Air Quality Modeling Technical Support Document: Boiler Source Sector Rules

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I Introduction

This document describes the air quality modeling performed by EPA in support of the National Emission Standards for Hazardous Air Pollutants for Industrial, Commercial, and Institutional Boilers and Process Heaters. 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 concentrations for particulate matter less than 2.5 microns (PM2.5) c, 8-hr maximum ozone, 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 boiler 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. Photochemical model source apportionment tracks the formation and transport of primarily and secondarily formed pollutants from emissions sources and allows the estimation of contributions at receptors. This type of emissions apportionment is useful to understand what types of sources or regions are contributing to pollutants estimated by photochemical grid models.

The 2005-based CAMx 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 platform is intended to support a variety of regulatory and research model applications and analyses. 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, 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 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

CAMx version 5.20 is a freely available computer model that simulates the formation and fate of photochemical oxidants, ozone, primary and secondary PM concentrations, and air toxics, over regional and urban spatial scales for given input sets of meteorological conditions and emissions. CAMx includes numerous science modules that simulate the emission, production, decay, deposition and transport of organic and inorganic gas-phase and particle-phase pollutants in the atmosphere (Baker and Scheff, 2007; Nobel et al., 2001; Russell, 2008). CAMx is applied with ISORROPIA inorganic chemistry (Nenes et al., 1999), a semi-volatile equilibrium scheme to partition condensable organic gases between gas and particle phase (Strader et al., 1999), Regional Acid Deposition Model (RADM) aqueous phase chemistry (Chang et al., 1987), and Carbon Bond 05 (CB05) gas-phase chemistry module (ENVIRON, 2008; Gery et al., 1989).

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

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

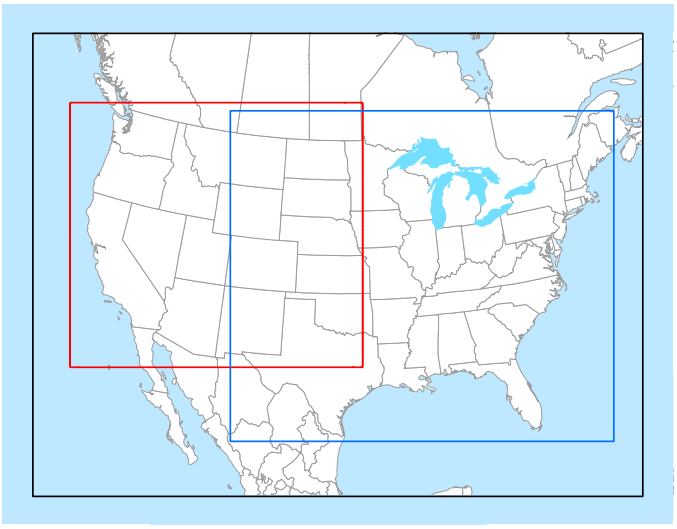
B. Model domain and grid resolution

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

2005 baseline emissions

The emissions data used in the 2005 base year are from the EPA's 2005-based v4.1 modeling platform. This platform is based on the 2005 National Emissions Inventory (NEI), version 2. Emissions were processed to photochemical model inputs with the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system (Houyoux et al., 2000).

This platform includes criteria pollutants and precursors: particulate matter less than 10 microns (PM10), PM2.5, nitrogen oxides (NO_X), sulfur dioxide (SO_2), carbon monoxide (CO), volatile organic compounds (VOC), ammonia (NH_3) and hazardous air pollutants (HAP): hydrogen chloride, chlorine and mercury. Additionally, for some sectors, HAP emissions of benzene, formaldehyde, acetaldehyde and methanol are used from the inventory for chemical speciation VOC. For this rule, mercury emissions were added to the v4.1 platform to reflect the needs for the rule development and these not intended for more general use. The mercury emissions included in this platform are primarily from the 2005 National Air Toxics Assessment (NATA) inventory, which was updated from the 2005 NEI v2 in order to incorporate updated data for particular source categories such as cement and hazardous waste incineration, and also revised from comments from state and local inventory providers as a result of NATA review.

This inventory was further modified to remove sources that were found to have shut down prior to 2005 and to update the gold mine emissions per information collected during the Gold Mine Ore and Production NESHAP. In addition, mercury emissions were revised for the boiler sector to allow for greater consistency with the Information Collection Request (ICR) data collected for this rule. In particular, we used the unit-specific ICR mercury emissions for all ICR facilities that could be mapped to the NATA Inventory.[1] We used the NEI to add important emissions release point information necessary for photochemical grid modeling such as geographic

[1] The "NEI_UNIQUE_ID" field was used to map the ICR facilities to the NATA inventory. We used 7032 units' Hg emissions out of 7,738 total units in the ICR. These 7032 units from the ICR sum to 4.66 tons. ICR emissions that were not included sum to 0.177 tons.

coordinates, stack coordinates, stack release height, exit temperature, exit velocity because the ICR lacks this information.

