



Air Quality Modeling Technical Support Document: EGU Mercury Analysis

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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_{2.5} 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_{2.5} 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_{2.5} 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) 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). Mercury estimates from CMAQ have been compared to observations and other mercury modeling systems in several peer reviewed publications (Bullock et al., 2008, 2009; Lin et al., 2007).

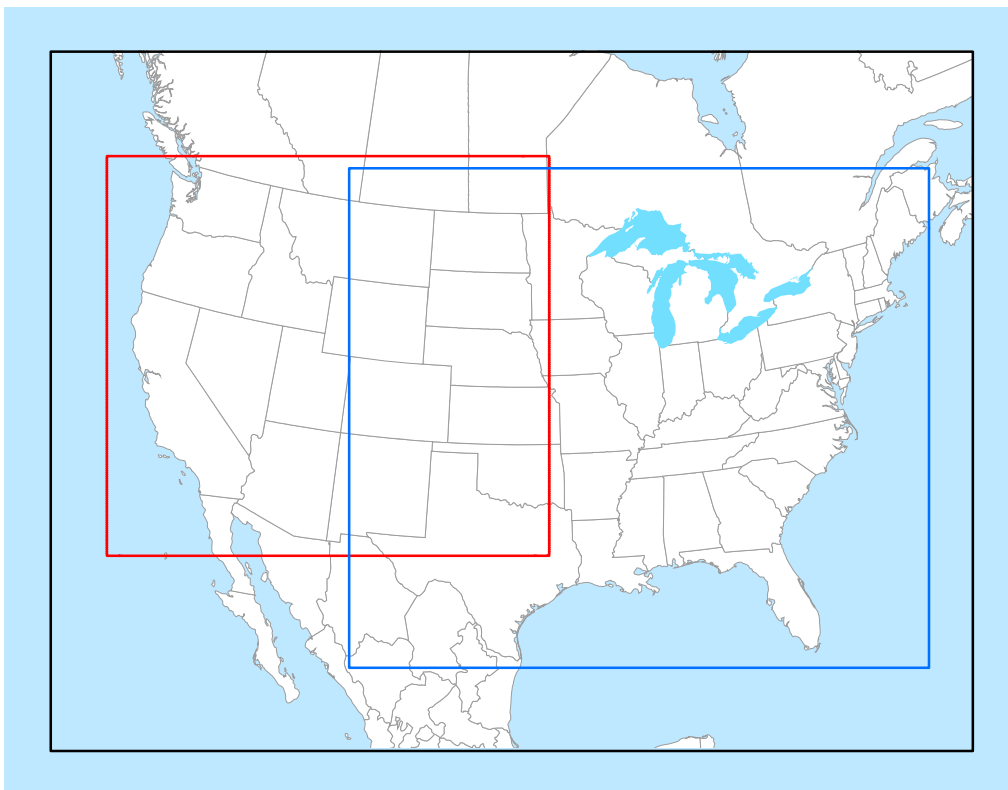
B. Model domain and grid resolution

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_{2.5}, 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.

All mercury emissions from facilities included in the PTIPM sector were removed, or “zeroed-out” in both the 2005 baseline and 2016 baseline scenarios to provide information about the contribution of mercury from this sector.

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-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. Initial and boundary conditions for the projected future year (2016) 36 km simulations are the same as the 2005 base year. The first 10 days of the 36 km modeling simulation are not used in the analysis, which is beyond the number of days necessary to remove the influence of initial conditions on mercury deposition estimates (Pongprueksa et al., 2008).

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). A comparison of global mercury emissions by continent for 2000 and 2006 is published in (Streets et al., 2009). Total mercury emissions from China (and Oceania) total 1,306 Mg/yr in 2000 and 1,317 Mg/yr in 2006 (Streets et al., 2009). Given these consistent emissions estimates from Asia, the 2005 boundary inflow to the 36 km CMAQ domain was not adjusted. Recent research has shown that ambient mercury concentrations have been decreasing in the northern hemisphere since 2000 (Slemr et al., 2011). Since emissions from China have not appreciably changed between 2000 and 2006, ambient mercury concentrations have been decreasing, and the large uncertainties surrounding projected mercury global inventories the mercury boundary conditions are the same for both the 2005 and 2016 simulations.

