



# Air Quality Modeling Technical Support Document: Point Source Sector Rules

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U.S. Environmental Protection Agency  
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## **I Introduction**

This document describes the air quality modeling performed by EPA in support of air quality and mercury deposition assessments related to large stationary point sources that generate electricity. A national scale air quality modeling analysis was performed to estimate the impact of the sector emissions changes on future year annual and 24-hour PM<sub>2.5</sub> concentrations, 8-hr maximum ozone, total mercury deposition, as well as visibility impairment. Air quality benefits are estimated with the Community Multi-scale Air Quality (CMAQ) model. CMAQ 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 CMAQ model, the modeling platform includes the emissions, meteorology, and initial and boundary condition data which are inputs to this model.

Emissions and air quality modeling decisions are made early in the analytical process. For this reason, it is important to note that the inventories used in the air quality modeling and the benefits modeling may be slightly different than the final utility sector inventories presented in the RIA. However, the air quality inventories and the final rule inventories are generally consistent, so the air quality modeling adequately reflects the effects of the rule.

## **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 CMAQ modeling platform was used as the basis for the air quality modeling for this rule. 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 and certain toxics including hydrogen chloride (HCL) and speciated mercury: Hg(0) (gaseous elemental), Hg(II) (oxidized gaseous), and Hg(p) (particle-bound). This modeling platform and analysis is described below.

As part of the analysis for this rulemaking, the modeling system was used to calculate daily and annual PM<sub>2.5</sub> concentrations, 8-hr maximum ozone, annual total mercury deposition levels and visibility impairment. Model predictions are used to estimate future-year design values of PM<sub>2.5</sub> and ozone. Specifically, we compare a 2016 reference scenario, a scenario without the boiler sector controls, to a 2016 control scenario which includes the adjustments to the boiler sector. 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). Additionally, the raw model outputs are also used in a relative sense as inputs to the health and welfare impact functions of the benefits analysis. Only model

predictions for mercury deposition were analyzed using absolute model changes, although percent changes between the control case and two future baselines are also estimated.

### A. Model version

The Community Multi-scale Air Quality (CMAQ) model v4.7.1 ([www.cmaq-model.org](http://www.cmaq-model.org)) is a state of the science three-dimensional Eulerian “one-atmosphere” photochemical transport model used to estimate air quality (Appel et al., 2008; Appel et al., 2007; Byun and Schere, 2006). CMAQ 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. CMAQ is applied with the AERO5 aerosol module, which includes the ISORROPIA inorganic chemistry (Nenes et al., 1998) and a secondary organic aerosol module (Carlton et al., 2010). The CMAQ model is applied with sulfur and organic oxidation aqueous phase chemistry (Carlton et al., 2008) and the carbon-bond 2005 (CB05) gas-phase chemistry module (Gery et al., 1989). Mercury oxidation pathways are represented for both the gas and aqueous phases in addition to aqueous phase reduction reactions (Bullock and Brehme, 2002).

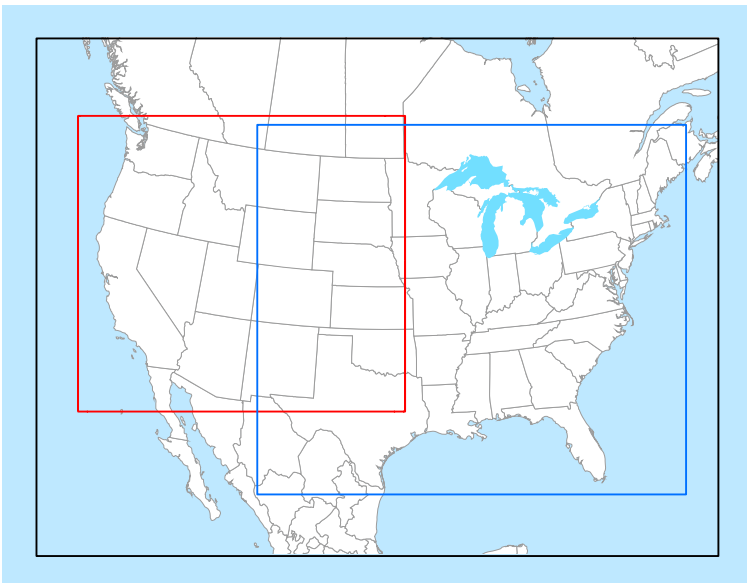
### B. Model domain and grid resolution

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 PM<sub>2.5</sub>, total mercury deposition, and visibility impacts from the regulation. 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 v4.1 platform. The emissions cases use different emissions data for some pollutants than the official v4 platform to use data intended only for this rule. Unlike the 2005 v4 platform, the configuration for this modeling application included mercury emissions from the National Air Toxics Assessment Inventory and some industrial boiler sector mercury emissions more consistent with the engineering analysis for the Industrial/Commercial/Institutional Boilers and Process Heaters NESHAP. Emissions for the future years for the EGU sector utilized information collected from the utility MACT information collection request. The information collection request informed existing HCL, NOX, HG, and PM controls. In addition this data was used to supply HCL removal rates from selected

