Air Quality Modeling Technical Support Document: Source Sector Assessments

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U.S. Environmental Protection Agency
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Air Quality Assessment Division
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I Introduction

This document describes the air quality modeling performed by EPA in support or air quality and deposition assessments related source sector groups. A national scale air quality modeling analysis was performed to estimate the impact of current and future year sector emissions on annual and 24-hour PM2.5 concentrations, 8-hr maximum ozone, as well as visibility impairment. Air quality benefits are estimated with the Comprehensive Air Quality Model with Extensions (CAMx) model. CAMx simulates the numerous physical and chemical processes involved in the formation, transport, and destruction of ozone, particulate matter and air toxics. In addition to the CAMx model, the modeling platform includes the emissions, meteorology, and initial and boundary condition data which are inputs to this model. It is important to note that the inventories used in the air quality modeling may be different than a final sector inventory presented in a Regulatory Impact Analyses.

II. Photochemical Model Version, Inputs and Configuration

Photochemical grid models use state of the science numerical algorithms to estimate pollutant formation, transport, and deposition over a variety of spatial scales that range from urban to continental. Emissions of precursor species are injected into the model where they react to form secondary species such as ozone and then transport around the modeling domain before ultimately being removed by deposition or chemical reaction.

The 2005-based CAMx modeling platform was used as the basis for the air quality modeling. This platform represents a structured system of connected modeling-related tools and data that provide a consistent and transparent basis for assessing the air quality response to projected changes in emissions. The base year of data used to construct this platform includes emissions and meteorology for 2005. The modeling system treats the emissions, transport, and fate of criteria pollutants.

The modeling system was used to calculate daily and annual PM2.5 concentrations, 8-hr maximum ozone, and visibility impairment. Model predictions are used to estimate future-year design values of PM2.5 and ozone using a 2016 reference scenario compared to a 2005 baseline. This is done by calculating the simulated air quality ratios between any particular future year simulation and the 2005 base. These predicted ratios are then applied to ambient base year design values. The design value projection methodology used here followed EPA guidance for such analyses (USEPA, 2007).

A. Model version

CAMx version 5.30 is a freely available computer model that simulates the formation and fate of photochemical oxidants, ozone, primary and secondary PM concentrations, and air toxics, over regional and urban spatial scales for given input sets of meteorological conditions and emissions. CAMx includes numerous science modules that simulate the emission, production, decay, deposition and transport of organic and inorganic gas-phase and particle-phase pollutants in the atmosphere (Baker and Scheff, 2007; Nobel et al., 2001; Russell, 2008). CAMx is applied with ISORROPIA inorganic chemistry (Nenes et al., 1999), a semi-volatile equilibrium scheme to

partition condensable organic gases between gas and particle phase (Strader et al., 1999), Regional Acid Deposition Model (RADM) aqueous phase chemistry (Chang et al., 1987), and Carbon Bond 05 (CB05) gas-phase chemistry module (ENVIRON, 2008; Gery et al., 1989).

CAMx 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 (ENVIRON, 2008). Ozone source apportionment tracers are treated using the standard model algorithms for vertical advection, vertical diffusion, and horizontal diffusion. Horizontal advective fluxes for each of the regular model species that make up nitrogen oxides (NO_X) and volatile organic compounds (VOC) are combined and normalized by a concentration based weighted mean. Separate ozone tracers are used in CAMx to track ozone formation that happens under NO_X and VOC limited conditions.

Particulate matter source apportionment technology (PSAT) implemented in CAMx estimates the contribution from specific emissions source groups to PM2.5 and all forms of mercury using reactive tracers (ENVIRON, 2008; Wagstrom et al., 2008). The tracer species are estimated with source apportionment algorithms rather than by the host model routines. PSAT tracks contribution to PM2.5 sulfate, nitrate, ammonium, secondary organic aerosol, and inert primarily emitted species. Non-linear processes like gas and aqueous phase chemistry are solved for bulk species and then apportioned to the tagged species. Emissions of nitrogen oxides are tracked through all intermediate nitrogen species to particulate nitrate ion. Ammonia emissions are tracked to particulate ammonium ion. This modeling assessment used the PSAT approach to estimate source contribution to PM2.5 species and the APCA method to estimate source contribution to modeled ozone.