The replacement of the NATA mercury with the ICR mercury is described in more detail below. ICR emissions were not used directly for any other pollutants used in the v4.1 platform; however they informed numerous corrections and updates to the inventory including the removal of duplicates and facilities that had shut down prior to 2005, and the inclusion of control information.

The stationary inventory used in the v4.1 platform is separated into modeling sectors such as EGU point (ptipm), non-EGU point (ptnonipm), and stationary emissions not included in the point source inventories (nonpt). This nonpoint category is generally referred to as the "area" source inventory, and this category is not a direct representation of sources classified as area sources for the purposes of National Emissions Standards for Hazardous Air Pollutants (NESHAP) and Maximum Available Control Technology (MACT) standards.

2005 ICR emissions data integration with NEI for stationary sources

For the non-EGU point sector (ptnonipm), a cross-walk was developed and applied to remove boiler and process heater mercury emissions from the 2005 NATA inventory at facilities with identification information that matched facilities in the ICR database. This cross-walk identified inventory sources with boiler and process header source classification codes (SCCs) in the inventory that were also associated with facilities that matched the ICR database. All nonpoint (nonpt) boiler mercury emissions were removed from the inventory to eliminate the possibility of double counting of emissions with those added from the boiler ICR data. The boiler mercury emissions from the ICR database were then added to the inventory in place of these emissions.

In addition, boiler mercury emissions were removed from facilities in the EGU point sector (ptipm) that matched facilities in the ICR database and that had unit design capacity less than 25 MW according to the 2006 version 3.02 National Electric Energy Database System (NEEDS) database (http://www.epa.gov/airmarkt/progsregs/epa-ipm/past-modeling.html#needs). If design capacity was missing and a unit had been identified in the NATA inventory as being subject to the Boiler MACT (based on the "MACT Code" inventory field) then its mercury emissions were also removed from this modeling sector inventory.

The specific procedure used to replace the Hg emissions in the NATA inventory with the ICR data is detailed below.

Non-EGU point (ptnonipm) sector:

- Apply a crosswalk containing Maximum Achievable Control Technology (MACT), Standard Industrial Classification (SIC) and Source Classification Codes (SCC) and North American Industry Classsification (NAICS) codes that map to the boiler source category to the NATA inventory. This crosswalk contains nearly 4500 combinations of the above codes.

- Remove only facilities that match facilities in the ICR database (based on the NEI_UNIQUE_ID field)
- Add all Hg emissions from the ICR database that include an NEI_UNIQUE_ID (this procedure added all but 0.177 tons (3.7% of the total) Hg in the ICR database.

EGU Point (ptipm) sector:

- Remove units from facilities that matched to the ICR database whereby
  - Design capacity of the unit is less than 25 Megawatts (MW)
  - Or, if no design capacity was available, removed units that had a MACT code representing the boiler MACT category in the NATA inventory

Non-point/area (nonpt) sector:

- Remove nonpoint boiler Hg emissions to prevent double counting.
- Boiler emissions in the nonpoint inventory utilized a crosswalk of MACT and SCC codes shown in Table II-5.

The resulting emissions for the boiler sector in the modeling inventory are 4.7[2] tons and all were included in the ptnonipm sector.

Future Year Baseline Emissions

The 2016 baseline emissions are intended to represent the emissions associated with growth and controls in 2016. The projections used for this effort are unique to this project and are not associated with a particular modeling platform.

The EGU point source (ptipm) emissions estimates for the future year reference were created by the Integrated Planning Model (IPM) version 3.02 for criteria pollutants, hydrochloric acid, and mercury in 2015[3]. For the non-EGU point (ptnonipm) and nonpoint (nonpt) sectors, both control and growth factors were applied to a subset of the 2005 v4.1 platform data to create the 2016 reference case. The 2014 projection factors developed for the Transport Rule proposal (see http://www.epa.gov/ttn/chief/emch/index.html#transport) were further enhanced and updated for these 2016 baseline projections.

The projected inventory incorporates emissions projections for the proposed Transport Rule, cement kiln NESHAP, RICE NESHAP, gold mine NESHAP, changes to boiler emissions based on the ICR database developed for this rule, and known consent decrees. A complete list of rules included in the future point source baseline inventory is shown in Table II-2.

