UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

# Air Quality Modeling
# Platform for the
# Ozone National Ambient Air Quality Standard
# Final Rule Regulatory Impact Analysis

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# Air Quality Modeling Platform for the Ozone National Ambient Air Quality Standard Final Rule Regulatory Impact Analysis

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 2002-Based Air Quality Modeling Platform (2002 Platform) used by EPA in support of the Ozone National Ambient Air Quality Standard (NAAQS) Final Rule Regulatory Impact Assessment (RIA). A modeling platform is a structured system of connected modeling-related tools and data that provide a consistent and transparent basis for assessing the air quality response to changes in emissions and/or meteorology. A platform typically consists of a specific air quality model, base year and future year emissions estimates, a set of meteorological inputs, and estimates of "boundary conditions" representing pollutant transport from source areas outside the region modeled. We used the Community Multiscale Air Quality (CMAQ)[1] as part of the 2002 Platform to provide a national scale air quality modeling analysis for the RIA. The CMAQ model simulates the multiple physical and chemical processes involved in the formation, transport, and destruction of ozone and fine particulate matter ($PM_{2.5}$). The 2002 base year and 2020 future base case emissions scenarios, which were developed as part of the Platform, were used in support of the RIA modeling. In brief, the 2020 base case 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.

For the RIA, the 2002 Platform was used to project ozone and $PM_{2.5}$ concentrations for 2020 which is the analysis year chosen for the NAAQS review. The model predictions are used to (a) estimate 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 $PM_{2.5}$ which are used for characterizing human health impacts from reducing ozone precursor emissions as part of the calculation of expected benefits of attainment of the NAAQS. The focus of the RIA is to evaluate the costs and benefits of reaching attainment with potential alternative ozone standards. Several 2020 emissions scenarios were modeled for this purpose. These include a 2020 baseline and 2020 control strategy which were both developed and modeled specifically for the Ozone NAAQS RIA. The 2020 baseline scenario includes control measures which EPA estimates would be needed to attain the current standard (0.08 ppm) in 2020. The 2020 control strategy represents a hypothetical scenario to illustrate one possible control pathway that could be adopted to help areas attain an alternative primary standard by 2020. The 2020 baseline and control strategy scenarios were modeled to provide a means for assessing the costs and benefits of a attaining a new, more stringent NAAQS incremental to attainment of the current NAAQS. Additional "across-the-board" emissions sensitivity scenarios were modeled to help determine the costs of attainment for those areas that were projected to remain nonattainment of the new NAAQS after the application of the modeled control strategy. Details on the control measures, geographic application of controls, emissions sensitivity scenarios, and the air quality modeling results for these model simulations can be found in chapters 3 and 4 of the RIA.

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[1] Byun, D.W., and K. L. Schere, 2006: Review of the Governing Equations, Computational Algorithms, and Other Components of the Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. Applied Mechanics Reviews, Volume 59, Number 2 (March 2006), pp. 51-77.

The remainder of is report provides a description of each of the main components of the 2002 Platform along with the results of a model performance evaluation in which the 2002 base year model predictions are compared to corresponding measured concentrations.

## II. CMAQ Model Version, Inputs and Configuration

### A. Model version

CMAQ is a non-proprietary computer model that simulates the formation and fate of photochemical oxidants, including $PM_{2.5}$ and ozone, for given input sets of meteorological conditions and emissions. This analysis employed a version of CMAQ based on the latest publicly-released version of CMAQ available at the time of the Ozone NAAQS modeling (i.e., version 4.6[2]). CMAQ version 4.6 reflects recent updates in a number of areas to improve the underlying science from version 4.5 as used in the proposal. These model enhancements include:

1) an updated Carbon Bond chemical mechanism (CB-05) and associated Euler Backward Iterative (EBI) solver was added;

2) an updated version of the ISORROPIA aerosol thermodynamics module was added;

3) the heterogeneous $N_2O_5$ reaction probability is now temperature- and humidity-dependent;

4) the gas-phase reactions involving $N_2O_5$ and $H_2O$ are now included; and

5) an updated version of the vertical diffusion module was added (ACM2).

Additionally, there were a few minor changes made to the release version of CMAQ by the EPA model developers subsequent to its release. The relatively minor changes and new features of this internal version that was ultimately used in this analysis (4.6.1i) are described elsewhere.[3]

### B. Model domain and grid resolution

The CMAQ 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.

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[2] CMAQ version 4.6 was released on September 30, 2006. It is available from the Community Modeling and Analysis System (CMAS) at: http://www.cmascenter.org .

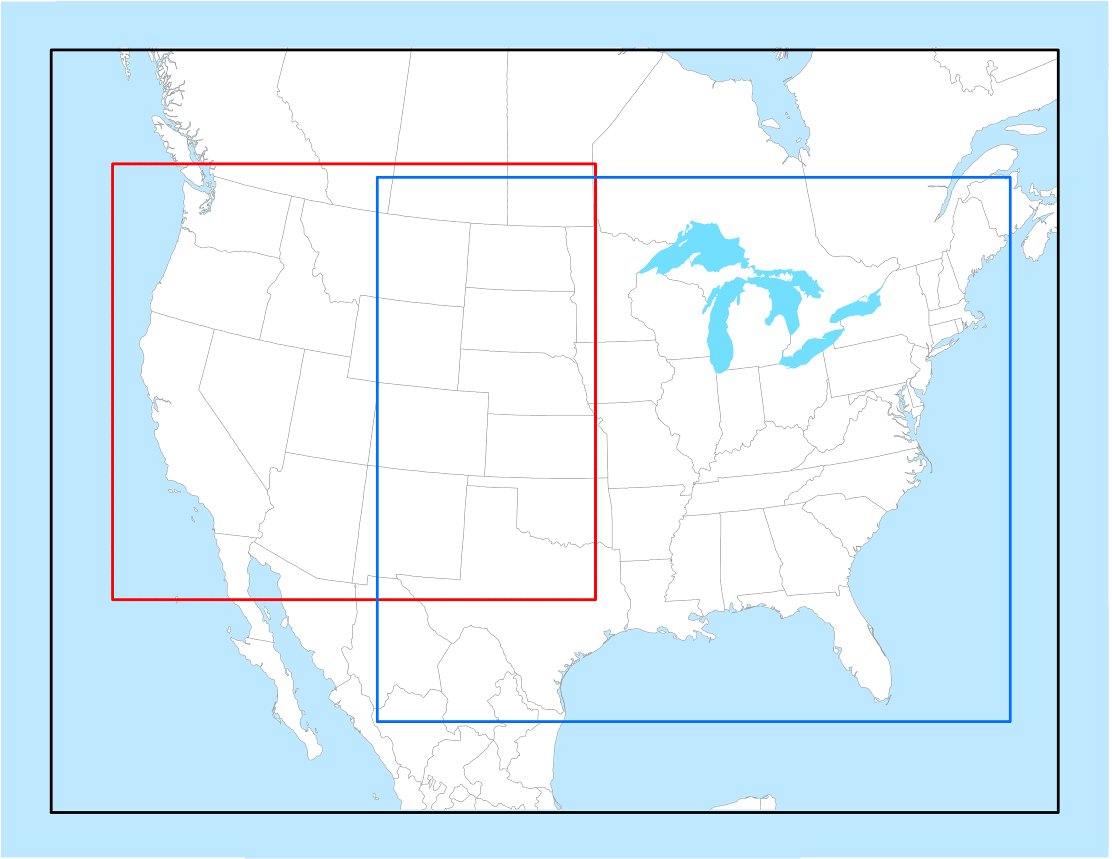
[3] See the 4/09/07 e-mail from Shawn Roselle, Office of Research and Development to Carey Jang, Office of Air Quality Planning and Standards which is included in the docket for this rulemaking.

All of the modeling results assessing the emissions scenarios for the RIA were taken from the 12 km grids. Table II-1 provides some basic geographic information regarding the CMAQ domains.

**Table II-1. Geographic information for modeling domains.**

| | CMAQ 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 CMAQ modeling domain. The black outer box denotes the 36 km national modeling domain; the red inner box is the 12 km western U.S. fine grid; and the blue inner box is the 12 km eastern U.S. fine grid.**



## C. Modeling Period / Ozone Episodes

The 36 km and both 12 km CMAQ modeling domains were modeled for the entire year of 2002[4]. All 365 model days were used in the annual average levels of $PM_{2.5}$. For the 8-hour ozone, we used modeling results from the period between May 1 and September 30, 2002. This 153-day period generally conforms to the ozone season across most parts of the U.S. and contains the majority of days that observed high ozone concentrations in 2002.

## D. Model Inputs: Emissions, Meteorology and Boundary Conditions

*1. Base Year and Future Baseline Emissions:* As noted in the introduction section, we switched from the 2001-Based Platform used for the proposed rule modeling to a 2002 Platform for the final rule modeling. The 2002 Platform builds upon the general concepts, tools and emissions modeling data from the 2001 Platform, while updating and enhancing many of the emission inputs and tools. A summary of the emissions inventory development is described below. More detailed documentation on the methods and data summaries of the 2002 Platform emissions for base and future years is also available separately.[5]

We used version 3 of the 2002 Platform which takes emission inventories from the 2002 National Emissions Inventory (NEI) version 3.0. These inventories, with the exception of California[6], include monthly onroad and nonroad emissions generated from the National Mobile Inventory Model (NMIM) using versions of MOBILE6.0 and NONROAD2005 consistent with recent national rule analyses[7,8]. The 2002 Platform and its associated chemical mechanism (CB05) employs updated speciation profiles using data included in the SPECIATE4.0 database[9]. In addition, the 2002 Platform incorporates several temporal profile updates for both mobile and stationary sources.

The 2002 Platform includes emissions for a 2002 base year model evaluation case, a 2002 base case and several projection years. As noted above, 2020 is the projection year for the

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[4] We also modeled 10 days at the end of December 2001 as a modeled "ramp up" period. These days are used to minimize the effects of initial conditions and are not considered as part of the output analyses.

[5] Technical Support Document: Preparation of Emissions Inventories for the 2002-based Platform, Version 3.0, Criteria Air Pollutants, and Appendices, January 2008. Files containing this TSD and the appendices are available in the docket for this rulemaking.

[6] The California Air Resources Board submitted annual emissions for California. These were allocated to monthly resolution prior to emissions modeling using data from the National Mobile Inventory Model (NMIM).

[7] MOBILE6 version was used in the Mobile Source Air Toxics Rule: *Regulatory Impact Analysis for Final Rule: Control of Hazardous Air Pollutants from Mobile Sources*, U.S. Environmental Protection Agency, Office of Transportation and Air Quality, Assessment and Standards Division, Ann Arbor, MI 48105, EPA420-R-07-002, February 2007.

[8] NONROAD2005 version was used in the proposed rule for small spark ignition (SI) and marine SI rule: Draft Regulatory Impact Analysis: *Control of Emissions from Marine SI and Small SI Engines, Vessels, and Equipment* , U.S. Environmental Protection Agency, Office of Transportation and Air Quality, Office of Transportation and Air Quality, Assessment and Standards Division, Ann Arbor, MI, EPA420-D-07-004, April 2007.

[9] See http://www.epa.gov/ttn/chief/software/speciate/index.html for more details.

Ozone NAAQS RIA. The model evaluation case uses prescribed burning and wildfire emissions specific to 2002, which were developed and modeled as day-specific, location-specific emissions using an updated version of Sparse Matrix Operator Kernel Emissions (SMOKE) system, version 2.3, which computes plume rise and vertically allocates the fire emissions. It also includes continuous emissions monitoring (CEM) data for 2002 for electric generating units (EGUs) with CEMs. The 2002 and future year base cases include an average fire sector and temporally averaged emissions (i.e., no CEM data) for EGUs. Projections from 2002 were developed to account for the expected impact of national regulations, consent decrees or settlements, known plant closures, and, for some sectors, activity growth.

*2. Meteorological Input Data:* The gridded meteorological input data for the entire year of 2002 were derived from simulations of the Pennsylvania State University / National Center for Atmospheric Research Mesoscale Model. This model, commonly referred to as MM5[10], 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 domains shown in Figure II-1. The MM5 simulations were run on the same map projection as CMAQ. The 36 km national domain was modeled using MM5 v.3.6.0 using land-surface modifications that were added in v3.6.3. The 12 km eastern U.S grid was modeled with MM5 v3.7.2. These two sets of meteorological inputs were developed by EPA. For the 12 km western U.S. domain, we utilized existing MM5 meteorological model data prepared by the Western Regional Air Partnership (WRAP)[11].

The three meteorological model runs used similar sets of physics options. All three simulations used the Pleim-Xiu planetary boundary layer and vertical diffusion scheme, the RRTM longwave radiation scheme, and the Reisner 1 microphysics scheme. The EPA cases used the Kain-Fritsch 2 subgrid convection scheme while the WRAP simulation used the Betts-Miller scheme for subgrid convection. In the EPA simulations, analysis nudging was utilized above the boundary layer for temperature and water vapor and in all locations for the wind components, using relatively weak nudging coefficients. The WRAP runs employed similar four-dimensional data assimilation, but also included observational nudging of surface winds. All three sets of model runs were conducted in 5.5 day segments with 12 hours of overlap for spin-up purposes. Additionally, all three domains contained 34 vertical layers with an approximately 38 m deep surface layer and a 100 millibar top. The MM5 and CMAQ vertical structures are shown in Table II-2 and do not vary by horizontal grid resolution.

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[10] Grell, G., J. Dudhia, and D. Stauffer, 1994: A Description of the Fifth-Generation Penn State/NCAR Mesoscale Model (MM5), NCAR/TN-398+STR., 138 pp, National Center for Atmospheric Research, Boulder CO.

[11] Kemball-Cook, S., Y. Jia, C. Emery, R. Morris, Z. Wang and G. Tonnesen. 2004. 2002 Annual MM5 Simulation to Support WRAP CMAQ Visibility Modeling for the Section 308 SIP/TIP – MM5 Sensitivity Simulations to Identify a More Optimal MM5 Configuration for Simulating Meteorology in the Western United States. Western Regional Air Partnership, Regional Modeling Center. December 10. (http://pah.cert.ucr.edu/aqm/308/reports/mm5/MM5SensitivityRevRep_Dec_10_2004.pdf)

**Table II-2. Vertical layer structure for MM5 and CMAQ (heights are layer top).**

| CMAQ Layers | MM5 Layers | Sigma P | Approximate Height (m) | Approximate Pressure (mb) |
|---|---|---|---|---|
| 0 | 0 | 1.000 | 0 | 1000 |
| 1 | 1 | 0.995 | 38 | 995 |
| 2 | 2 | 0.990 | 77 | 991 |
| 3 | 3 | 0.985 | 115 | 987 |
|  | 4 | 0.980 | 154 | 982 |
| 4 | 5 | 0.970 | 232 | 973 |
|  | 6 | 0.960 | 310 | 964 |
| 5 | 7 | 0.950 | 389 | 955 |
|  | 8 | 0.940 | 469 | 946 |
| 6 | 9 | 0.930 | 550 | 937 |
|  | 10 | 0.920 | 631 | 928 |
|  | 11 | 0.910 | 712 | 919 |
| 7 | 12 | 0.900 | 794 | 910 |
|  | 13 | 0.880 | 961 | 892 |
|  | 14 | 0.860 | 1,130 | 874 |
| 8 | 15 | 0.840 | 1,303 | 856 |
|  | 16 | 0.820 | 1,478 | 838 |
|  | 17 | 0.800 | 1,657 | 820 |
| 9 | 18 | 0.770 | 1,930 | 793 |
|  | 19 | 0.740 | 2,212 | 766 |
| 10 | 20 | 0.700 | 2,600 | 730 |
|  | 21 | 0.650 | 3,108 | 685 |
| 11 | 22 | 0.600 | 3,644 | 640 |
|  | 23 | 0.550 | 4,212 | 595 |
| 12 | 24 | 0.500 | 4,816 | 550 |
|  | 25 | 0.450 | 5,461 | 505 |
|  | 26 | 0.400 | 6,153 | 460 |
| 13 | 27 | 0.350 | 6,903 | 415 |
|  | 28 | 0.300 | 7,720 | 370 |
|  | 29 | 0.250 | 8,621 | 325 |
|  | 30 | 0.200 | 9,625 | 280 |
| 14 | 31 | 0.150 | 10,764 | 235 |
|  | 32 | 0.100 | 12,085 | 190 |
|  | 33 | 0.050 | 13,670 | 145 |
|  | 34 | 0.000 | 15,674 | 100 |

The meteorological outputs from all three MM5 sets were processed to create model-ready inputs for CMAQ using the Meteorology-Chemistry Interface Processor (MCIP)[12], version 3.1, to derive the specific inputs to CMAQ.

Before initiating the air quality simulations, it is important to identify the biases and errors associated with the meteorological modeling inputs. The EPA 2002 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. Qualitatively, the model fields closely matched the observed synoptic patterns, which is expected given the use of nudging. The operational

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[12] Byun, D.W., and Ching, J.K.S., Eds, 1999. Science algorithms of EPA Models-3 Community Multiscale Air Quality (CMAQ modeling system, EPA/600/R-99/030, Office of Research and Development).

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, four meteorological parameters were investigated: temperature, humidity, wind speed, and wind direction. The operational piece of the analyses focuses on surface parameters. The Atmospheric Model Evaluation Tool (AMET) was used to conduct the analyses as described in this report.[13] The three individual MM5 evaluations are described elsewhere.[14,15,16] It was ultimately determined that the bias and error values associated with all three sets of 2002 meteorological data were generally within the range of past meteorological modeling results that have been used for air quality applications.[17]

*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[18] model. 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 2002 with a grid resolution of 2.0 degree x 2.5 degree (latitude-longitude) and 20 vertical layers. The predictions were used to provide one-way dynamic boundary conditions at three-hour intervals and an initial concentration field for the CMAQ simulations. More information is available about the GEOS-CHEM model and other applications using this tool at: http://www-as.harvard.edu/chemistry/trop/geos.

## E. CMAQ Base Case Model Performance Evaluation

An operational model performance evaluation for ozone and $PM_{2.5}$ and its related speciated components was conducted using 2002 State/local monitoring sites data in order to estimate the ability of the CMAQ modeling system to replicate the base year concentrations for the 12-km eastern and western domains. In summary, model performance statistics were calculated for observed-predicted pairs of daily, monthly, seasonal, and annual concentrations. Statistics were generated for the following geographic groupings: the entire 12-km Eastern US domain (EUS), the entire 12-km Western US domain (WUS), and five large subregions[19]:

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[13] Gilliam, R. C., W. Appel, and S. Phillips. The Atmospheric Model Evaluation Tool (AMET): Meteorology Module. Presented at 4th Annual CMAS Models-3 Users Conference, Chapel Hill, NC, September 26 - 28, 2005.

[14] Brewer J., P. Dolwick, and R. Gilliam. Regional and Local Scale Evaluation of MM5 Meteorological Fields for Various Air Quality Modeling Applications, Presented at the 87th Annual American Meteorological Society Annual Meeting, San Antonio, TX, January 15-18, 2007.

[15] Dolwick, P, R. Gilliam, L. Reynolds, and A. Huffman. Regional and Local-scale Evaluation of 2002 MM5 Meteorological Fields for Various Air Quality Modeling Applications, Presented at 6th Annual CMAS Models-3 Users Conference, Chapel Hill, NC, October 1 - 3, 2007.

[16] Kemball-Cook, S., Y. Jia, C. Emery, R. Morris, Z. Wang, and G. Tonnesen. Annual 2002 MM5 Meteorological Modeling to Support Regional Haze Modeling of the Western United States,
Prepared for The Western Regional Air Partnership (WRAP), 1515 Cleveland Place, Suite 200
Denver, CO 80202, March 2005.

[17] Environ, Enhanced Meteorological Modeling and Performance Evaluation for Two Texas Episodes, August 2001.

[18] Yantosca, B., 2004. GEOS-CHEMv7-01-02 User's Guide, Atmospheric Chemistry Modeling Group, Harvard University, Cambridge, MA, October 15, 2004.

[19] The subregions are defined by States where: Midwest is IL, IN, MI, OH, and WI; Northeast is CT, DE,

Midwest, Northeast, Southeast, Central, and West U.S. The "acceptability" of model performance was judged by comparing our CMAQ 2002 performance results to the range of performance found in the 2001 CMAQ results used in the proposal, as well as recent regional ozone and $PM_{2.5}$ model applications (e.g., Clean Air Interstate Rule, Final PM NAAQS Rule)[20]. These other modeling studies represent a wide range of modeling analyses which cover various models, model configurations, domains, years and/or episodes, chemical mechanisms, and aerosol modules.

There are various statistical metrics available and used by the science community for model performance evaluation. For a robust evaluation, the principal evaluation statistics used to evaluate CMAQ performance were two bias metrics, normalized mean bias and fractional bias; and two error metrics, normalized mean error and fractional error. