Air Quality Modeling Technical Support Document: National Emission Standards for Hazardous Air Pollutants from the Portland Cement Manufacturing Industry

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U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Air Quality Assessment Division
Research Triangle Park, NC 27711
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I Introduction

This document describes the air quality modeling performed by EPA in support of the Portland Cement NESHAP. 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, total mercury deposition, 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.

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 are slightly different than the final adjusted cement kiln 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

The 2005-based CAMx modeling platform was used as the basis for the air quality modeling for this final 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 platform is intended to support a variety of regulatory and research model applications and analyses. This modeling platform and analysis is described below.

A. Model version

CAMx version 5.10 is a freely available computer model that simulates the formation and fate of photochemical oxidants, 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 (Nobel, McDonald-Buller et al. 2001; Baker and Scheff 2007; Russell 2008). CAMx is applied with ISORROPIA inorganic chemistry (Nenes, Pandis 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, Brost et al. 1987), and Carbon Bond 05 (CB05) gas-phase chemistry module (Gery, Whitten et al. 1989; ENVIRON 2008).

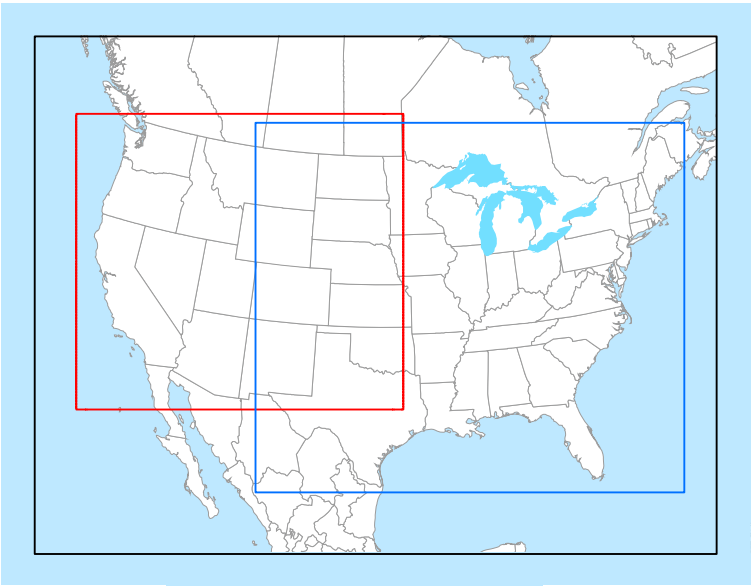
B. Model domain and grid resolution

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 did not change over the simulations. In turn, 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 emission standard program changes. Table II-1 provides some basic geographic information regarding 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 domain. 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.

D. Model Inputs: Emissions, Meteorology and Boundary Conditions

The 2005-based modeling platform was used for the air quality modeling of future emissions scenarios. As noted in the introduction, in addition to the CAMx model, the modeling platform also consists of the base- and future-year emissions estimates (both anthropogenic and biogenic), 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 platform. The emissions cases use some different emissions data than the official v4 platform to use data intended only for the rule development and not for general use. Unlike the 2005 v4 platform, the configuration for this modeling application included some additional hazardous air pollutants (HAPs) and a cement kiln sector emissions inventory more consistent with the engineering analysis of potential control options.

The 2013 reference case is intended to represent the emissions associated with growth and controls in that year. The US 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 2013 (though hydrochloric acid was not modeled). Both control and growth factors were applied to a subset of the 2005 non-EGU point and nonpoint to create the 2013 reference case. The 2002 v3.1 platform 2020 projection factors were the starting point for most of the 2013 SMOKE-based projections.