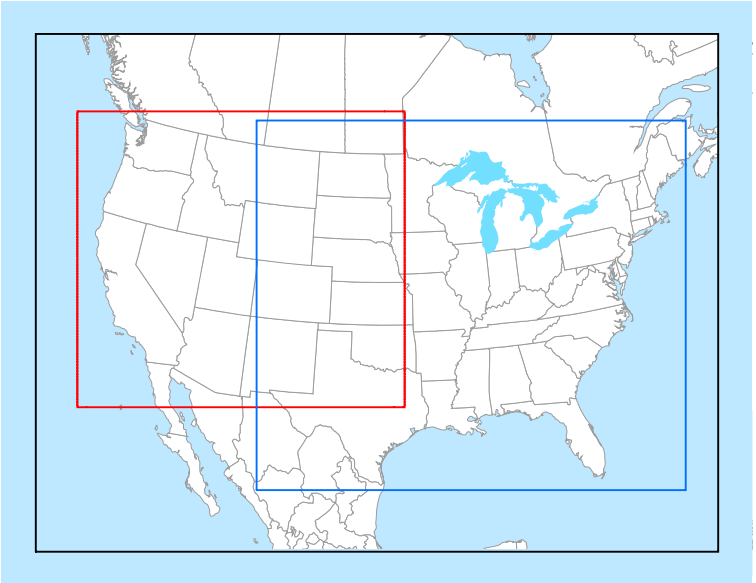
B. Model domain and grid resolution

The modeling analyses were performed for a domain covering the continental United States as shown in Figure II-1. This domain has a parent horizontal grid of 36 km with two finer-scale 12 km grids over portions of the eastern and western U.S. The model extends vertically from the surface to 100 millibars (approximately 15 km) using a sigma-pressure coordinate system. Air quality conditions at the outer boundary of the 36 km domain were taken from a global model and vary in time and space. The 36 km grid was only used to establish the incoming air quality concentrations along the boundaries of the 12 km grids. Only the finer grid data were used in determining the impacts of the emissions changes. Table II-1 provides geographic information about the photochemical model domains.

Table II-1. Geographic elements of domains used in photochemical modeling.

	Photochemical Modeling Configuration		
	National Grid	**Western U.S. Fine Grid**	**Eastern U.S. Fine Grid**
Map Projection	Lambert Conformal Projection		
Grid Resolution	36 km	12 km	12 km
Coordinate Center	97 deg W, 40 deg N		
True Latitudes	33 deg N and 45 deg N		
Dimensions	148 x 112 x 14	213 x 192 x 14	279 x 240 x 14
Vertical extent	14 Layers: Surface to 100 millibar level (see Table II-3)		

Figure II-1. Map of the photochemical modeling domains. The black outer box denotes the 36 km national modeling domain; the red inner box is the 12 km western U.S. grid; and the blue inner box is the 12 km eastern U.S. grid.



C. Modeling Time-period

The 36 km and both 12 km modeling domains were modeled for the entire year of 2005. Data from the entire year were utilized when looking at the estimation of PM2.5 and visibility impacts. Data from April through October is used to estimate ozone impacts.

D. Model Inputs: Emissions, Meteorology and Boundary Conditions

The 2005-based modeling platform was used for the air quality modeling of future emissions scenarios. In addition to the photochemical model, the modeling platform also consists of the

base- and future-year emissions estimates, meteorological fields, as well as initial and boundary condition data which are all inputs to the air quality model.

1. Emissions Input Data

The emissions data used in the base year and future reference and future emissions adjustment case are based on the 2005 v4.3 platform. Emissions are processed to photochemical model inputs with the SMOKE emissions modeling system (Houyoux et al., 2000). The 2016 reference case is intended to represent the emissions associated with growth and controls in that year projected from the 2005 simulation year. The United States EGU point source emissions estimates for the future year reference and control case are based on an Integrated Planning Model (IPM) run for criteria pollutants. Both control and growth factors were applied to a subset of the 2005 non-EGU point and non-point emissions to create the 2016 reference case. The 2005 v4 platform projection factors were the starting point for most of the 2016 SMOKE-based projections.

Table II.2 Domain total estimated sector emissions (TPY) for 2016 modeling scenario.

Sector	Year	VOC	NOX	Primary PM2.5	SO2	NH3
Biogenics	2016	59,388,365	2,218,207	0	0	0
Cement Kilns	2016	3,059	130,536	1,106	48,737	679
Pulp & Paper	2016	121,597	240,139	10,067	170,393	10,859
Refineries	2016	111,391	118,206	7,379	132,337	3,556
Coke Ovens	2016	7,821	16,110	368	27,952	1,084
Iron/Steel Foundries	2016	14,384	5,867	1,366	3,590	166
Integrated Iron/Steel	2016	9,620	31,925	2,856	29,045	167
Electric Arc Furnaces	2016	3,560	15,707	622	6,088	119
Taconite Mining	2016	606	41,350	884	8,823	4
Ferroalloy Production	2016	150	3,412	201	4,580	510
Residential Wood	2016	538,466	33,786	192,492	4,720	6,586
Non-point Other	2016	9,380,925	1,633,261	325,820	1,243,154	126,802
Non-EGU point Other	2016	1,259,745	1,263,276	67,614	877,620	140,948
Average Fires	2016	1,874,035	189,428	459,641	49,094	36,777
Air/Locomotives/Marine	2016	43,547	1,342,849	35,604	9,087	940
Nonroad mobile	2016	1,953,067	1,259,578	106,975	2,879	2,345
Onroad mobile	2016	2,357,108	4,239,971	118,986	26,786	82,094
Canada + Mexico	2016	5,615,200	2,841,702	242,412	2,855,974	1,077,333
Point EGU	2016	63,198	1,826,582	30,078	3,793,362	36,706
Commercial Marine (SECA-C3)	2016	66,093	1,534,234	7,407	439,987	0
Area Fugutive Primary PM2.5	2016	0	0	47,438	0	0

The future year projection includes emissions reductions related to the NOx SIP Call, Boiler MACT, RICE, and the proposed Transport Rule (TR1). The residential wood combustion category is defined based on SCC codes 2104008 and 2104009. Certain sectors are based on a list of facilities that would likely be subject to a NESHAP related to that sector: cement kilns, pulp & paper, refineries, coke ovens, iron/steel foundries, integrated ion/steel, electric arc

furnaces, taconite mining, and ferroalloy production. The model domain total estimated emissions by source sector used in this modeling assessment are shown in Table II.2 for 2016 and Table II.3 for 2005.

Table II.3 Domain total estimated sector emissions (TPY) for 2005 modeling scenario

Sector	Year	VOC	NOX	Primary PM2.5	SO2	NH3
Biogenics	2005	59,388,365	2,218,207	0	0	0
Cement Kilns	2005	9,044	217,948	2,342	157,163	861
Pulp & Paper	2005	128,390	246,714	11,979	345,917	10,990
Refineries	2005	112,622	150,924	7,750	246,351	3,556
Coke Ovens	2005	7,914	16,145	416	29,239	1,089
Iron/Steel Foundries	2005	15,522	5,985	1,435	3,611	166
Integrated Iron/Steel	2005	9,687	31,961	2,862	32,646	167
Electric Arc Furnaces	2005	3,630	15,707	622	6,088	119
Taconite Mining	2005	607	41,350	1,035	11,285	4
Ferroalloy Production	2005	150	3,412	201	4,580	510
Residential Wood	2005	647,141	38,190	222,081	5,280	7,238
Non-point Other	2005	12,453,787	1,659,651	326,140	1,251,930	126,802
Non-EGU point Other	2005	1,747,491	1,297,668	71,899	1,215,203	141,230
Average Fires	2005	1,874,035	189,428	459,641	49,094	36,777
Air/Locomotives/Marine	2005	58,890	1,909,526	53,671	154,016	773
Nonroad mobile	2005	3,353,497	2,083,093	181,038	195,597	1,969
Onroad mobile	2005	4,734,097	9,006,389	258,251	176,525	156,276
Canada + Mexico	2005	5,615,200	2,841,702	242,412	2,855,974	1,077,333
Point EGU	2005	63,404	3,726,455	39,544	10,380,773	21,684
Commercial Marine (SECA-C3)	2005	42,438	1,169,907	10,501	740,998	0
Area Fugutive Primary PM2.5	2005	0	0	47,315	0	0

Other North American emissions of criteria and toxic pollutants (including mercury) are based on a 2006 Canadian inventory and 1999 Mexican inventory. Both inventories are not grown or controlled when used as part of future year baseline inventories. Global emissions of criteria are included in the modeling system through boundary condition inflow.

2. Meteorological Input Data

The gridded meteorological input data for the entire year of 2005 were derived from simulations of the Pennsylvania State University / National Center for Atmospheric Research Mesoscale Model. This model, commonly referred to as MM5, is a limited-area, nonhydrostatic, terrain-following system that solves for the full set of physical and thermodynamic equations which govern atmospheric motions. Meteorological model input fields were prepared separately for each of the three domains shown in Figure II-1 using MM5 version 3.7.4. The MM5 simulations were run on the same map projection as shown in Figure II-1.

All three meteorological model runs were configured similarly. The selections for key MM5 physics options are shown below:

- Pleim-Xiu PBL and land surface schemes
- Kain-Fritsh 2 cumulus parameterization
- Reisner 2 mixed phase moisture scheme
- RRTM longwave radiation scheme
- Dudhia shortwave radiation scheme

Three dimensional analysis nudging for temperature and moisture was applied above the boundary layer only. Analysis nudging for the wind field was applied above and below the boundary layer. The 36 km domain nudging weighting factors were 3.0×10^4 for wind fields and temperatures and 1.0×10^5 for moisture fields. The 12 km domain nudging weighting factors were 1.0×10^4 for wind fields and temperatures and 1.0×10^5 for moisture fields.

Table II-4. Vertical layer structure (heights are layer top).

CAMX Layers	MM5 Layers	Sigma P	Approximate Height (m)	Approximate Pressure (mb)
0	0	1.000	0	1000
1	1	0.995	38	995
2	2	0.990	77	991
3	3	0.985	115	987
	4	0.980	154	982
4	5	0.970	232	973
	6	0.960	310	964
5	7	0.950	389	955
	8	0.940	469	946
6	9	0.930	550	937
	10	0.920	631	928
	11	0.910	712	919
7	12	0.900	794	910
	13	0.880	961	892
	14	0.860	1,130	874
8	15	0.840	1,303	856
	16	0.820	1,478	838
	17	0.800	1,657	820
9	18	0.770	1,930	793
	19	0.740	2,212	766
10	20	0.700	2,600	730
	21	0.650	3,108	685
11	22	0.600	3,644	640
	23	0.550	4,212	595
12	24	0.500	4,816	550
	25	0.450	5,461	505
	26	0.400	6,153	460
13	27	0.350	6,903	415
	28	0.300	7,720	370
	29	0.250	8,621	325
	30	0.200	9,625	280
14	31	0.150	10,764	235
	32	0.100	12,085	190
	33	0.050	13,670	145
	34	0.000	15,674	100

All three sets of model runs were conducted in 5.5 day segments with 12 hours of overlap for spin-up purposes. All three domains contained 34 vertical layers with an approximately 38 m deep surface layer and a 100 millibar top. The MM5 and CAMx vertical structures are shown in Table II-4 and do not vary by horizontal grid resolution. The meteorological outputs from all

three MM5 sets were processed to create model-ready inputs for CAMx using the MCIP processor.

Before initiating the air quality simulations, it is important to identify the biases and errors associated with the meteorological modeling inputs. The 2005 MM5 model performance evaluations used an approach which included a combination of qualitative and quantitative analyses to assess the adequacy of the MM5 simulated fields. The qualitative aspects involved comparisons of the model-estimated synoptic patterns against observed patterns from historical weather chart archives. Additionally, the evaluations compared spatial patterns of estimated to observed monthly average rainfall and checked maximum planetary boundary layer (PBL) heights for reasonableness.

Qualitatively, the model fields closely matched the observed synoptic patterns, which is not unexpected given the use of nudging. The operational evaluation included statistical comparisons of model/observed pairs (e.g., mean normalized bias, mean normalized error, index of agreement, root mean square errors, etc.) for multiple meteorological parameters. For this portion of the evaluation, five meteorological parameters were investigated: temperature, humidity, shortwave downward radiation, wind speed, and wind direction. The three individual MM5 evaluations are described elsewhere (Baker, 2009a, b, c). It was ultimately determined that the bias and error values associated with all three sets of 2005 meteorological data were generally within the range of past meteorological modeling results that have been used for air quality applications.

3. Initial and Boundary Conditions

The lateral boundary and initial species concentrations are provided by a three-dimensional global atmospheric chemistry model, the GEOS-CHEM model (standard version 7-04-11). The global GEOS-CHEM model simulates atmospheric chemical and physical processes driven by assimilated meteorological observations from the NASA's Goddard Earth Observing System (GEOS). This model was run for 2005 with a grid resolution of 2.0 degree x 2.5 degree (latitude-longitude) and 30 vertical layers up to 100 mb. The predictions were used to provide one-way dynamic boundary conditions at three-hour intervals and an initial concentration field for the 36 km CAMx simulations. The 36 km photochemical model simulation is used to supply initial and hourly boundary concentrations to the 12 km domains. The 36 km domain simulation includes 10 days of spin-up before the start of each calendar quarter that are not used in the analysis. The 12 km domain simulations include 3 days of spin-up before each calendar quarter. The future base conditions from the 36 km coarse grid modeling were used as the initial/boundary state for all subsequent future year 12 km finer grid modeling scenarios.

