas in the region including Voyageurs and Boundary Waters in Minnesota and Isle Royale and Seney in Michigan.

Source apportionment results will be estimated on an annual average basis and on a daily basis to be relevant to the annual and 24-hr PM2.5 NAAQS. Days with 24-hr averaged model estimated PM2.5 greater than 30 $\mu g/m^3$ are averaged together to represent higher concentration days that would be more relevant to the daily average PM2.5 NAAQS. The 24-hr average source apportionment results for the 20% worst and 20% best observed days at the Class I area receptors will be converted to light extinction using the latest IMPROVE Steering Committee recommended equation then averaged together to estimate contribution to the 20% worst and 20% best days (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.

METHODS

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; Chen et al. 2003; Morris, Mansell, Tai, 2004). The model is applied with ISORROPIA inorganic chemistry (Nenes et al, 1998),

SOAP organic chemistry, regional acid deposition model (RADM) aqueous phase chemistry, and the carbon-bond 2005 (CB05) gas phase chemistry module (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, which includes additional PM2.5 secondary organic aerosol formation (ENVIRON, 2007). An updated dry deposition scheme that is based on AERMOD is chosen for these simulations. This scheme uses gridded monthly leaf area index to adjust dry deposition velocities (Kemball-Cook et al, 2007). The photochemical model is initiated at midnight Eastern Standard Time and run for 24 hours for each episode day. The annual 2005 simulation is run separately by calendar quarter and is initiated 2 weeks prior to each quarter: December 17 (2004), March 15, June 15, and September 15.

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. 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 (Bey et al, 2001; Jacob et al, 2005). 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.

Meteorological input data for the photochemical modeling runs are processed using the National Center for Atmospheric Research (NCAR) 5th generation Mesoscale Model (MM5) version 3.6.3 (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).

Emissions developed for the 2018 future year inventory 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 the annual simulation. 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. The Model of Emissions of Gases and Aerosols from Nature (MEGAN) has been implemented into the CONsolidated Community Emissions Processing Tool (CONCEPT) emissions modeling framework (Wilkinson, 2006; Guenther and Wiedinmyer, 2006). Biogenic emissions are estimated for each day of the simulation using the MEGAN model as implemented in CONCEPT (Baker, 2007). MEGAN explicitly outputs important biogenic secondary organic aerosol pre-cursor species including monoterpenes and sesquiterpenes that are used by the CAMx SOA chemistry module. Ammonia emissions are based on the July

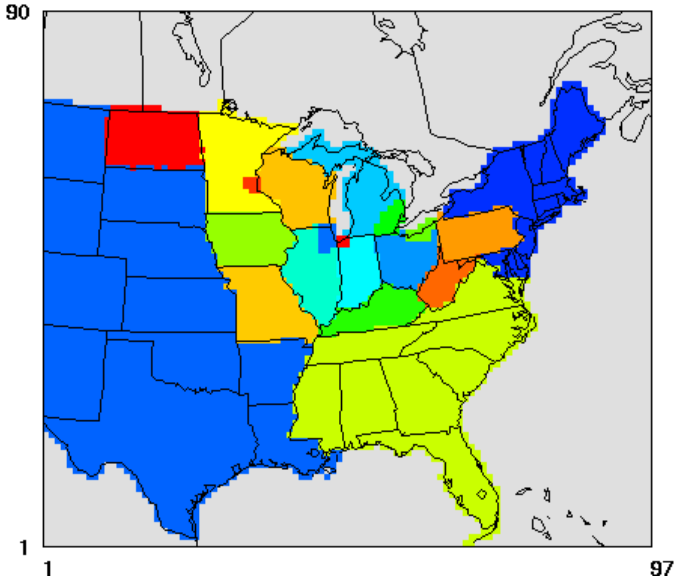
2004 version of the Carnegie Mellon University ammonia model (Strader et al. 2005; Pinder et al., 2004; Goebes et al., 2003).

The meteorological, emissions, and photochemical 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 (Figure 1). CAMx is applied with the vertical atmosphere resolved with 16 layers up to approximately 15 kilometers above ground level. 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.

Table 1. Complete list of source regions tracked for contribution

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

Figure 1. Model domain and source regions tracked with PSAT



Six emissions source sectors are tracked for contribution to particulate matter: onroad mobile, offroad mobile, area, electrical generating units, non-electrical generating units,

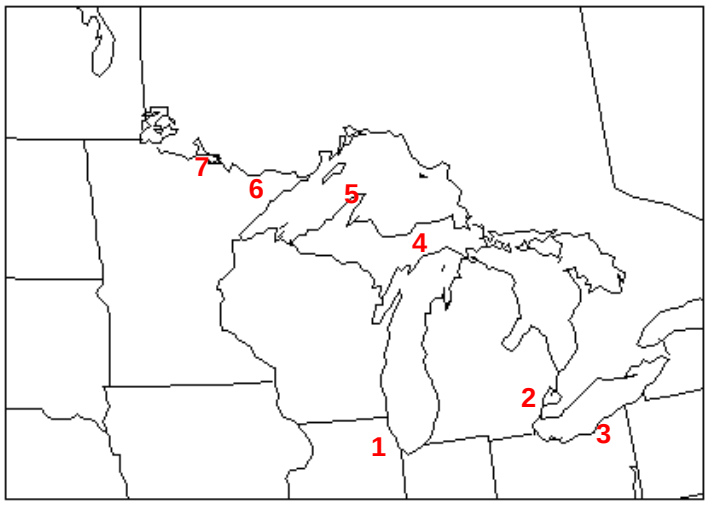
and agricultural ammonia. Offroad mobile emissions include sources such as construction equipment, locomotives, commercial marine vessels, and airports. Two distinct groups of stationary point sources are tracked for contribution to particulate matter: electrical generating units and non-electrical generating units. Additionally, secondary organic aerosol is a standard model output and presented as a unique contribution group to present a complete picture of predicted PM2.5.

The boundary contribution represents particulate matter entering the model through the lateral and top boundaries, which may represent a hemispheric or global background contribution. The emphasis of the modeling exercise is the estimation of potentially controllable pollution in the central and eastern United States, meaning minimal effort was made to determine the validity of particulate matter concentrations entering the model from boundaries.

An option in CAMx is employed to force elevated point sources into particular regions rather than placement based on coordinates and the 36 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 36 km grid cell source region map. This option improves the confidence in the source apportionment results for stationary point sources.

The receptors used for this analysis are shown Figure 2. These receptors represent large urban centers and all 4 Class I areas in the Great Lakes region. The urban center receptors include monitor locations in Chicago (1; AIRS ID = 170310052), Detroit (2; AIRS ID = 261630033), and Cleveland (3; AIRS ID = 390350013). The 4 Class I areas include Seney (4), Isle Royale (5), Boundary Waters (6), and Voyageurs (7).

Figure 2. Receptor Locations



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KEY WORDS

Particulate matter, visibility, source apportionment, CAMx, photochemical model, PSAT