The 2013 reference scenario for the cement kiln sector assumed no growth or control for the industry from the 2005 sector emissions estimates with the exception that facilities that closed between 2005 and 2010 were removed from the 2013 inventory. The length of time required to conduct emissions and photochemical modeling preclude the use of the final facility specific emissions estimates based on controls implemented for this rule. A 2013 “control” or emissions adjustment case was developed by removing all Portland Cement sector emissions from the 2013 baseline inventory. Portland Cement sector emissions in this analysis refer to facilities that burn hazardous waste and those that do not burn hazardous waste. This “zero-out” of the sector creates a policy space where potential controls would be maximized at all locations. Since this is unrealistic, the air quality estimates from the 2013 “zero-out” or “control” case are adjusted to reflect nation-wide estimates of control percentages by pollutant.

As part of the analysis for this rulemaking, the modeling system was used to calculate daily and annual PM2.5 concentrations, annual total mercury deposition levels and visibility impairment.

Model predictions are used in a relative sense to estimate scenario-specific, future-year design values of PM2.5 and ozone. Specifically, we compare a 2013 reference scenario, a scenario without the cement kiln controls, to a 2013 control scenario which includes the adjustments to the cement kiln 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 these parameters also considered percent changes between the control case and two future baselines.

Table II.2 2005 and estimated future year sector emissions

	Cement Kiln Emissions (TPY)	
Specie	**2005**	**Future Year Baseline**
Nitrogen Oxides	216,525	199,391
Volatile Organic Compounds	8,817	8,419
Sulfur Dioxide	158,560	149,013
Primary PM2.5	16,758	15,403
PM2.5 Mercury	0.8	0.7
Reactive Gas Phase Mercury	6.2	6.0
Elemental Mercury	3.8	3.6

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 x 10^5 for moisture fields. The 12 km domain nudging weighting factors were 1.0 x 10^4 for wind fields and temperatures and 1.0 x 10^5 for moisture fields.

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-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 CAMx using the MM5CAMx processor to derive the specific inputs.

Table II-3. 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

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 2009; Baker 2009; Baker 2009). 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 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.

E. Base Case Model Performance Evaluation

1. PM2.5

An operational model performance evaluation for PM2.5 and its related speciated components (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 CAMx hourly species predictions were aggregated to the averaging times of the measurements.

Model performance statistics were calculated for observed/predicted pairs of daily concentrations. These metrics are averaged by season. Statistics were generated for the following geographic groupings: domain wide Eastern and Western United States. The "acceptability" of model performance was judged by comparing our 2005 performance results to the range of performance found in recent regional PM2.5 model applications for other, non-EPA studies. Overall, the mean bias (bias) and gross mean error (error) statistics shown in Table II-4 and Table II-5 are within the range or close to that found by other groups in recent applications. The model performance results give us confidence that our application of CAMx using this modeling platform provides a scientifically credible approach for assessing PM2.5 concentrations for the purposes of this assessment. The number (N) of monitor locations used to estimate the aggregated metrics are shown by chemical specie, quarter, network, and domain in Table II-6.

TABLE II-4. Bias ($\mu g/m^3$) metric by quarter, network, and model domain.

Domain	Network	Quarter	Metric	SO4	NO3	NH4	OC	EC	CRUSTAL
EAST	IMPROVE	1	bias (ug/m3)	1.02	0.37	0.75	0.33	0.09	1.93
EAST	IMPROVE	2	bias (ug/m3)	0.37	-0.03	0.91	-0.14	-0.07	1.03
EAST	IMPROVE	3	bias (ug/m3)	-0.34	-0.06	0.88	0.08	-0.09	1.07
EAST	IMPROVE	4	bias (ug/m3)	0.79	0.34	0.98	0.08	0.01	1.54
EAST	CSN	1	bias (ug/m3)	1.53	0.55	0.54	0.61	0.49	3.82
EAST	CSN	2	bias (ug/m3)	0.58	0.11	0.28	-0.62	0.28	2.40
EAST	CSN	3	bias (ug/m3)	-0.42	-0.15	-0.15	-0.54	0.28	2.62
EAST	CSN	4	bias (ug/m3)	1.21	0.49	0.50	-0.13	0.29	3.41
WEST	IMPROVE	1	bias (ug/m3)	0.31	-0.04		0.03	0.03	0.66
WEST	IMPROVE	2	bias (ug/m3)	0.05	-0.24		-0.08	0.01	0.42
WEST	IMPROVE	3	bias (ug/m3)	-0.28	-0.21		0.39	0.05	0.70
WEST	IMPROVE	4	bias (ug/m3)	0.14	0.04		-0.17	-0.02	0.55
WEST	CSN	1	bias (ug/m3)	0.42	-0.44	0.14	-0.08	0.55	3.32
WEST	CSN	2	bias (ug/m3)	-0.04	-0.54	0.01	-0.26	0.35	1.61
WEST	CSN	3	bias (ug/m3)	-0.66	-0.82	-0.29	-0.13	0.44	1.90
WEST	CSN	4	bias (ug/m3)	0.14	-0.78	-0.13	-1.57	0.18	2.63