III. Base Case Model Performance Evaluation

A. PM_{2.5}

An operational model performance evaluation for the speciated components of PM_{2.5} (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 PM_{2.5} component species includes comparisons of predicted

and observed concentrations of sulfate (SO₄), nitrate (NO₃), ammonium (NH₄), elemental carbon (EC), and organic carbon (OC). PM_{2.5} 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.

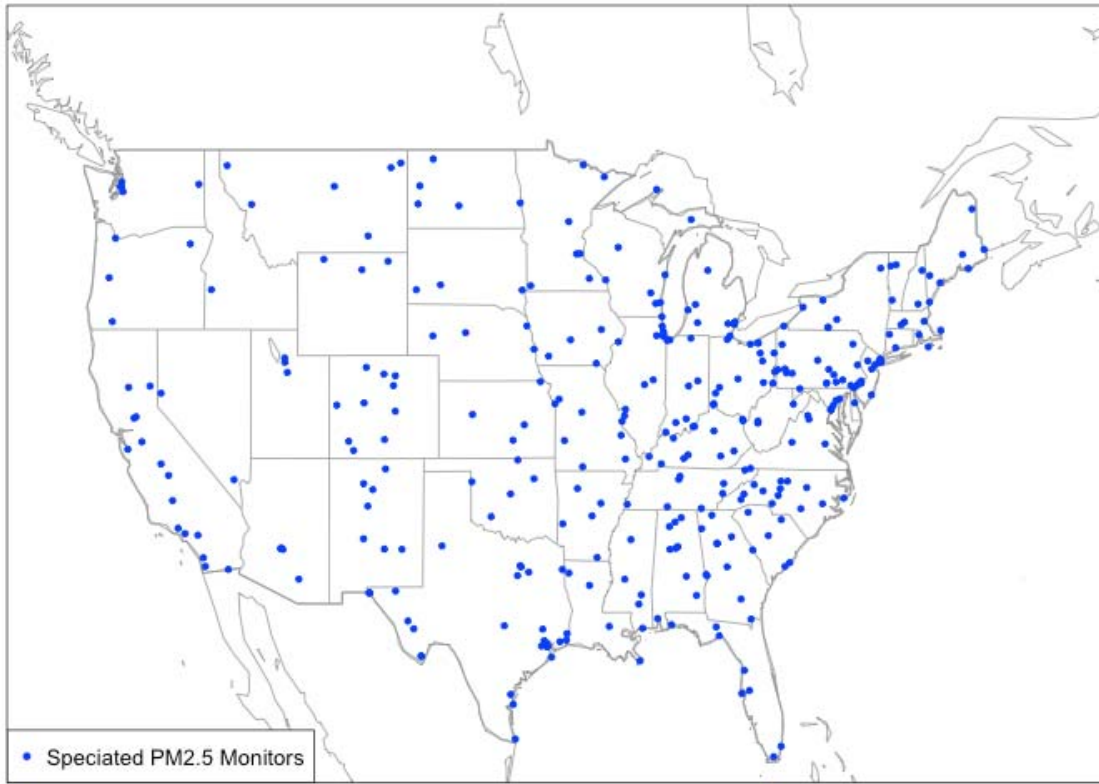


Figure III-1. Speciated PM_{2.5} monitors used in the model performance evaluation.

Model performance statistics were calculated for observed/predicted pairs of daily concentrations. Estimated metrics include bias, error, fractional bias, and fractional error (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. The “acceptability” of model performance was judged by comparing our 2005 performance results to the range of performance found in recent regional PM_{2.5} 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_{2.5} concentrations for the purposes of this assessment.