[2] 4.66 tons from the ICR and 0.02 tons from NATA Hg inventory sources that were not covered by the ICR but were in the NATA Hg inventory and were added to the universe to be tagged as Boiler MACT sources.
[3] The 2015 IPM run represents the average of 2014 to 2016.

Table II-2. Control strategies and/or growth assumptions included in the 2016 projection

Projections Carried Forward from the proposed Transport Rule[1,2]	
Description	**Pollutants**
MACT rules, national, VOC: national applied by SCC, MACT	VOC
Consent Decrees and Setttlements, including refinery consent decrees, and settlements for: 1) Alcoa, TX and 2) Premcor (formerly MOTIVA), DE	All
Municipal Waste Combustor Reductions –plant level	PM
Hazardous Waste Combustion	PM
Hospital/Medical/Infectious Waste Incinerator Regulations under Section 129d/11 1d	NOX, PM, SO_2
Large Municipal Waste Combustors – growth applied to specific plants	All
MACT rules, plant-level, VOC: Auto Plants	VOC
MACT rules, plant-level, PM & SO2: Lime Manufacturing	PM, SO_2
MACT rules, plant-level, PM: Taconite Ore	PM
Municipal Waste Landfills: project factor of 0.25 applied	All
Livestock Emissions Growth from year 2002 to 2016	NH_3, PM
Residential Wood Combustion Growth and Changeouts from year 2005 to year 2016	All
Gasoline Stage II growth and control from year 2005 to year 2016	VOC
Portable Fuel Container MSAT2 inventory growth and control from year 2005 to year 2016	VOC
Additional Projections Used In Boiler MACT modeling[3]	
Emission Reductions resulting from controls put on specific boiler units (not due to MACT) after 2005, identified through analysis of the control data gathered from the ICR from the ICI Boiler NESHAP.	NOX, SO2, HCL
NESHAP: Portland Cement (09/09/10) – plant level based on Industrial Sector Integrated Solutions (ISIS) policy emissions in 2013. The ISIS results are from the ISIS-Cement model runs for the NESHAP and NSPS analysis of July 28, 2010.	HG, NOX, SO_2, PM, HCL
NESHAP: Gold Mine Ore Processing and Production Area Source Category (based on proposed rule 04-15-10) – finalized 12/2010	HG
New York SIP reductions	VOC, NOX
Additional plant and unit closures	All
NESHAP: Reciprocating Internal Combustion Engines[4]	NOX, CO, PM

1. They were only changed in that the projection year was 2015 or 2016, rather than 2012 / 2014.
2. We inadvertently did not apply closures that had been applied for the Transport Rule proposal; emissions from these plants sum to 3300 tons VOC, 178 tons PM2.5, 1982 tons SO2, 1639 tons NOX, 6 tons NH3 and 379 tons CO. At the state level, the largest impact is in West Virginia (717 tons NOX, which is 2% of emissions in ptnonipm) and 1604 tons SO2 which is 7% of the ptnonipm sector. When considering emissions from other sectors, the percentages will be much smaller. All other errors are under 500 tons (less than 1% of the ptnonipm sector)
3. We inadvertently did not apply LaFarge and SaintGobain consent decrees- since one of the LaFarge facilities was already covered in the cement ISIS projections, the reductions missed were lower than estimated by the consent decree were on the order of 20,000 tons SO2, 15,000 tons NOX, 400 tons HCL, 200 tons PM2.5
4. Note that SO2 reductions are expected to occur to due fuel sulfur limits but were excluded from the projection. They were expected to reduce SO2 by 27,000 tons, nationwide

The 2016 onroad emissions reflect control program implementation through 2016 and include the Light-Duty Vehicle Tier 2 Rule, the Onroad Heavy-Duty Rule, and the Mobile Source Air Toxics (MSAT) final rule and the category 3 marine diesel engines Clean Air Act and

International Maritime Organization standards which includes the establishment of emission control areas for these ships. Emission reductions and increases from the Renewable Fuel Standard version 2 (RFS2) are not included. The future baseline case nonroad mobile emissions reductions for these years include reductions to locomotives, various nonroad engines including diesel engines and various marine engine types, fuel sulfur content, and evaporative emissions standards. A summary of the mobile source control programs included in the projected future year baseline is shown in Table II-3.