control technology. 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, hydrochloric acid, and mercury in 2016. Both control and growth factors were applied to a subset of the 2005 non-EGU point and non-point to create the 2016 reference case. The 2005 v4 platform 2014 projection factors were the starting point for most of the 2016 SMOKE-based projections. The mercury projections for non-EGU point sources accounted for emission reductions expected in the future due to NESHAP for various non-EGU source categories that were finalized or expected to be finalized prior to the rule proposal including the Boiler MACT, Gold Mine NESHAP and Electric Arc Furnace NESHAP. The estimated total anthropogenic emissions and emissions for the utility sector used in this modeling assessment are shown in Table II.2.

**Table II.2** Estimated total inventory and EGU sector emissions for each modeling scenario.

Scenario	Sector	Emissions (tons/year)					
		VOC	NOx	CO	SO2	PM10	PM2.5
2005 baseline	EGU (PTIPM)	40,950	3,726,459	601,564	10,380,786	615,095	508,903
	All	17,613,543	22,216,093	83,017,436	15,050,209	13,031,716	4,400,680
2016 baseline	EGU (PTIPM)	40,845	1,769,764	691,310	3,577,698	523,504	384,320
	All	14,390,421	15,019,836	59,148,384	7,245,595	12,772,091	4,022,846
2016 control case	EGU (PTIPM)	38,217	1,618,199	656,245	1,220,379	358,165	291,044
	All	14,387,792	14,868,270	59,113,319	4,888,276	12,606,752	3,929,570
Scenario	Sector	Emissions (tons/year)					
		Hg(0)	Hg(II)	Hg(p)	HCL	CL2	NH3
2005 baseline	EGU (PTIPM)	30	21	1.6	351,592	99	21,684
	All	64	33	8.5	429,223	6,409	3,762,641
2016 baseline	EGU (PTIPM)	21	7	0.7	74,089		36,655
	All	42	16	5.9	140,638	6,050	3,897,033
2016 control case	EGU (PTIPM)	5	2	0.4	8,802		36,982
	All	26	11	5.6	75,351	6,050	3,897,360

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 and toxic pollutants (including mercury) 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  $3.0 \times 10^4$  for wind fields and temperatures and  $1.0 \times 10^5$  for moisture fields. The 12 km domain nudging weighting factors were  $1.0 \times 10^4$  for wind fields and temperatures and  $1.0 \times 10^5$  for moisture fields.

**Table II-3.** Vertical layer structure (heights are layer top).

CMAQ 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 CMAQ vertical structures are shown in Table II-3 and do not vary by horizontal grid resolution. The meteorological outputs from all three MM5 sets were processed to create model-ready inputs for CMAQ 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 CMAQ simulations. The 36 km photochemical model simulation is used to supply initial and hourly boundary concentrations to the 12 km domains. 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. Mercury initial and boundary conditions were based on a GEOS-CHEM simulation using a 2000 based global anthropogenic emissions inventory that includes 1,278 Mg/yr of Hg(0), 720 Mg/yr of Hg(II), and 192 Mg/yr of particle bound mercury (Selin et al., 2007).

## **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 state/local 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 (SO<sub>4</sub>), nitrate (NO<sub>3</sub>), ammonium (NH<sub>4</sub>), 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. The aggregated metrics and number (N) of prediction-observation pairs are

shown by chemical specie and quarter in Table III-1. The “acceptability” of model performance was judged by comparing our 2005 performance results to the range of performance found in recent regional PM<sub>2.5</sub> model applications for other, non-EPA studies. Overall, the mean bias (bias) and mean error (error) statistics shown in Table III-1 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 CMAQ using this modeling platform provides a scientifically credible approach for assessing PM<sub>2.5</sub> concentrations for the purposes of this assessment.

