

Chapter 2: Characterizing Ozone and Modeling Tools Used in This Analysis

Synopsis

This chapter describes the chemical and physical properties of ozone, general ozone air quality patterns, key health and environmental impacts associated with exposure to ozone, and key sources of ozone precursor emissions. In order to evaluate the health and environmental impacts of trying to reach a tighter ozone standard in the year 2020, it was necessary to use models to predict concentrations in the future. The tools and methodology used for the air quality modeling are described in this chapter. Subsequent chapters of this RIA rely heavily on the results of this modeling.

2.1 Ozone Chemistry

Ozone occurs both naturally in the stratosphere to provide a protective layer high above the earth, and at ground-level (troposphere) as the prime ingredient of smog. Tropospheric ozone, which is regulated by the NAAQS, is formed by both naturally occurring and anthropogenic sources. Ozone is not emitted directly into the air, but is created when its two primary components, volatile organic compounds (VOC) and oxides of nitrogen (NO_x), combine in the presence of sunlight. VOC and NO_x are often referred to as ozone precursors, which are, for the most part, emitted directly into the atmosphere.

Ambient ozone concentrations are directly affected by temperature, solar radiation, wind speed and other meteorological factors. Ultraviolet radiation from the sun plays a key role in initiating the processes leading to ozone formation. However, there is little empirical evidence directly linking day-to-day variations in observed surface ultraviolet radiation levels with variations in tropospheric ozone levels.

The rate of ozone production can be limited by either VOCs or NO_x. In general, ozone formation using these two precursors is reliant upon the relative sources of hydroxide (OH) and NO_x. When the rate of OH production is greater than the rate of production of NO_x, indicating that NO_x is in short supply, the rate of ozone production is NO_x-limited. In this situation, ozone concentrations are most effectively reduced by lowering current and future NO_x emissions, rather than lowering emissions of VOCs. When the rate of OH production is less than the rate of production of NO_x, ozone production is VOC-limited. Here, ozone is most effectively reduced by lowering VOCs. Between the NO_x- and VOC-limited extremes there is a transitional region where ozone is nearly equally sensitive to each species. However ozone is relatively insensitive to marginal changes in both NO_x and VOC in this situation. In urban areas with a high population concentration, ozone is often VOC-limited. Ozone is generally NO_x-limited in rural areas and downwind suburban areas. Additional information on ozone formation can be found in “Atmospheric Chemistry and Physics” (Seinfeld et. al., 1998).

Due to the complex photochemistry of ozone production, NO_x emissions lead to both the formation and destruction of ozone, depending on the local quantities of NO_x, VOC, and ozone catalysts such as the OH and HO₂ radicals. In areas dominated by fresh emissions of NO_x, ozone

catalysts are removed via the production of nitric acid, which slows the ozone formation rate. Because NO_x is generally depleted more rapidly than VOC, this effect is usually short-lived and the emitted NO_x can lead to ozone formation later and further downwind. The terms “NO_x disbenefits” or “ozone disbenefits” refer to the ozone increases that can result from NO_x emission reductions in these localized areas.¹

2.1.1 Temporal Scale

Ground-level ozone forms readily in the atmosphere, usually during hot weather. The effects of sunlight on ozone formation depend on its intensity and its spectral distribution. Ozone levels tend to be highest during the daytime, during the summer or warm season. Changing weather patterns contribute to day to day and interannual differences in ozone concentrations. Differences in climatic regime, amount and mixture of emissions, and the extent of transport contribute to variations in ozone from city to city.

2.1.2 Geographic Scale and Transport

In many urban areas, ozone nonattainment is not caused by emissions from the local area alone. Due to atmospheric transport, contributions of precursors from the surrounding region can also be important. Thus, in designing control strategies to reduce ozone concentrations in a local area, it is often necessary to account for regional transport within the U.S.