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

		Quarter			
		1	2	3	4
N	Sulfate Ion	6,927	7,248	6,819	6,372
	Nitrate Ion	6,577	6,850	6,532	6,240
	Ammonium Ion	4,752	4,777	4,576	4,303
	Organic Carbon	7,049	7,219	6,726	6,386
	Elemental Carbon	6,977	7,182	6,830	6,464
Mean Observed (ug/m ³)	Sulfate Ion	2.5	3.6	5.1	2.3
	Nitrate Ion	2.5	0.9	0.6	1.6
	Ammonium Ion	1.7	1.4	1.7	1.3
	Organic Carbon	0.6	0.5	0.5	0.7
	Elemental Carbon	0.4	0.7	0.8	0.6
Mean Predicted (ug/m ³)	Sulfate Ion	2.3	3.2	4.1	2.2
	Nitrate Ion	2.3	1.2	0.5	1.8
	Ammonium Ion	1.5	1.4	1.3	1.3
	Organic Carbon	0.9	0.7	0.7	0.9
	Elemental Carbon	5.5	4.1	4.8	5.8
Bias (ug/m ³)	Sulfate Ion	-0.2	-0.3	-0.8	-0.1
	Nitrate Ion	-0.1	0.4	0.0	0.3
	Ammonium Ion	0.0	0.3	-0.1	0.2
	Organic Carbon	0.4	0.2	0.2	0.3
	Elemental Carbon	5.1	3.6	4.1	5.3
Error (ug/m ³)	Sulfate Ion	1.0	1.2	1.6	0.7
	Nitrate Ion	1.5	0.9	0.5	1.3
	Ammonium Ion	0.8	0.7	0.7	0.7
	Organic Carbon	0.5	0.4	0.4	0.5
	Elemental Carbon	5.2	3.7	4.3	5.3
Fractional Bias (%)	Sulfate Ion	-6.6	-6.0	-13.4	1.0
	Nitrate Ion	-17.9	-24.8	-67.0	-6.3
	Ammonium Ion	6.2	28.5	10.4	31.1
	Organic Carbon	33.3	17.7	15.6	18.5
	Elemental Carbon	159.6	124.0	127.9	151.8
Fractional Error (%)	Sulfate Ion	42.9	35.8	38.7	36.8
	Nitrate Ion	76.7	95.8	111.7	91.1
	Ammonium Ion	51.8	58.3	57.8	60.8
	Organic Carbon	61.9	61.1	59.1	55.8
	Elemental Carbon	161.5	134.0	136.9	154.0

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 bias, error, fractional bias, and fractional error for both daily maximum 1-hr ozone and daily maximum 8-hr ozone (Boylan and Russell, 2006).