III. Base Case Model Performance Evaluation

A. PM2.5

An operational model performance evaluation for the speciated components of PM2.5 (e.g., sulfate, nitrate, elemental carbon, organic carbon, etc.) was conducted using 2005 monitoring data in order to estimate the ability of the modeling system to replicate base year concentrations. The evaluation of PM2.5 component species includes comparisons of predicted and observed concentrations of sulfate (SO4), nitrate (NO3), ammonium (NH4), elemental carbon (EC), and organic carbon (OC). PM2.5 ambient measurements for 2005 were obtained from the Chemical Speciation Network (CSN) and the Interagency Monitoring of PROtected Visual Environments (IMPROVE). The CSN sites are generally located within urban areas and the IMPROVE sites are typically in rural/remote areas. The measurements at CSN and IMPROVE sites represent 24-hour average concentrations. In calculating the model performance metrics, the modeled hourly species predictions were aggregated to the averaging times of the measurements.

Model performance statistics were calculated for observed/predicted pairs of daily concentrations (Boylan and Russell, 2006). The aggregated metrics and number (N) of prediction-observation pairs are shown by chemical specie and quarter in Table III-1. Model performance was compared to the performance found in recent regional PM2.5 model applications for other, non-EPA studies. Overall, the mean bias (bias) and mean error (error) statistics are within the range or close to that found by other groups in recent applications (Doraiswamy, 2010; Tesche et al., 2006). The model performance results give us confidence that our application of CAMx using this modeling platform provides a scientifically credible approach for estimating PM2.5 concentrations for the purposes of this assessment.

TABLE III-1. Model performance metrics for speciated PM2.5 averaged by quarter.

Specie	Quarter	N	Observed	Predicted	Bias	Error
PM2.5 Sulfate Ion	1	6,218	2.7	4.2	1.6	2.0
	2	6,537	3.8	4.4	0.7	1.6
	3	6,108	5.4	5.2	0.0	1.9
	4	5,894	2.5	3.7	1.3	1.5
PM2.5 Nitrate Ion	1	5,870	2.4	1.9	-0.4	1.3
	2	6,146	0.8	0.6	-0.1	0.6
	3	5,828	0.5	0.2	-0.2	0.4
	4	5,757	1.3	1.1	-0.1	0.8
PM2.5 Ammonium Ion	1	4,045	1.7	1.8	0.4	0.8
	2	4,075	1.5	1.5	0.3	0.7
	3	3,869	1.8	1.5	0.0	0.8
	4	3,763	1.3	1.4	0.4	0.7
PM2.5 Organic Carbon	1	5,882	1.7	2.2	0.6	1.1
	2	6,180	2.1	1.7	-0.4	0.9
	3	5,836	2.4	2.3	-0.1	0.9
	4	5,600	2.0	2.0	0.1	1.0
PM2.5 Elemental Carbon	1	6,368	0.5	1.0	0.5	0.6
	2	6,552	0.5	0.7	0.3	0.4
	3	6,061	0.5	0.8	0.3	0.4
	4	5,937	0.6	0.9	0.4	0.5

B. Ozone

An operational model performance evaluation for hourly and eight-hour daily maximum ozone was conducted in order to estimate the ability of the modeling system to replicate the base year concentrations. Ozone measurements were taken from the 2005 State/local monitoring site data in the Air Quality System (AQS) Aerometric Information Retrieval System (AIRS). The ozone metrics covered in this evaluation include one-hour and eight-hour average daily maximum ozone bias and error. The evaluation principally consists of statistical assessments of model versus observed pairs that are paired in time and space. This ozone model performance was limited to the prediction-observation pairs where observed ozone exceeded or equaled 60 ppb. This cutoff was applied to evaluate the model on days of elevated ozone which are more policy relevant. Aggregated performance metrics by quarter are shown in Table III-2 for daily maximum 1-hr average ozone and Table III-3 for daily maximum 8-hr average ozone.

TABLE III-2. Model performance metrics for daily maximum 1-hr avg ozone by quarter.

Quarter	N	Observed	Predicted	Bias	Error	Fractional Bias	Fractional Error
2	19,821	76	65	-11	12	-16	18
3	22,699	80	71	-9	13	-13	17

TABLE III-3. Model performance metrics for daily maximum 8-hr avg ozone by quarter.

Quarter	N	Observed	Predicted	Bias	Error	Fractional Bias	Fractional Error
2	19,833	69	60	-9	11	-15	17
3	22,714	70	64	-6	10	-10	16

This model performance is consistent with photochemical modeling used to support other national regulations (USEPA, 2010).

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