United States Environmental Protection Agency

Air Quality Modeling Technical Support Document: Final EGU NESHAP

EPA-454/R-11-009
October 2011

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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 the final National Emissions Standard for Hazardous Air Pollutants (NESHAP) related to electrical generating utilities. 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 PM2.5 concentrations, 8-hr maximum ozone, 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 other air pollutants. 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 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. 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 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. Specifically, we compare a 2017 reference scenario to a 2017 control scenario. 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

The Community Multi-scale Air Quality (CMAQ) model v4.7.1 (www.cmaq-model.org) is a state of the science three-dimensional Eularian “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 other pollutants 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).

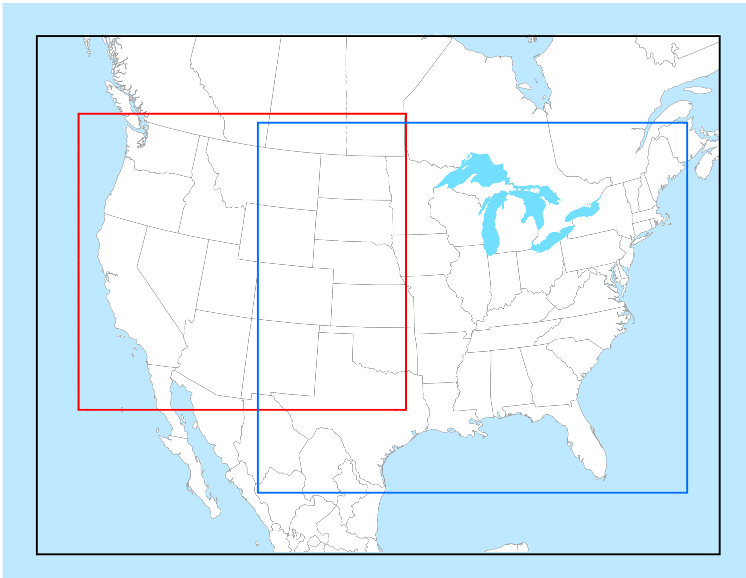
B. Model domain and grid resolution

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, 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 v4.3 platform. Emissions are processed to photochemical model inputs with the SMOKE emissions modeling system (Houyoux et al., 2000). The 2017 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 2017 reference case. The 2005 v4 platform projection factors were the starting point for most of the 2017 SMOKE-based projections. The estimated total anthropogenic emissions and emissions for the utility sector used in this modeling assessment over the entire model domain are shown in Table II.2.

Table II.2 Model domain total estimated total inventory and EGU sector emissions for each modeling scenario.

Scenario	Sector	CO	NOX	NH3	SO2	SULF	Primary PM2.5
2005 baseline	EGU (PTIPM)	603,788	3,729,157	21,995	10,380,870	224,859	496,874
	All Other	102,946,238	22,523,479	4,805,389	6,675,740	88,714	4,567,808
2017 baseline	EGU (PTIPM)	873,345	1,930,767	40,259	3,281,361	73,994	276,428
	All Other	71,652,291	16,171,166	4,998,214	6,063,388	50,506	4,040,380
2017 control case	EGU (PTIPM)	707,641	1,789,788	35,493	1,866,245	41,592	223,319
	All Other	71,652,291	16,171,166	4,998,214	6,063,388	50,506	4,040,380

Other North American emissions 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 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-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 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. Initial and boundary conditions for the projected future year 36 km simulations are the same as the 2005 base year.

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 (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.