Table II-3. Summary of mobile source control programs included in 2016 baseline

National Onroad Rules:
- Tier 2 Rule (*Signature date:* February 28, 2000)
- Onroad Heavy-Duty Rule (February 24, 2009)
- Final Mobile Source Air Toxics Rule (MSAT2) (February 9, 2007)
- Renewable Fuel Standard (March 26, 2010)

Local Onroad Programs:
- National Low Emission Vehicle Program (NLEV) (March 2, 1998)
- Ozone Transport Commission (OTC) LEV Program (January, 1995)

National Nonroad Controls:
- Tier 1 nonroad diesel rule (June 17, 2004)
- Phase 1 nonroad SI rule (July 3, 1995)
- Marine SI rule (October 4, 1996)
- Nonroad diesel rule (October 23, 1998)
- Phase 2 nonroad nonhandheld SI rule (March 30, 1999)
- Phase 2 nonroad handheld SI rule (April 25, 2000)
- Nonroad large SI and recreational engine rule (November 8, 2002)
- Clean Air Nonroad Diesel Rule - Tier 4 (June 29, 2004)
- Locomotive and marine rule (May 6, 2008)
- Nonroad SI rule (October 8, 2008)

Aircraft:
- Itinerant (ITN) operations at airports adjusted to year 2014

Locomotives:
- Clean Air Nonroad Diesel Final Rule – Tier 4 (June 29, 2004)
- Locomotive rule (April 16, 2008)
- Locomotive and marine rule (May 6, 2008)

Commercial Marine:
- Locomotive and marine rule (May 6, 2008)
- Category 3 marine diesel engines Clean Air Act and International Maritime Organization standards (April, 30, 2010)

As with the 2005 emissions, the 2016 onroad emissions were based on MOVES 2010. Future-year vehicle miles travelled (VMT) were projected from the 2005 NEI v2 VMT using growth rates from the 2009 Annual Energy Outlook (AEO) data. The same MOVES-based $PM_{2.5}$ temperature adjustment factors were also applied as in 2005 for running mode emissions because these are not dependent on year; however, cold start emissions used 2015-specific temperature adjustment factors.

2016 nonroad mobile emissions were created with NMIM using an approach that is consistent with that used for 2005, but emissions were calculated using NMIM 2016 equipment population

estimates and control programs for 2016. Emissions for locomotives and category 1 and 2 (C1 and C2) commercial marine vessels were derived for 2016 based on emissions published in the Locomotive Marine Rule, Regulatory Impact Assessment, Chapter 3 (see http://www.epa.gov/otaq/locomotives.htm#2008final). Emissions for Category 3 marine vessels (seca_c3) were computed by projecting the 2005 C3 marine using regional projection factors that include the impacts of the International Maritime Organization standards.

Future Year Sector Contribution Approach

The 2016 reference scenario for the boilers affected by the rule includes 2005 emissions estimates with some emissions removed from the inventory because of shut downs. The length of time required to conduct emissions and photochemical modeling precluded the use of the final facility-specific emissions estimates based on controls implemented for this rule. A 2016 "control" or emissions adjustment scenario was developed by tracking the total contribution from potentially controllable boiler sector emissions from the 2016 baseline inventory. This total contribution estimate, essentially a "zero-out", of the sector creates a policy space where potential control impacts would be maximized at all locations. Since emissions reductions at controllable sources are not 100% (100% ~ total contribution), the boiler sector air quality contribution estimates from the 2016 source apportionment model simulation are adjusted based on nation-wide estimates of control percentages by pollutant to create a final 2016 "control" emissions scenario.

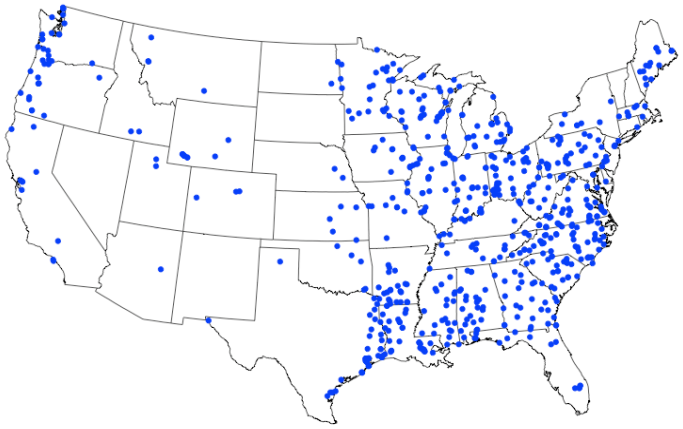
The 2016 estimated controllable emissions for the boiler sector are shown in Table II-4. Boiler sector emissions are contained in several different general classes of emissions used for emissions modeling: non-point or area (nonpt), point EGU (ptipm), and point non-EGU (ptnonipm). These totals are the sum of emissions in the eastern and western U.S. modeling domains so the non-point (area) category contains some double-counting of emissions where the model domains overlap in the central United States (see Figure II-1).

Table II-4. Estimated future year controllable boiler sector emissions

	Sector	VOC	NOX	SO2	PM25	NH3	HG0	HG2	PM25 HG
Total (TPY)	Non-point - Boiler (nonpt)	14,107	394,459	1,149,402	108,386	8,489	0	0	0
Total (TPY)	EGU Point - Boiler (ptipm)	57	0	54,337	826	0	0	0	0
Total (TPY)	Non-EGU Point - Boiler (ptnonipm)	15,451	215,809	492,676	28,838	706	1	2	1
Pct of Sector	Non-point - Boiler (nonpt)	0	19	82	9	5			
Pct of Sector	EGU Point - Boiler (ptipm)	0	0	1	0	0			
Pct of Sector	Non-EGU Point - Boiler (ptnonipm)	1	9	26	6	0	10	7	12

Figure II-2 shows the locations of boilers in the NEI point source inventory used in the modeling analysis. Non-point boilers in the NEI do not have stack location information and are not shown. These boilers are spatially distributed in the modeling domain using spatial surrogates appropriate for this sector.

Figure II-2. Locations of boilers in the NEI point inventory for the future baseline (2016).



Boiler emissions in the non-point/area (nonpt) modeling sector are used as the basis of estimating air quality impacts and health benefits for the area source rule. These emissions are based on SCC codes shown in Table II-5. Boiler emissions in the point non-EGU (ptnonipm) and point EGU (ptipm) are used to estimate impacts of the major source rule. Facilities were identified for the major source rule based on meeting several criteria: 1) NEI facility ID and process level fuel type matched to a facility in the boiler ICR database, 2) NEI source had a boiler SCC code, and 3) unit design capacity was less than 25 MW.

Table II-5. SCC codes used to identify area source sector emissions

MACT Code	MACT Source Category	SCC
		2101002000
		2101004000
		2101005000
107	Industrial/Commercial/ Institutional Boilers & Process Heaters	2102011000
107	Industrial/Commercial/ Institutional Boilers & Process Heaters	2103011000
107	Industrial/Commercial/ Institutional Boilers & Process Heaters	2103011005
107	Industrial/Commercial/ Institutional Boilers & Process Heaters	2199011000
0107-1	Industrial/Commercial/ Institutional Boilers & Process Heaters - coal	2102001000
0107-1	Industrial/Commercial/ Institutional Boilers & Process Heaters - coal	2102002000
0107-1	Industrial/Commercial/ Institutional Boilers & Process Heaters - coal	2103001000
0107-1	Industrial/Commercial/ Institutional Boilers & Process Heaters - coal	2103002000
0107-1	Industrial/Commercial/ Institutional Boilers & Process Heaters - coal	2199001000
0107-3	Industrial/Commercial/ Institutional Boilers & Process Heaters - oil	2102004000
0107-3	Industrial/Commercial/ Institutional Boilers & Process Heaters - oil	2102005000
0107-3	Industrial/Commercial/ Institutional Boilers & Process Heaters - oil	2102012000
0107-3	Industrial/Commercial/ Institutional Boilers & Process Heaters - oil	2103004000
0107-3	Industrial/Commercial/ Institutional Boilers & Process Heaters - oil	2103005000
0107-3	Industrial/Commercial/ Institutional Boilers & Process Heaters - oil	2199004000
0107-3	Industrial/Commercial/ Institutional Boilers & Process Heaters - oil	2199004001
0107-3	Industrial/Commercial/ Institutional Boilers & Process Heaters - oil	2199005000
0107-4	Industrial/Commercial/ Institutional Boilers & Process Heaters - wood or waste	2102008000
0107-4	Industrial/Commercial/ Institutional Boilers & Process Heaters - wood or waste	2103008000

Table II-5. SCC codes used to identify area source sector emissions (continued)