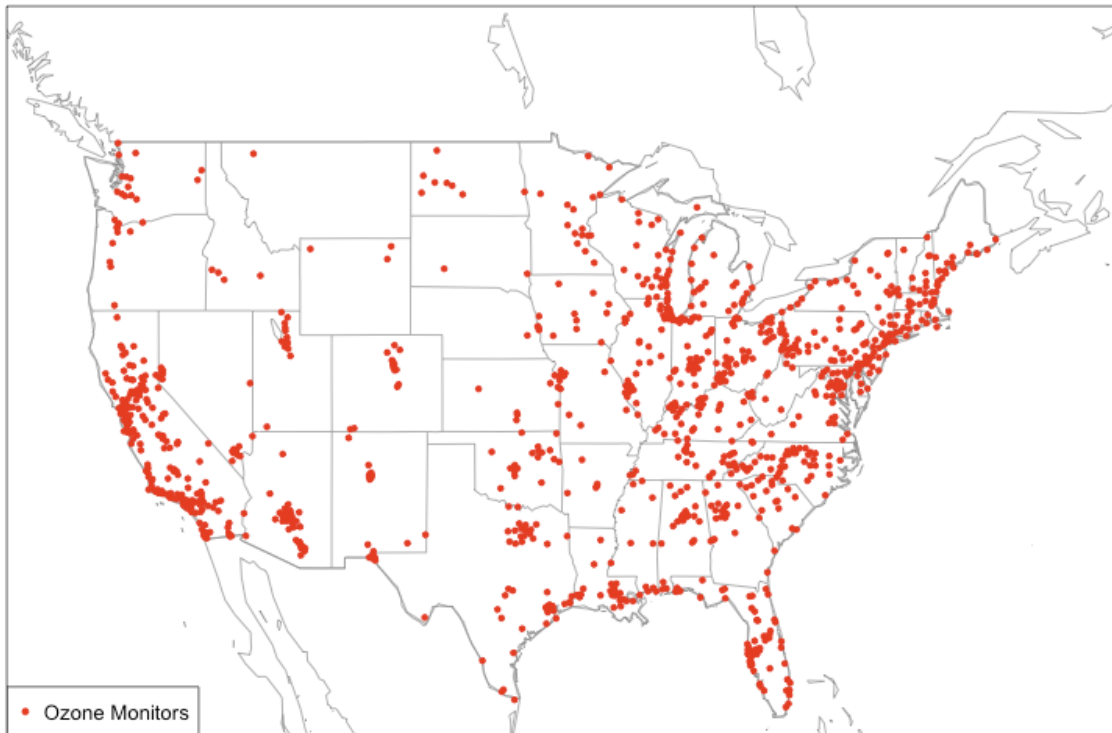


Figure III-2. Ozone monitors used in the model performance evaluation.

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.

		Month				
		5	6	7	8	9
N	Daily peak 1-hr ozone	7,173	9,553	9,522	8,433	7,118
	Daily peak 8-hr ozone	7,180	9,557	9,529	8,437	7,120
Mean observed (ppb)	Daily peak 1-hr ozone	75	79	81	81	78
	Daily peak 8-hr ozone	68	71	72	71	70
Mean predicted (ppm)	Daily peak 1-hr ozone	68	74	78	77	72
	Daily peak 8-hr ozone	63	68	70	69	64
Bias (ppb)	Daily peak 1-hr ozone	-7	-5	-3	-4	-6
	Daily peak 8-hr ozone	-6	-4	-1	-2	-5
Error (ppb)	Daily peak 1-hr ozone	9	9	11	11	10
	Daily peak 8-hr ozone	8	8	9	9	9
Fractional bias (%)	Daily peak 1-hr ozone	-9	-7	-5	-6	-9
	Daily peak 8-hr ozone	-9	-6	-2	-4	-8
Fractional error (%)	Daily peak 1-hr ozone	13	12	14	14	14
	Daily peak 8-hr ozone	12	11	12	13	13

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. Previous versions of the CMAQ modeling system has been applied by other researchers at a continental and regional scale and evaluation has been published (Bullock et al., 2008, 2009; Lin et al., 2007; Pongprueksa et al., 2008; Vijayaraghavan et al., 2007).

Model performance is characterized using a variety of statistical metrics common in photochemical model evaluation journal articles: bias, error, fractional bias, and fractional error (Boylan and Russell, 2006). These metrics are estimated for total mercury wet deposition and for rainfall. Performance is best when the metrics approach 0. The fractional bias and error metrics are bound by $\pm 200\%$, which would be considered poor performance.