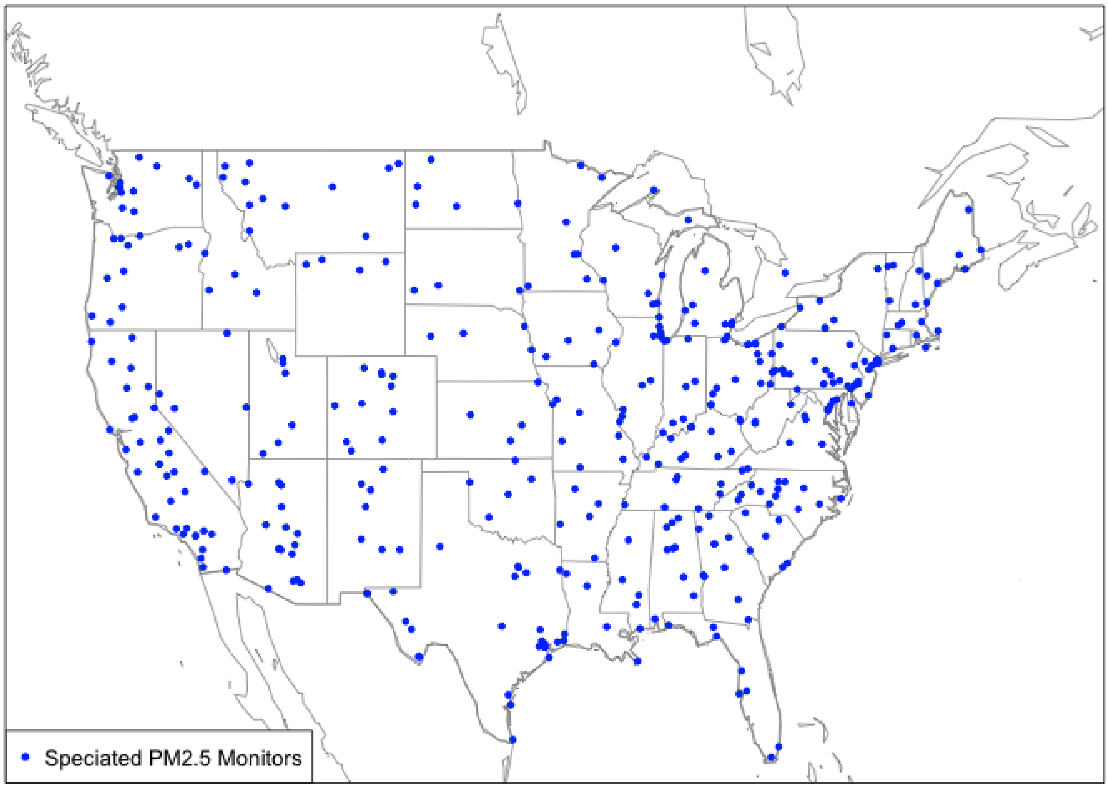


Figure III-1. Speciated PM2.5 monitors included in the model performance evaluation.

Model performance statistics were calculated for observed/predicted pairs of daily concentrations. Metrics estimated include bias, error, fractional bias, and fractional error (Boylan and Russell, 2006; USEPA, 2007). The aggregated metrics and number (N) of prediction-observation pairs are shown by chemical specie and quarter in Table III-1. Performance is best when metrics approach 0. The fractional bias and error metrics are bound by 200%, which would represent poor model performance. 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 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 PM2.5 concentrations for the purposes of this assessment.

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

		Quarter			
	Specie	1	2	3	4
N	Sulfate Ion	8,493	8,916	8,229	8,155
	Nitrate Ion	8,143	8,518	7,942	8,016
	Ammonium Ion	4,723	4,746	4,546	4,461
	Organic Carbon	8,038	8,485	7,939	7,874
	Elemental Carbon	8,543	8,857	8,145	8,218
Mean Observed (ug/m^3)	Sulfate Ion	2.1	3.0	4.3	2.0
	Nitrate Ion	2.1	0.8	0.5	1.4
	Ammonium Ion	1.7	1.4	1.7	1.3
	Organic Carbon	1.7	1.8	2.3	2.2
	Elemental Carbon	0.5	0.4	0.5	0.6
Mean Predicted (ug/m^3)	Sulfate Ion	1.9	2.7	3.4	1.9
	Nitrate Ion	1.9	0.9	0.4	1.4
	Ammonium Ion	1.2	1.2	1.1	1.1
	Organic Carbon	1.7	1.2	1.6	1.5
	Elemental Carbon	0.8	0.6	0.7	0.8
Bias (ug/m^3)	Sulfate Ion	-0.2	-0.2	-0.8	-0.1
	Nitrate Ion	-0.1	0.2	-0.1	0.1
	Ammonium Ion	0.0	0.2	-0.2	0.2
	Organic Carbon	0.0	-0.7	-0.7	-0.6
	Elemental Carbon	0.3	0.2	0.2	0.2
Error (ug/m^3)	Sulfate Ion	0.9	1.0	1.4	0.6
	Nitrate Ion	1.3	0.7	0.5	1.1
	Ammonium Ion	0.8	0.7	0.7	0.7
	Organic Carbon	1.0	1.0	1.2	1.2
	Elemental Carbon	0.5	0.3	0.4	0.4
Fractional Bias (%)	Sulfate Ion	0.2	-3.8	-11.9	6.2
	Nitrate Ion	-33.0	-47.2	-85.5	-25.5
	Ammonium Ion	4.5	27.3	7.6	27.5
	Organic Carbon	0.8	-35.8	-33.1	-23.2
	Elemental Carbon	29.8	16.9	22.3	13.4
Fractional Error (%)	Sulfate Ion	43.3	35.3	39.6	39.1
	Nitrate Ion	86.3	103.5	119.8	97.8
	Ammonium Ion	50.9	56.4	56.6	59.4
	Organic Carbon	55.2	62.2	59.9	60.1
	Elemental Carbon	63.3	60.9	60.8	58.1

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).