TABLE II-5. Gross error (μg/m^3) metric by quarter, network, and model domain.

Domain	Network	Quarter	Metric	SO4	NO3	NH4	OC	EC	CRUSTAL
EAST	IMPROVE	1	error (ug/m3)	1.23	0.99	0.86	0.63	0.20	1.93
EAST	IMPROVE	2	error (ug/m3)	1.43	0.40	1.09	0.61	0.19	1.04
EAST	IMPROVE	3	error (ug/m3)	1.77	0.21	1.14	0.55	0.17	1.08
EAST	IMPROVE	4	error (ug/m3)	1.03	0.74	1.01	0.57	0.17	1.54
EAST	CSN	1	error (ug/m3)	1.99	1.76	0.90	1.36	0.61	3.83
EAST	CSN	2	error (ug/m3)	1.85	0.84	0.76	1.18	0.45	2.41
EAST	CSN	3	error (ug/m3)	2.38	0.52	0.80	1.09	0.45	2.64
EAST	CSN	4	error (ug/m3)	1.55	1.22	0.73	1.39	0.57	3.45
WEST	IMPROVE	1	error (ug/m3)	0.43	0.54		0.35	0.13	0.67
WEST	IMPROVE	2	error (ug/m3)	0.50	0.34		0.42	0.12	0.43
WEST	IMPROVE	3	error (ug/m3)	0.56	0.25		0.80	0.16	0.71
WEST	IMPROVE	4	error (ug/m3)	0.34	0.49		0.49	0.14	0.58
WEST	CSN	1	error (ug/m3)	0.91	2.33	0.89	2.83	0.84	3.35
WEST	CSN	2	error (ug/m3)	0.79	0.84	0.44	1.23	0.52	1.62
WEST	CSN	3	error (ug/m3)	1.00	0.90	0.50	1.23	0.58	1.90
WEST	CSN	4	error (ug/m3)	0.71	2.46	0.96	3.21	0.85	2.74

TABLE II-6. Number (N) of monitors used for metric estimation by quarter, network, and model domain.

Domain	Network	Quarter	Metric	SO4	NO3	NH4	OC	EC	CRUSTAL
EAST	IMPROVE	1	N	2,586	2,586	409	2,666	2,670	2,419
EAST	IMPROVE	2	N	2,868	2,868	406	2,861	2,867	2,704
EAST	IMPROVE	3	N	2,633	2,633	394	2,585	2,573	2,411
EAST	IMPROVE	4	N	2,513	2,513	382	2,503	2,511	2,388
EAST	CSN	1	N	3,640	3,292	3,640	3,224	3,706	3,580
EAST	CSN	2	N	3,669	3,278	3,669	3,319	3,685	3,609
EAST	CSN	3	N	3,475	3,195	3,475	3,251	3,488	3,441
EAST	CSN	4	N	3,381	3,244	3,381	3,097	3,426	3,359
WEST	IMPROVE	1	N	2,833	2,833	0	2,740	2,760	2,548
WEST	IMPROVE	2	N	3,043	3,043	0	2,994	3,002	2,879
WEST	IMPROVE	3	N	2,648	2,648	0	2,632	2,615	2,462
WEST	IMPROVE	4	N	2,809	2,809	0	2,714	2,733	2,632
WEST	CSN	1	N	1,089	1,010	1,087	970	1,086	1,046
WEST	CSN	2	N	1,085	990	1,076	975	1,055	1,032
WEST	CSN	3	N	1,080	1,011	1,076	1,011	1,037	1,027
WEST	CSN	4	N	1,100	1,052	1,088	1,021	1,071	1,051

III. Model Results

As described above, we performed a series of air quality modeling simulations for the continental U.S in order to assess the impacts of emissions adjustments to the Portland cement kiln sector. We looked at impacts on future ambient PM2.5, total mercury deposition levels and visibility impairment. In this section, we present information on current and projected levels of pollution for 2013.

A. Impacts of Sector on Total Mercury Deposition

This section summarizes the results of our modeling of differences in total mercury deposition impacts in the future based on changes to the cement kiln emissions. Specifically, we compare a 2013 reference scenario to a 2013 emissions change scenario. Model results for the eastern and central United States indicate that total mercury deposition (wet and dry forms) would be reduced by a total of 44,946 µg/m^2. A reduction of 19,231 µg/m^2 is estimated for the western United States.

Figure III-1. Changes in Total Mercury Deposition (µg/m^2) Between the Reference Case and the Emissions Reduction Scenario for the Eastern and Central United States

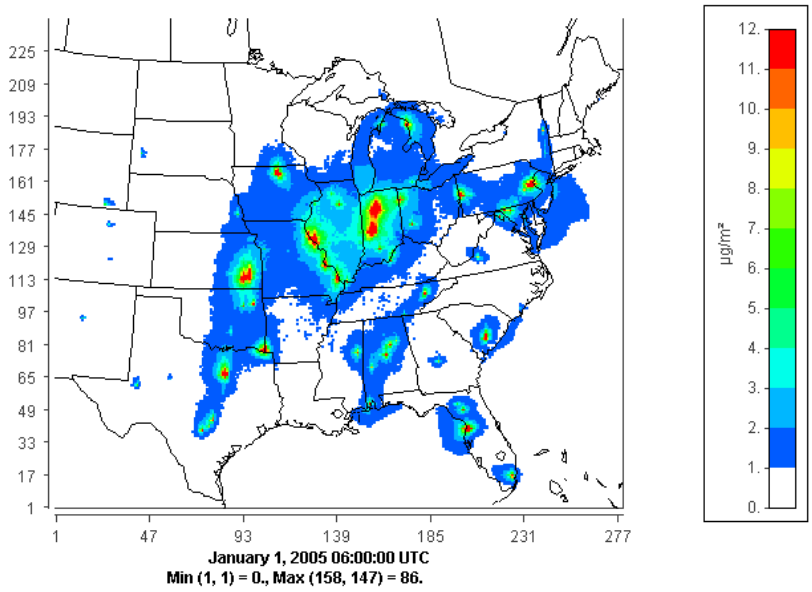
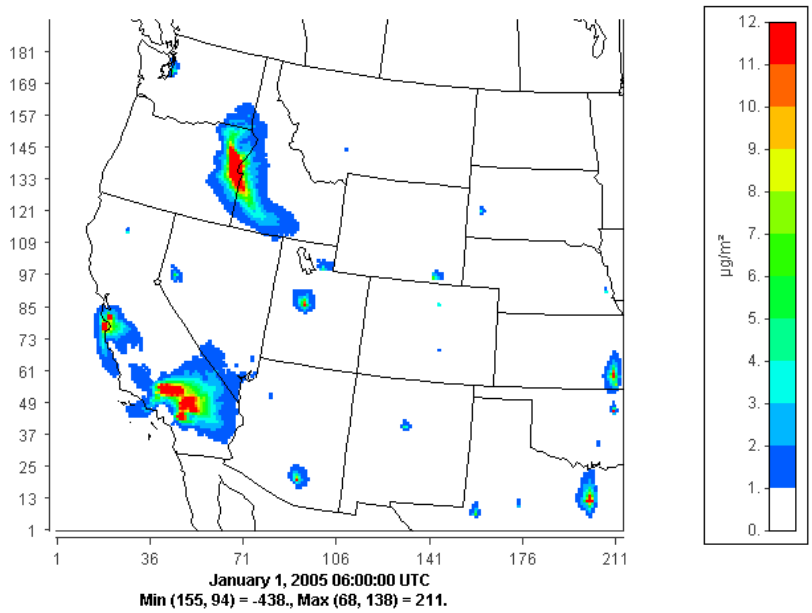


Figure III-2. Changes in Total Mercury Deposition (µg/m^2) Between the Reference Case and the Emissions Reduction Scenario for the Eastern and Central United States



The reductions to total annual mercury deposition estimated by the photochemical model show that the reductions tend to be greatest nearest the sources.

B. Impacts of Sector on Future Annual $PM_{2.5}$ Levels

This section summarizes the results of our modeling of annual average $PM_{2.5}$ air quality impacts in the future due to reductions in emissions from this sector. Specifically, we compare a 2013 reference scenario to a 2013 control scenario. The modeling assessment indicates a decrease up to 0.3 $\mu g/m^3$ in annual $PM_{2.5}$ design values is possible given an area's proximity to controlled sources and the amount of reduced sulfur dioxide and primary PM2.5 emissions. The median reduction over all monitor locations is 0.09 $\mu g/m^3$. An annual $PM_{2.5}$ design value is the concentration that determines whether a monitoring site meets the annual NAAQS for $PM_{2.5}$. The full details involved in calculating an annual $PM_{2.5}$ design value are given in appendix N of 40 CFR part 50. Projected air quality benefits are estimated using procedures outlined by United States Environmental Protection Agency modeling guidance (USEPA 2007).

C. Impacts of Sector on Future 24-hour $PM_{2.5}$ Levels

This section summarizes the results of our modeling of 24-hr average $PM_{2.5}$ air quality impacts in the future due to reductions in emissions from this sector. Specifically, we compare a 2013 reference scenario to a 2013 control scenario. The modeling assessment indicates a decrease up to 0.5 $\mu g/m^3$ in 24-hr average $PM_{2.5}$ design values at most monitor locations in the United States is possible given an area's proximity to controlled sources and the amount of reduced sulfur dioxide and primary PM2.5 emissions. The median reduction over all monitor locations is 0.1 $\mu g/m^3$. The maximum reduction was 1.5 $\mu g/m^3$ at a monitor located in Oklahoma. A 24-hour $PM_{2.5}$ design value is the concentration that determines whether a monitoring site meets the 24-hour NAAQS for $PM_{2.5}$. The full details involved in calculating a 24-hour $PM_{2.5}$ design value are given in appendix N of 40 CFR part 50. Projected air quality benefits are estimated using procedures outlined by United States Environmental Protection Agency modeling guidance (USEPA 2007).

D. Impacts of Sector on Future Visibility Levels

Air quality modeling conducted for this final rule was used to project visibility conditions in 138 mandatory Class I federal areas across the U.S. in 2013 (USEPA 2007). The level of visibility impairment in an area is based on the light-extinction coefficient and a unitless visibility index, called a "deciview", which is used in the valuation of visibility. The deciview metric provides a scale for perceived visual changes over the entire range of conditions, from clear to hazy. Under many scenic conditions, the average person can generally perceive a change of one deciview. Higher deciview values are indicative of worse visibility. Thus, an improvement in visibility is a decrease in deciview value. The modeling assessment indicates a decrease up to 0.31 deciviews in annual 20% worst visibility days is possible given an area's proximity to controlled sources and the amount of reduced sulfur dioxide and primary PM2.5 emissions. Median reductions are 0.01 deciviews to the 20% worst days and 20% best days over all monitor locations.

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