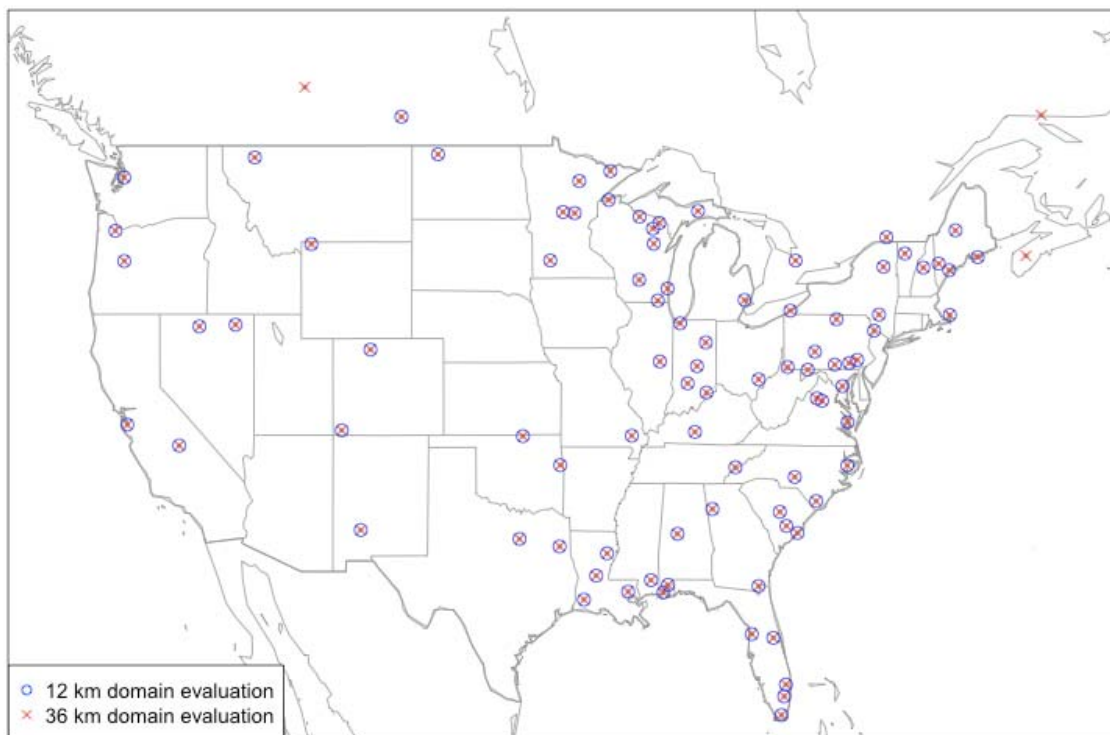


Figure III-1. Mercury deposition network monitors used for evaluation of the 12 and 36 km domains.

CMAQ estimates of total mercury wet deposition are paired in space and time with MDN observations. Model performance metrics are averaged by season and shown in Table III-3 for the 12 km domain and Table III-4 for the 36 km model domain. Other published mercury modeling studies show a positive bias for annual total mercury wet deposition (Bullock et al., 2009; Lin et al., 2007; Vijayaraghavan et al., 2007). This CMAQ application also shows an over prediction bias except during the summer months in the eastern United States.

An annual mercury modeling application done by ENVIRON and Atmospheric and Environmental Research for Lake Michigan Air Directors Consortium show seasonal average normalized bias between 70 and 158% and seasonal average normalized error between 72 and 503% (Yarwood et al, 2003). The model performance shown by EPA is consistent with other long term mercury modeling applications and often more robust in terms of estimated metrics that are more stringently paired in space and time before averaging to an annual or seasonal temporal scale (Seigneur et al., 2006; Vijayaraghavan et al., 2008).

TABLE III-3. Model performance metrics for mercury wet deposition and rainfall by quarter. 12 km domain.

		12 km Domain			
Quarter		1	2	3	4
Total Mercury Wet Deposition	N	753	795	773	733
	Observed (ng/m ²)	155	255	317	134
	Predicted (ng/m ²)	290	314	183	209
	Bias (ng/m ²)	135	59	-134	75
	Error (ng/m ²)	185	240	246	136
	Fractional Bias (%)	37	11	-46	28
	Fractional Error (%)	80	83	97	81
Rainfall	N	753	795	773	733
	Observed (mm)	23	24	27	27
	Predicted (mm)	23	28	31	23
	Bias (mm)	-0.04	3.43	4.67	-3.52
	Error (mm)	10	16	23	11
	Fractional Bias (%)	3	5	1	-3
	Fractional Error (%)	14	19	22	15

TABLE III-4. Model performance metrics for mercury wet deposition and rainfall by quarter. 36 km domain.

		36 km Domain			
Quarter		1	2	3	4
Total Mercury Wet Deposition	N	783	822	797	754
	Observed (ng/m ²)	152	252	313	133
	Predicted (ng/m ²)	262	276	187	183
	Bias (ng/m ²)	110	24	-125	50
	Error (ng/m ²)	165	211	235	114
	Fractional Bias (%)	29	6	-40	19
	Fractional Error (%)	82	84	91	79
Rainfall	N	783	822	797	754
	Observed (mm)	23	24	27	27
	Predicted (mm)	21	24	29	21
	Bias (mm)	-1.73	-0.09	1.87	-6.16
	Error (mm)	10	15	20	12
	Fractional Bias (%)	1	2	0	-5
	Fractional Error (%)	14	19	21	15

IV. Post Processing Mercury Deposition

CMAQ outputs hourly wet and dry deposition estimates (kg/ha) in each grid cell of speciated mercury: Hg⁰, Hg², and PM_{2.5} Hg. Hourly outputs are summed 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. Where both the eastern and western 12 km domains intersect in the integrated 12 km domain, the average of the 12 km eastern US and 12 km western US is assigned to the integrated 12 km domain. Total mercury deposition is defined as the sum of all wet and dry deposition of elemental mercury, divalent gas-phase mercury, and PM_{2.5} mercury.