In some areas, such as California, global transport of ozone from beyond North America can contribute to nonattainment areas. In a very limited number of areas, including areas such as Buffalo, Detroit and El Paso, which are located near borders, emissions from Canada or Mexico may contribute to nonattainment. In these areas, our illustrative implementation strategies may have included more controls on domestic sources than would be required if cross-border transport did not occur. However, we have not conducted formal analysis, and as such cannot determine the contribution of non-U.S. sources to ozone design values. The transport of ozone is determined by meteorological and chemical processes which typically extend over spatial scales of several hundred kilometers. Additionally, convection is capable of transporting ozone and its precursors vertically through the troposphere, with resulting mixing of stratospheric ozone for periods of a month or more with tropospheric ozone.

The Technical Support Document (TSD) for the Clean Air Interstate Rule (CAIR) suggests that ozone transport constitutes a sizable portion of projected nonattainment in most eastern areas based on a 2010 analysis. A listing of Eastern states and the extent of transported ozone they receive in the CAIR analysis is located in the CAIR TSD.² We used this information to help guide the design of emissions control strategies in this analysis.

¹ U.S. EPA. Final Regulatory Impact Analysis: Control of Emissions from Nonroad Diesel Engines. EPA420-R-04-007. May 2004.

² <http://www.epa.gov/interstateairquality/pdfs/finaltech02.pdf>, Table VI-2.

2.2 Sources of Ozone

The anthropogenic precursors of ozone originate from a wide variety of stationary and mobile sources. In urban areas, both biogenic (natural) and anthropogenic VOCs are important for ozone formation. Hundreds of VOCs are emitted by evaporation and combustion processes from a large number of anthropogenic sources. Current data show that solvent use and highway vehicles are the two main sources of VOCs, with roughly equal contributions to total emissions. Emissions of VOCs from highway vehicles account for roughly two-thirds of the transportation-related emissions.³ By 2020, EPA emission projections show that VOC emissions from highway vehicles decrease significantly. Solvent use VOC decreases as well, but by 2020 solvent use VOC is projected to be a slightly more significant VOC contributor than mobile VOC. On the regional and global scales, emissions of VOCs from vegetation are much larger than those from anthropogenic sources.

Anthropogenic NO_x emissions are associated with combustion processes. The two largest sources of NO_x are electric power generation plants (EGUs) and motor vehicles. EGU NO_x is approximately 40% less than onroad mobile NO_x in 2001. Both decrease between 2001 and 2020, with onroad mobile NO_x decreasing more, so that their emissions are similar in 2020. It is not possible to make an overall statement about their relative impacts on ozone in all local areas because EGUs are more sparse than mobile sources, particularly in the west and south (See Chapter 3 for a discussion of emission reductions projected in 2020 for the 8-hr ozone current standard baseline and the more stringent alternative control scenario). Natural NO_x sources include stratospheric intrusions, lightning, soils, and wildfires. Lightning, fertilized soils, and wildfires are the major natural sources of NO_x in the United States. Uncertainties in natural NO_x inventories are much larger than for anthropogenic NO_x emissions.

A complete list of emissions source categories, for both NO_x and VOCs, is compiled in the final ozone Staff Paper (EPA, 2007a, pp. 2-3 to 2-6).

2.3 Modeling Ozone Levels in the Future

In order to evaluate the predicted air quality in 2020, it is necessary to use modeling to derive estimated air quality concentrations. The modeling analysis uses an emissions inventory and historical meteorological conditions to simulate pollutant concentrations. The predictions from the modeling are used to (a) project future ozone design values (a representation of the resultant air quality concentration in 2020 representing the 4th highest maximum 8-hr concentration) and (b) create spatial fields of ozone and PM_{2.5} for characterizing human health impacts from reducing ozone precursors, which in the case of NO_x will also affect the formation of PM_{2.5}. The air quality model used in this RIA is the Community Multi-Scale Air Quality (CMAQ) model⁴. The modeling for ozone and PM_{2.5} was performed for a one year time period. All controls in the illustrative 0.070 scenario were applied similarly to all months. There were no controls applied

³ U.S EPA. 2007. Review of the National Ambient Air Quality Standards for Ozone: Policy Assessment of Scientific and Technical Information. OAQPS Staff Paper. North Carolina. EPA-452/R-07-003.

⁴ See CMAQ references listed at end of this chapter.

specifically for PM_{2.5} co-benefits because the controls developed to reduce summer ozone were applied to all months (see Chapter 3).