SCC	SCC Description
2101002000	Stationary Source Fuel Combustion, Electric Utility, Bituminous/Subbituminous Coal, Total: All Boiler Types
2101004000	Stationary Source Fuel Combustion, Electric Utility, Distillate Oil, Total: Boilers and IC Engines
2101005000	Stationary Source Fuel Combustion, Electric Utility, Residual Oil, Total: All Boiler Types
2102011000	Stationary Source Fuel Combustion, Industrial, Kerosene, Total: All Boiler Types
2103011000	Stationary Source Fuel Combustion, Commercial/Institutional, Kerosene, Total: All Combustor Types
2103011005	Stationary Source Fuel Combustion, Commercial/Institutional, Kerosene, All Boiler Types
2199011000	Stationary Source Fuel Combustion, Total Area Source Fuel Combustion, Kerosene, Total: All Heater Types
2102001000	Stationary Source Fuel Combustion, Industrial, Anthracite Coal, Total: All Boiler Types
2102002000	Stationary Source Fuel Combustion, Industrial, Bituminous/Subbituminous Coal, Total: All Boiler Types
2103001000	Stationary Source Fuel Combustion, Commercial/Institutional, Anthracite Coal, Total: All Boiler Types
2103002000	Stationary Source Fuel Combustion, Commercial/Institutional, Bituminous/Subbituminous Coal, Total: All Boiler Types
2199001000	Stationary Source Fuel Combustion, Total Area Source Fuel Combustion, Anthracite Coal, Total: All Boiler Types
2102004000	Stationary Source Fuel Combustion, Industrial, Distillate Oil, Total: Boilers and IC Engines
2102005000	Stationary Source Fuel Combustion, Industrial, Residual Oil, Total: All Boiler Types
2102012000	Stationary Source Fuel CombustionIndustrialWasteOil Total: All Boiler Types
2103004000	Stationary Source Fuel Combustion, Commercial/Institutional, Distillate Oil, Total: Boilers and IC Engines
2103005000	Stationary Source Fuel Combustion, Commercial/Institutional, Residual Oil, Total: All Boiler Types
2199004000	Stationary Source Fuel Combustion, Total Area Source Fuel Combustion, Distillate Oil, Total: Boilers and IC Engines
2199004001	Stationary Source Fuel Combustion, Total Area Source Fuel Combustion, Distillate Oil, All Boiler Types
2199005000	Stationary Source Fuel Combustion, Total Area Source Fuel Combustion, Residual Oil, Total: All Boiler Types
2102008000	Stationary Source Fuel Combustion, Industrial, Wood, Total: All Boiler Types
2103008000	Stationary Source Fuel Combustion, Commercial/Institutional, Wood, Total: All Boiler Types

Major source mercury emissions were identified as the units added from the boiler ICR database plus units in the NATA Hg inventory that were not in the ICR but were considered part of the Boiler MACT Universe. A percent emissions reduction was estimated based on the rule proposal unit-specific facility-fuel combination in the ICR database. Each facility/process matching the facility-fuel combinations that had emission reductions larger than 1% based on the proposed rule were tracked for source contribution.

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.
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-6 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.

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.

Table II-6. 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

3. Initial and Boundary Conditions

The lateral boundary and initial species concentrations are provided by a three-dimensional global atmospheric chemistry model, the GEOS-CHEM model (standard version 7-04-11). The global GEOS-CHEM model simulates atmospheric chemical and physical processes driven by assimilated meteorological observations from the NASA's Goddard Earth Observing System (GEOS). This model was run for 2005 with a grid resolution of 2.0 degree x 2.5 degree (latitude-longitude) and 30 vertical layers up to 100 mb. The predictions were used to provide one-way dynamic boundary conditions at three-hour intervals and an initial concentration field for the 36 km CAMx simulations. The 36 km photochemical model simulation is used to supply initial and hourly boundary concentrations to the 12 km domains. The future base conditions from the 36 km coarse grid modeling were used as the initial/boundary state for all subsequent future year 12 km finer grid modeling scenarios.

III. Base Case Model Performance Evaluation

1. 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.

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

Metric	Quarter	Sulfate Ion	Nitrate Ion	Ammonium Ion	Organic Carbon	Elemental Carbon
Number	1	6,218	5,870	4,045	5,882	6,368
	2	6,537	6,146	4,075	6,180	6,552
	3	6,108	5,828	3,869	5,836	6,061
	4	5,894	5,757	3,763	5,600	5,937
Mean Observed	1	2.7	2.4	1.7	1.7	0.5
($\mu g/m^3$)	2	3.8	0.8	1.5	2.1	0.5
	3	5.4	0.5	1.8	2.4	0.5
	4	2.5	1.3	1.3	2.0	0.6
Mean Predicted	1	4.2	2.1	1.8	2.3	1.1
($\mu g/m^3$)	2	4.5	0.7	1.5	1.8	0.8
	3	5.4	0.3	1.5	2.4	0.8
	4	3.7	1.3	1.4	2.1	1.0
Bias	1	1.6	-0.2	0.4	0.7	0.6
($\mu g/m^3$)	2	0.8	-0.1	0.3	-0.2	0.3
	3	0.2	-0.2	0.0	0.0	0.3
	4	1.3	0.1	0.5	0.2	0.4
Error	1	1.9	1.3	0.8	1.2	0.6
($\mu g/m^3$)	2	1.7	0.6	0.8	0.9	0.4
	3	2.0	0.4	0.8	0.9	0.5
	4	1.6	0.9	0.7	1.1	0.6

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 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. 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.