V. References

- Appel, K.W., Bhave, P.V., Gilliland, A.B., Sarwar, G., Roselle, S.J., 2008. Evaluation of the community multiscale air quality (CMAQ) model version 4.5: Sensitivities impacting model performance; Part II - particulate matter. *Atmospheric Environment* 42, 6057-6066.
- Appel, K.W., Gilliland, A.B., Sarwar, G., Gilliam, R.C., 2007. Evaluation of the Community Multiscale Air Quality (CMAQ) model version 4.5: Sensitivities impacting model performance Part I - Ozone. *Atmospheric Environment* 41, 9603-9615.
- Baker, K., Dolwick, P., 2009a. Meteorological Modeling Performance Evaluation for the Annual 2005 Continental U.S. 36-km Domain Simulation. US Environmental Protection Agency OAQPS.
- Baker, K., Dolwick, P., 2009b. Meteorological Modeling Performance Evaluation for the Annual 2005 Eastern U.S. 12-km Domain Simulation. US Environmental Protection Agency OAQPS, RTP.
- Baker, K., Dolwick, P., 2009c. Meteorological Modeling Performance Evaluation for the Annual 2005 Western U.S. 12-km Domain Simulation, in: EPA, U. (Ed.). US Environmental Protection Agency OAQPS.
- Boylan, J.W., Russell, A.G., 2006. PM and light extinction model performance metrics, goals, and criteria for three-dimensional air quality models. *Atmospheric Environment* 40, 4946-4959.
- Bullock, O.R., Atkinson, D., Braverman, T., Civerolo, K., Dastoor, A., Davignon, D., Ku, J.Y., Lohman, K., Myers, T.C., Park, R.J., Seigneur, C., Selin, N.E., Sistla, G., Vijayaraghavan, K., 2008. The North American Mercury Model Intercomparison Study (NAMMIS): Study description and model-to-model comparisons. *Journal of Geophysical Research-Atmospheres* 113.
- Bullock, O.R., Atkinson, D., Braverman, T., Civerolo, K., Dastoor, A., Davignon, D., Ku, J.Y., Lohman, K., Myers, T.C., Park, R.J., Seigneur, C., Selin, N.E., Sistla, G., Vijayaraghavan, K., 2009. An analysis of simulated wet deposition of mercury from the North American Mercury Model Intercomparison Study. *Journal of Geophysical Research-Atmospheres* 114.
- Bullock, O.R., Brehme, K.A., 2002. Atmospheric mercury simulation using the CMAQ model: formulation description and analysis of wet deposition results. *Atmospheric Environment* 36, 2135-2146.
- Byun, D., Schere, K.L., 2006. Review of the governing equations, computational algorithms, and other components of the models-3 Community Multiscale Air Quality (CMAQ) modeling system. *Applied Mechanics Reviews* 59, 51-77.
- Carlton, A.G., Bhave, P.V., Napelenok, S.L., Edney, E.D., Sarwar, G., Pinder, R.W., Pouliot, G.A., Houyoux, M., 2010. Model Representation of Secondary Organic Aerosol in CMAQv4.7. *Environmental Science & Technology* 44, 8553-8560.
- Carlton, A.G., Turpin, B.J., Altieri, K.E., Seitzinger, S.P., Mathur, R., Roselle, S.J., Weber, R.J., 2008. CMAQ Model Performance Enhanced When In-Cloud Secondary Organic Aerosol is Included: Comparisons of Organic Carbon Predictions with Measurements. *Environmental Science & Technology* 42, 8798-8802.
- Doraiswamy, P., Hogrefe, C., Hao, W., Civerolo, K., Ku, J., Sistla, G., 2010. A Retrospective Comparison of Model-Based Forecasted PM_{2.5} Concentrations with Measurements. *Journal of Air & Waste Management Association* 60, 1293-1308.
- Gery, M.W., Whitten, G.Z., Killus, J.P., Dodge, M.C., 1989. A Photochemical Kinetics Mechanism for Urban and Regional Scale Computer Modeling. *Journal of Geophysical Research-Atmospheres* 94, 12925-12956.