**TABLE III-1.** Model performance metrics for speciated PM<sub>2.5</sub> averaged by quarter.

Metric	Quarter	Sulfate Ion	Nitrate Ion	Ammonium Ion	Organic Carbon	Elemental Carbon
Number	1	6,218	5,870	4,045	6,368	6,305
	2	6,537	6,146	4,075	6,552	6,516
	3	6,108	5,828	3,869	6,061	6,152
	4	5,894	5,757	3,763	5,697	5,792
Mean Observed ( $\mu\text{g}/\text{m}^3$ )	1	2.69	2.39	1.72	0.51	0.40
	2	3.80	0.83	1.49	0.48	0.66
	3	5.43	0.45	1.84	0.52	0.78
	4	2.45	1.28	1.26	0.61	0.52
Mean Predicted ( $\mu\text{g}/\text{m}^3$ )	1	2.37	2.36	1.50	0.82	5.20
	2	3.45	1.21	1.47	0.64	4.06
	3	4.39	0.48	1.39	0.66	4.69
	4	2.31	1.84	1.32	0.81	5.46
Bias ( $\mu\text{g}/\text{m}^3$ )	1	-0.27	0.12	0.05	0.34	4.87
	2	-0.28	0.49	0.33	0.15	3.50
	3	-0.88	0.07	-0.12	0.16	4.03
	4	-0.08	0.63	0.36	0.24	5.01
Error ( $\mu\text{g}/\text{m}^3$ )	1	1.05	1.37	0.77	0.47	4.90
	2	1.25	0.89	0.81	0.35	3.65
	3	1.73	0.46	0.80	0.35	4.24
	4	0.74	1.17	0.66	0.44	5.05

## 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 were 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.

**TABLE III-2.** Model performance metrics for daily maximum ozone by quarter.

1-hr Daily Maximum Ozone (ppb)					
Quarter	N	Observed	Predicted	Bias	Error
2	24,357	76.0	69.6	-6.4	9.2
3	27,430	79.7	75.3	-4.4	10.6
8-hr Daily Maximum Ozone (ppb)					
Quarter	N	Observed	Predicted	Bias	Error
2	24,370	69.3	63.9	-5.4	8.1
3	27,447	70.5	68.0	-2.5	8.6

\*metrics estimated where observed ozone > 60 ppb

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

### C. Mercury Wet Deposition

Model estimated weekly mercury wet deposition is compared to observation data to assess model skill simulating this component of mercury deposition. Mercury wet deposition measurements are weekly totals taken at sites that are part of the Mercury Deposition Network (<http://nadp.sws.uiuc.edu/MDN/>) which operates under the National Atmospheric Deposition Program. In addition to mercury wet deposition, the network sites also collect rainfall data which is also evaluated against estimates used by the photochemical model from prognostic meteorological model output.

**TABLE III-3.** Model performance metrics for mercury wet deposition and rainfall by quarter.

Total Mercury Wet Deposition ( $\mu\text{g}/\text{m}^2$ )					
Quarter	N	Observed	Predicted	Bias	Error
1	798	0.15	0.23	0.14	0.18
2	853	0.26	0.28	0.06	0.24
3	840	0.31	0.16	-0.12	0.24
4	748	0.13	-0.80	-1.27	1.47
Rainfall (mm)					
Quarter	N	Observed	Predicted	Bias	Error
1	1,073	17.27	18.10	0.83	8.34
2	1,082	19.41	23.50	4.09	14.45
3	1,118	20.64	26.51	5.87	19.77
4	1,037	20.18	17.22	-2.97	10.38

A comparison of observed and predicted mercury wet deposition is shown in Table III-3. Mercury wet deposition performance (annual average normalized mean bias of 34% and annual

average normalized mean error of 52%) compares well to other photochemical model applications published in literature (Bullock and Brehme, 2002; Vijayaraghavan et al., 2007).

#### **IV. Post Processing Mercury Deposition**

CMAQ outputs hourly wet and dry deposition estimates (kg/ha) in each grid cell of speciated mercury: Hg<sub>0</sub>, Hg<sub>2</sub>, and PM<sub>2.5</sub> Hg. Hourly outputs are averaged by day, then month, and then to an annual estimate. CMAQ model estimates of annual total mercury deposition from both 12 km model domains (12EUS1 and 12WUS1) were joined into a single 12 km model file covering the entire continental United States. Total mercury deposition is defined as the sum of all wet and dry deposition of elemental mercury, divalent gas-phase mercury, and PM<sub>2.5</sub> mercury. Gridded 12 km total mercury estimates from 2005, 2016, and emissions sensitivity CMAQ simulations were linked to an ArcInfo shape file of the model domain. ArcGIS software was then used to calculate weighted areal ratios between the 12 km grid cells and 12 digit hydrologic unit code (HUC) boundaries to produce a shape file of emissions estimates for each HUC within the domain.

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