2.3.1 CMAQ Model and Inputs

A national scale air quality modeling analysis was performed to estimate future year attainment/nonattainment of the current and alternative ozone standards. In addition, the model-based projections of ozone and PM_{2.5} were used as inputs to the calculation of expected incremental benefits from the alternative ozone standards considered in this assessment. The 2002-based modeling platform (EPA, 2008) was used as the basis for air quality modeling of the future baseline emissions and illustrative control scenario. This modeling platform includes a number of updates and improvements to data and tools compared to the 2001-based platform that was used for the proposal modeling. For the final rule modeling we used the new 2002 National Emissions Inventory along with updated versions of the models used to project future emissions from electric generating units (EGUs) and onroad and nonroad vehicles. The proposal modeling was based on the 2001 National Emissions Inventory. The new platform also includes 2002 meteorology and more recent ambient design values which were used as the starting point for projecting future air quality. For proposal, we used meteorology for 2001 for modeling the East and 2002 for modeling the West. The updates⁵ to CMAQ between proposal and final include (1) an in-cloud sulfate chemistry module that accounts for the nonlinear sensitivity of sulfate formation to varying pH; (2) improved vertical convective mixing; (3) heterogeneous reaction involving nitrate formation; (4) an updated gas-phase chemistry mechanism, Carbon Bond 2005 (CB05); and (5) an aqueous chemistry mechanism that provides a comprehensive simulation of aerosol precursor oxidants.

The key non-emissions inputs to the CMAQ model include meteorological data, and initial and boundary concentrations. The CMAQ meteorological input files were derived from simulations of the Pennsylvania State University/National Center for Atmospheric Research Mesoscale Model (Grell, Dudhia, and Stauffer, 1994). 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. The lateral boundary and initial species concentrations for the 36 km continental scale modeling domain, described below, were obtained from a three-dimensional global atmospheric chemistry model, the GEOSChem model (Yantosca, 2004). The global GEOSChem model simulates atmospheric chemical and physical processes driven by assimilated meteorological observations from the NASA's Goddard Earth Observing System (GEOS). We used GEOSChem results for 2002 to provide initial and boundary concentrations for our final rule air quality modeling. For proposal we used GEOSChem results for 2001.

EPA performed an extensive evaluation of CMAQ using the 2002 inputs for emissions, meteorology, and boundary conditions. Details of the model performance methodology and results are described in the 2002-Based Modeling Platform Report (EPA, 2008). As in the evaluation for previous model applications, the "acceptability" of model performance for the ozone RIA modeling was judged by comparing the results to those found in recent regional

⁵ Additional documentation on the updates in CMAQ version 4.6 can be found at the following web site: <http://www.emascenter.org/>.

ozone model applications for other EPA and non-EPA studies (see Appendix B of EPA, 2007b). Overall, the performance for the CMAQ application is generally within the range of these other applications.

Figure 2.1 shows the modeling domains that were used as a part of this analysis. The geographic specifications for these domains are provided in Table 2.1. All three modeling domains contain 14 vertical layers with a top at about 16,200 meters, or 100 mb. Two domains with 12 km horizontal resolution were used for modeling the 2002 base year, 2020 baseline and 2020 control strategy scenarios. These domains are labeled as the East and West 12 km domains in Figure 2.1. Simulations for the 36 km domain were only used to provide initial and boundary concentrations for the 12 km domains. As indicated above, the model produces spatial fields of gridded air quality concentrations on an hourly basis for the entire modeling domain. These gridded concentrations can be processed to produce a number of air quality metrics, including the 8-hr ozone design values, and can be used as inputs for the analysis of costs and benefits. The air quality modeling results are used in a relative sense to project concentrations for the future year scenarios using procedures consistent with EPA guidance (EPA, 2007b). For the final rule projections we used ambient design values for the period 2000 through 2004 as the starting point for projections. For the proposal, design values from 1999 through 2003 were used. The change between proposal and final in terms of the period of design values was made, in accordance with EPA guidance, in order to align the central year of design values with the base year of the emissions (i.e., 2001 for the proposed rule and 2002 for the final rule).

For this analysis, predictions from the East domain were used to provide data for all areas that are east of approximately 104 degrees longitude. Model predictions from the West domain we used for all areas west of this longitude.

Figure 2.1: Map of the CMAQ Modeling Domains Used for Ozone NAAQS RIA

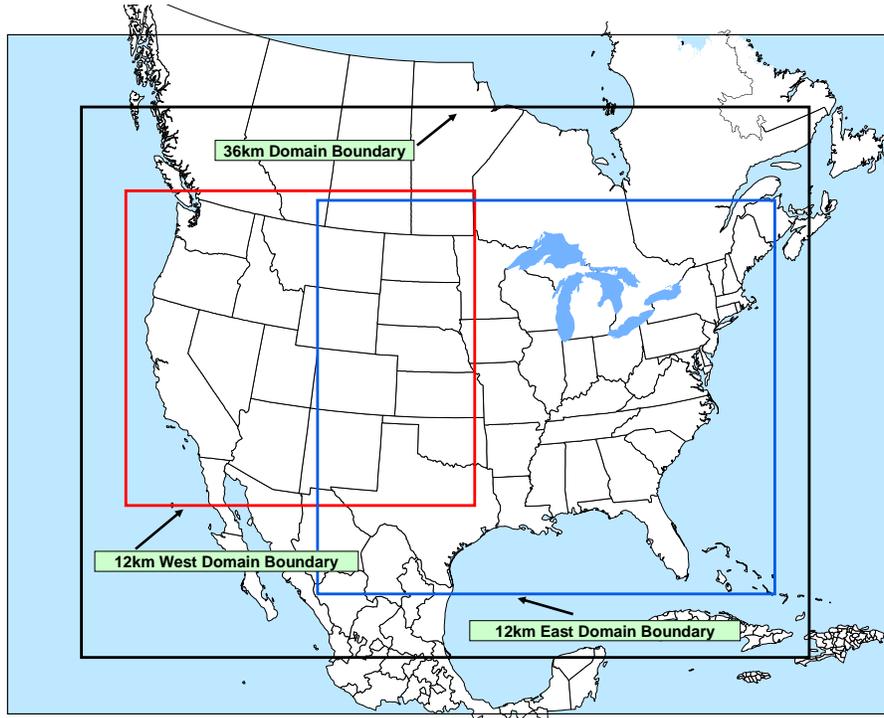


Table 2.1: Geographic Specifications of Modeling Domains

36 km Domain (148 x 112 Grid Cells)			12 km East Domain (279 x 240 Grid Cells)			12 km West Domain (213 x 192 Grid Cells)		
	Lon	lat		lon	lat		lon	lat
SW	-121.77	18.17	SW	-106.79	24.99	SW	-121.65	28.29
NE	-58.54	52.41	NE	-65.32	47.63	NE	-94.94	51.91

2.3.2 Emissions Inventory

The 2020 inventory, projected from the 2002 Version 3 emissions modeling platform (EPA, 2008), is the starting point for the baseline and control strategy for the Final Ozone NAAQS emissions inventory. The 2002 documentation describes the 2002 base year inventory as well as the projection methodology and controls applied to create year 2020 emissions. The 2020 inventory includes activity growth for some sectors, and controls including: the Clean Air Interstate Rule, the Clean Air Mercury Rule, the Clean Air Visibility Rule, the Clean Air Nonroad Diesel Rule, the Light-Duty Vehicle Tier 2 Rule, the Heavy Duty Diesel Rule, known plant closures, and consent decrees and settlements. Table 2.2 provides a comprehensive list of the rules/control strategies and projection assumptions in the 2020 inventory; full discussion of the 2020 inventory is provided in the 2002 Version 3 emissions modeling platform (EPA, 2008a). The data for the controls and projection strategies can be found in the Loco-Marine docket (EPA, 2008b).