- Houyoux, M.R., Vukovich, J.M., Coats, C.J., Wheeler, N.J.M., Kasibhatla, P.S., 2000. Emission inventory development and processing for the Seasonal Model for Regional Air Quality (SMRAQ) project. *Journal of Geophysical Research-Atmospheres* 105, 9079-9090.
- Lin, C.J., Pongprueks, P., Russell Bullock, O., Lindberg, S.E., Pehkonen, S.O., Jang, C., Braverman, T., Ho, T.C., 2007. Scientific uncertainties in atmospheric mercury models II: Sensitivity analysis in the CONUS domain. *Atmospheric Environment* 41, 6544-6560.
- Nenes, A., Pandis, S.N., Pilinis, C., 1998. ISORROPIA: A new thermodynamic equilibrium model for multiphase multicomponent inorganic aerosols. *Aquatic Geochemistry* 4, 123-152.
- Pongprueksa, P., Lin, C.J., Lindberg, S.E., Jang, C., Braverman, T., Bullock, O.R., Ho, T.C., Chu, H.W., 2008. Scientific uncertainties in atmospheric mercury models III: Boundary and initial conditions, model grid resolution, and Hg(II) reduction mechanism. *Atmospheric Environment* 42, 1828-1845.
- Seigneur, C., Lohman, K., Vijayaraghavan, K., Jansen, J., Levin, L., 2006. Modeling atmospheric mercury deposition in the vicinity of power plants. *Journal of the Air & Waste Management Association* 56, 743-751.
- Selin, N.E., Jacob, D.J., Park, R.J., Yantosca, R.M., Strode, S., Jaegle, L., Jaffe, D., 2007. Chemical cycling and deposition of atmospheric mercury: Global constraints from observations. *Journal of Geophysical Research-Atmospheres* 112.
- Slemr, F., Brunke, E.G., Ebinghaus, R., Kuss, J., 2011. Worldwide trend of atmospheric mercury since 1995. *Atmospheric Chemistry and Physics* 11, 4779-4787.
- Streets, D.G., Zhang, Q., Wu, Y., 2009. Projections of Global Mercury Emissions in 2050. *Environmental Science & Technology* 43, 2983-2988.
- Tesche, T.W., Morris, R., Tonnesen, G., McNally, D., Boylan, J., Brewer, P., 2006. CMAQ/CAMx annual 2002 performance evaluation over the eastern US. *Atmospheric Environment* 40, 4906-4919.
- USEPA, 2007. Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM_{2.5}, and Regional Haze, RTP.
- USEPA, 2010. Air Quality Modeling Technical Support Document: Boiler Source Sector Rules (EPA-454/R-10-006), Research Triangle Park, North Carolina.
- Vijayaraghavan, K., Karamchandani, P., Seigneur, C., Balmori, R., Chen, S.-Y., 2008. Plume-in-grid modeling of atmospheric mercury. *Journal of Geophysical Research-Atmospheres* 113.
- Vijayaraghavan, K., Seigneur, C., Karamchandani, P., Chen, S.Y., 2007. Development and application of a multipollutant model for atmospheric mercury deposition. *Journal of Applied Meteorology and Climatology* 46, 1341-1353.
- Yarwood, G, Lau, S., Jia, Y., Karamchandani, P., Vijayaraghavan, K. 2003. Final Report: Modeling Atmospheric Mercury Chemistry and Deposition with CAMx for a 2002 Annual Simulation. Prepared for Wisconsin Department of Natural Resources. http://www.gypsymoth.wi.gov/air/toxics/mercury/hg_X97579601_appB.pdf

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