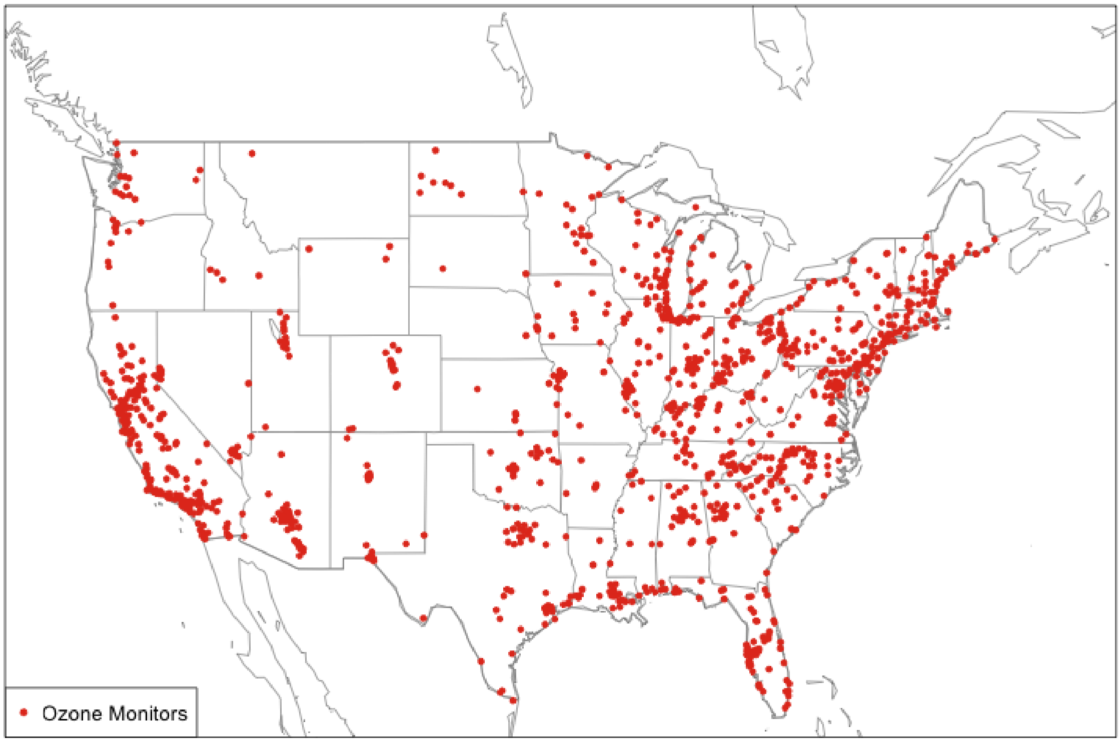


Figure III-2. Ozone monitors included in model performance evaluation.

The ozone metrics covered in this evaluation include one-hour and eight-hour average daily maximum ozone bias, error, fractional bias, and fractional error (Boylan and Russell, 2006; USEPA, 2007). 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 ozone season month are shown in Table III-2.

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

		Month					
		4	5	6	7	8	9
N	Daily 1-hr maximum	5,704	7,173	9,553	9,522	8,433	7,118
	Daily 8-hr maximum	5,705	7,180	9,557	9,529	8,437	7,120
Mean observed (ppb)	Daily 1-hr maximum	73	75	79	81	81	78
	Daily 8-hr maximum	68	68	71	72	71	70
Mean predicted (ppb)	Daily 1-hr maximum	64	67	72	77	75	70
	Daily 8-hr maximum	59	62	66	70	68	64
Bias (ppb)	Daily 1-hr maximum	-9	-8	-7	-4	-5	-8
	Daily 8-hr maximum	-9	-7	-5	-2	-3	-6
Error (ppb)	Daily 1-hr maximum	10	10	10	11	11	10
	Daily 8-hr maximum	9	8	8	9	9	9
Fractional bias (%)	Daily 1-hr maximum	-13	-12	-10	-6	-7	-11
	Daily 8-hr maximum	-14	-11	-8	-3	-5	-10
Fractional error (%)	Daily 1-hr maximum	14	14	14	14	15	14
	Daily 8-hr maximum	15	13	12	12	13	13

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

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United States Environmental Protection Agency	Office of Air Quality Planning and Standards Air Quality Assessment Division Research Triangle Park, NC	Publication No. EPA-454/R-11-009 October 2011