Table 2.2: Control Strategies and Projection Assumptions in the 2020 Emissions Inventory

Control Strategies (Grouped by Affected Pollutants or Standard and Approach Used to Apply to the Inventory)	Pollutants Affected	Approach or Reference
Non-EGU Point Controls		
NOx SIP Call (Phase II): Cement Manufacturing Large Boiler/Turbine Units Large IC Engines	NOx	1
DOJ Settlements: plant SCC controls Alcoa, TX MOTIVA, DE	NOx, SO ₂	2
Refinery Consent Decrees: plant/SCC controls	NOx, PM, SO ₂	3
Closures, pre-2007: plant control of 100% Auto plants Pulp and Paper Municipal Waste Combustors Plants closed in preparation for 2005 inventory	all	4
Industrial Boiler/Process Heater plant/SCC controls for PM	PM	5
MACT rules, national, VOC: national applied by SCC, MACT Boat Manufacturing Polymers and Resins III (Phenolic Resins) Polymers and Resins IV (Phenolic Resins) Wood Building Products Surface Coating Generic MACT II: Spandex Production, Ethylene manufacture Large Appliances Miscellaneous Organic NESHAP (MON): Alkyd Resins, Chelating Agents, Explosives, Phthalate Plasticizers, Polyester Resins, Polymerized Vinylidene Chloride Manufacturing Nutritional Yeast Oil and Natural Gas Petroleum Refineries—Catalytic Cracking, Catalytic Reforming, & Sulfur Plant Units Pesticide Active Ingredient Production Publicly Owned Treatment Works Reinforced Plastics Rubber Tire Manufacturing Asphalt Processing & Roofing Combustion Sources at Kraft, Soda, and Sulfite Paper Mills Fabric Printing, Coating and Dyeing Iron & Steel Foundries Metal: Can, Coil Metal Furniture Miscellaneous Metal Parts & Products Municipal Solid Waste Landfills Paper and Other Web Plastic Parts Plywood and Composite Wood Products Wet Formed Fiberglass Production Wood Building Products Surface Coating Carbon Black Production Cellulose Products Manufacturing Cyanide Chemical Manufacturing	VOC	EPA, 2007f

(continued)

**Table 2.2: Control Strategies and Projection Assumptions in the 2020 Emissions Inventory
(continued)**

Control Strategies (Grouped by Affected Pollutants or Standard and Approach Used to Apply to the Inventory)	Pollutants Affected	Approach or Reference
Friction Products Manufacturing Leather Finishing Operations Miscellaneous Coating Manufacturing Organic Liquids Distribution (Non-Gasoline) Refractory Products Manufacturing Sites Remediation		
Solid Waste Rules (Section 129d/111d)		
Hospital/Medical/Infectious Waste Incinerator Regulations	NO _x , PM, SO ₂	EPA, 2005
MACT rules, national, PM:		
Portland Cement Manufacturing Secondary Aluminum	PM	6
MACT rules, plant-level, VOC:		
Auto Plants	VOC	7
MACT rules, plant-level, PM & SO₂:		
Lime Manufacturing	PM, SO ₂	8
MACT rules, plant-level, PM:		
Taconite Ore	PM	9
Stationary Non-point (Area) Assumptions		
Municipal Waste Landfills: projection factor of 0.25 applied	VOC	EPA, 2007f
Livestock Emissions Growth	NH ₃ , PM	10
Residential Wood Combustion Growth reflects increase in use of lower polluting wood stoves, and decrease in use of higher polluting stoves	all	11
Gasoline Stage II growth and control (also impacts non-EGU point sources in a couple of states)	VOC	12
Portable Fuel Container growth and control	VOC	13
EGU Point Controls		
CAIR/CAMR/CAVR IPM Model 3.0	NO _x , SO ₂ , PM	14
Onroad Mobile and Nonroad Mobile Growth and Controls		
Onroad and Nonroad Growth: Onroad growth is based on VMT growth from Annual Energy Outlook (AEO) 2006 estimates of growth by vehicle type. Nonroad growth is based on activity increases from NONROAD model default growth estimates	all	
National Onroad Rules: Tier 2 Rule 2007 Onroad Heavy-Duty Rule Final Mobile Source Air Toxics Rule (MSAT2) Renewable Fuel Standard	all	
Local Onroad Programs: National Low Emission Vehicle Program (NLEV) Ozone Transport Commission (OTC) LEV Program	VOC	15

(continued)

**Table 2.2: Control Strategies and Projection Assumptions in the 2020 Emissions Inventory
(continued)**

Control Strategies (Grouped by Affected Pollutants or Standard and Approach Used to Apply to the Inventory)	Pollutants Affected	Approach or Reference
National Nonroad Controls:		
Clean Air Nonroad Diesel Final Rule—Tier 4	all	16
Control of Emissions from Nonroad Large-Spark Ignition Engines and Recreational Engines (Marine and Land Based): “Pentathlon Rule”		
Aircraft, Locomotives, and Commercial Marine Assumptions		
Aircraft:		
Itinerant (ITN) operations at airports	all	17
Locomotives:		
Energy Information Administration (EIA) fuel consumption projections for freight rail	all	EPA, 2007e, 18
Clean Air Nonroad Diesel Final Rule—Tier 4		
Locomotive Final Rulemaking, December 17, 1997		
Commercial Marine:		
EIA fuel consumption projections for diesel-fueled vessels	all	18, (EPA, 2007e)
Freight-tonnage growth estimates for residual-fueled vessels		
Clean Air Nonroad Diesel Final Rule—Tier 4		
Emissions Standards for Commercial Marine Diesel Engines, December 29, 1999 Tier 1 Marine Diesel Engines, February 28, 2003		
APPROACHES:		
1. Used <i>Emission Budget Inventories</i> report (EPA, 1999) for list of SCCs for application of controls, and for percent reductions (except IC Engines). Used Federal Register on Response to Court decisions (Federal Register, 2004) for IC Engine percent reductions and geographic applicability		
2. For ALCOA consent decree, used http:// cfpub.epa.gov/compliance/cases/index.cfm ; for MOTIVA: used information sent by State of Delaware		
3. Used data provided by Brenda Shine, EPA, OAQPS		
4. Closures obtained from EPA sector leads; most verified using the world wide web.		
5. Used data list of plants provided by project lead from 2001-based platform; required mapping the 2001 plants to 2002 NEI plants due to plant id changes across inventory years		
6. Same as used in CAIR, except added SCCs appeared to be covered by the rule: both reductions based on preamble to final rule. (Portland Cement used a weighted average across two processes)		
7. Percent reductions recommended and plants to apply to reduction to were based on recommendations by rule lead engineer, and are consistent with the reference: EPA, 2007e		
8. Percent reductions recommended are determined from the existing plant estimated baselines and estimated reductions as shown in the Federal Register Notice for the rule. SO ₂ % reduction will therefore be 6147/30,783 = 20% and PM ₁₀ and PM _{2.5} reductions will both be 3786/13588 = 28%		
9. Same approach used in CAIR: FR notice estimates reductions of “PM emissions by 10,538 tpy, a reduction of about 62%.” Used same list of plants as were identified based on tonnage and SCC from CAIR.		
10. Except for dairy cows and turkeys (no growth), based in animal population growth estimates from USDA and Food and Agriculture Policy and Research Institute.		
11. Expected benefits of woodstoves change-out program: http://www.epa.gov/woodstoves/index.html		
12. VOC emission ratios of year 2020 to year 2002 from the National Mobile Inventory Model (NMIM) results for onroad refueling including activity growth from VMT, Stage II control programs at gasoline stations, and phase in of newer vehicles with onboard Stage II vehicle controls.		
13. VOC emission ratios of year 2020 to year 2002 from MSAT rule (EPA, 2007c, EPA, 2007d)		
14. http://www.epa.gov/airmarkets/progsregs/epa-ipm/docs/summary2006.pdf		
15. Only for states submitting these inputs: http://www.epa.gov/otaq/lev-nlev.htm		
16. http://www.epa.gov/nonroad-diesel/2004fr.htm		
17. Federal Aviation Administration (FAA) Terminal Area Forecast (TAF) System, February 2006: http://www.apo.data.faa.gov/main/taf.asp		
18. http://www.epa.gov/nonroad-diesel/2004fr.htm		

Differences between the 2020 emissions modeling platforms—particularly the inventories—used in the Ozone NAAQS Proposal and here in the Ozone NAAQS Final are discussed in the Appendix for Chapter 2.

The development of the 2020 baseline inventory and the modeled control scenarios are discussed in Chapter 3. The 2020 baseline inventory includes the same year 2020 Canada and year 1999 Mexico emissions as the Final PM NAAQS (EPA, 2006b).

2.4 References

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