2. 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 on an hourly and/or daily basis, depending on the sampling frequency of each measurement site (measured data). 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
1	692	71.1	58.4	-12.7	13.3
2	24,357	76.0	67.0	-9.0	11.2
3	27,430	79.7	73.7	-6.0	11.3
4	1,626	75.8	69.3	-6.5	9.9
	8-hr Daily Maximum Ozone (ppb)				
Quarter	N	Observed	Predicted	Bias	Error
1	692	64.5	53.9	-10.6	11.1
2	24,370	69.3	61.9	-7.4	9.6
3	27,447	70.5	67.1	-3.4	9.2
4	1,629	66.8	63.2	-3.5	8.4
*metrics estimated where observed ozone > 60 ppb					

3. 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 (μg/m^2)				
Quarter	N	Observed	Predicted	Bias	Error
1	866	0.15	0.03	-0.12	0.12
2	943	0.27	0.04	-0.23	0.23
3	907	0.31	0.05	-0.25	0.26
4	808	0.13	0.02	-0.10	0.11
	Rainfall (mm)				
Quarter	N	Observed	Predicted	Bias	Error
1	1,162	17.32	18.15	0.83	8.55
2	1,192	20.19	24.41	4.22	14.85
3	1,213	20.50	26.34	5.84	19.58
4	1,124	19.78	17.92	-1.86	9.31

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APPENDIX A

Emissions Source Sectors in the 2005-based modeling platform, version 4.1

Table 3-1. Emissions Source Sectors for Current and Future-Year Inventories, 2005-based Platform, Version 4.1

Platform Sector and corresponding 2005 NEI sector	Description and resolution of the data input to SMOKE, 2005 v4.1 platform
IPM sector: *ptipm* **NEI Sector= Point**	For all pollutants other than mercury (Hg): 2005v2 NEI point source EGUs mapped to the Integrated Planning Model (IPM) model using the National Electric Energy Database System (NEEDS) database. Revisions of 2005v2 NOX and SO2 emissions for some units were made due to the availability of additional data (ORIS codes) which allowed use of the 2005 CEM data to replace annual emissions for these units. For Hg: 6/18/2010 version of the inventory used for the 2005 National Air Toxics Assessment (NATA) mapped to IPM using NEEDS. The NATA inventory is an update to the 2005v2 and was divided into IPM and non-IPM sectors consistent with the other pollutants. We removed Hg from sources that were identified in the industrial, commercial and institutional (ICI) database developed as part of the ICI rule because we included these emissions in the ptnonipm sector.
Non-IPM sector: *ptnonipm* **NEI Sector=Point**	For all pollutants other than Hg: All 2005v2 NEI point source records not matched to the ptipm sector, annual resolution. Includes all aircraft emissions. Updates to 2005v2 were made to remove duplicates, improve estimates from ethanol plants, and reflect new information collected from industry from the Information Collection Request (ICR) for the ICI rule. For Hg: The 6/18/2010 version of NATA inventory was used except for ICI boilers, modifications to gold mine emissions and removal of Hg from facilities that closed prior to 2005. For ICI boilers, the Hg emissions developed for the ICI rule were used.
Average-fire sector: *avefire* **No NEI Sector**	Average-year wildfire and prescribed fire emissions derived from the 2002-based Platform avefire sector, county and annual resolution.
Agricultural sector: *ag* **NEI Sector= Nonpoint**	NH_3 emissions from NEI nonpoint livestock and fertilizer application, county and annual resolution.
Area fugitive dust sector: *afdust* **NEI Sector= Nonpoint**	PM_{10} and $PM_{2.5}$ from fugitive dust sources from the NEI nonpoint inventory (e.g., building construction, road construction, paved roads, unpaved roads, agricultural dust), county and annual resolution.
Remaining nonpoint sector: *nonpt* **NEI Sector= Nonpoint**	Primarily 2002 NEI nonpoint sources not otherwise included in other SMOKE sectors, county and annual resolution. Also includes updated Residential Wood Combustion emissions, year 2005 non-California WRAP oil and gas Phase II inventory and year 2005 Texas and Oklahoma oil and gas emissions. Removed Hg emissions from ICI boilers to prevent potential double counting by inclusion of the ICI boiler Hg emissions from the MACT database in the Non-IPM sector.
Nonroad sector:	Monthly nonroad emissions from the National Mobile Inventory Model

Platform Sector and corresponding 2005 NEI sector	Description and resolution of the data input to SMOKE, 2005 v4.1 platform
nonroad **NEI Sector= Nonroad**	(NMIM) using NONROAD2005 (version nr05c-BondBase) for all states except California. Monthly emissions for California created from annual emissions submitted by the California Air Resources Board (CARB) for the 2005v2 NEI**.**
Locomotive, and non-C3 commercial marine: *alm_no_c3* **NEI Sector= Nonroad**	Year 2002 non-rail maintenance locomotives, and category 1 and category 2 commercial marine vessel (CMV) emissions sources, county and annual resolution. Aircraft emissions are now included in the ptnonipm sector and category 3 emissions are now contained in the seca_c3 sector.
C3 commercial marine: *seca_c3* **NEI Sector= Nonroad**	Annual point source-formatted, year 2005 category 3 (C3) CMV emissions, developed for the rule called "Control of Emissions from New Marine Compression-Ignition Engines at or Above 30 Liters per Cylinder", usually described as the Emissions Control Area (ECA) study, (originally called SO2 ["S"] ECA -see http://www.epa.gov/otaq/oceanvessels.htm). Utilized final projections from 2002, developed for the C3 ECA proposal to the International Maritime Organization (EPA-420-F-10-041, August 2010).
Onroad California, NMIM-based, and MOVES sources not subject to temperature adjustments: *on_noadj* **NEI Sector= Onroad**	Three, monthly, county-level components: 1) California onroad, created using annual emissions submitted by CARB for the 2005v2 NEI. 2) Onroad gasoline and diesel vehicle emissions from MOVES2010 not subject to temperature adjustments: exhaust CO, N_{OX}, VOC, benzene, formaldehyde, acetaldehyde, 1,3 butadiene, acrolein, naphthalene, brake and tirewear PM, and evaporative VOC, benzene, and naphthalene. 3) Onroad emissions for certain HAPs, including Hg, from NMIM using MOBILE6.2, other than for California.
Onroad cold-start gasoline exhaust mode vehicle from MOVES subject to temperature adjustments: *on_moves_startpm* **NEI Sector= Onroad**	Monthly, county-level MOVES2010 onroad gasoline vehicle emissions subject to temperature adjustments. Limited to exhaust mode only for PM species and Naphthalene. California emissions not included. This sector is limited to cold start mode emissions that contain different temperature adjustment curves from running exhaust (see on_moves_runpm sector).
Onroad running gasoline exhaust mode vehicle from MOVES subject to temperature adjustments: *on_moves_runpm* **NEI Sector= Onroad**	Monthly, county-level MOVES2010 onroad gasoline vehicle emissions subject to temperature adjustments. Limited to exhaust mode only for PM species and Naphthalene. California emissions not included. This sector is limited to running mode emissions that contain different temperature adjustment curves from cold start exhaust (see on_moves_startpm sector).
Biogenic: *biog*	Hour-specific, grid cell-specific emissions generated from the BEIS3.14

Platform Sector and corresponding 2005 NEI sector	Description and resolution of the data input to SMOKE, 2005 v4.1 platform
No NEI Sector	model -includes emissions in Canada and Mexico.
Other point sources not from the NEI: *othpt* **No NEI Sector**	Point sources from Canada's 2006 inventory and Mexico's Phase III 1999 inventory, annual resolution. Also includes annual U.S. offshore oil 2005v2 NEI point source emissions.
Other point sources not from the NEI, Hg only: *othpt_hg* **No NEI Sector**	Year 2000 Canada speciated mercury point source emissions; annual resolution.
Other nonpoint and nonroad not from the NEI: *othar* **No NEI Sector**	Year 2006 Canada (province resolution) and year 1999 Mexico Phase III (municipio resolution) nonpoint and nonroad mobile inventories, annual resolution.
Other nonpoint sources not from the NEI, Hg only: *othar_hg* **No NEI Sector**	Year 2000 Canada speciated mercury from nonpoint sources; annual resolution.
Other onroad sources not from the NEI: *othon* **No NEI Sector**	Year 2006 Canada (province resolution) and year 1999 Mexico Phase III (municipio resolution) onroad mobile inventories, annual resolution.

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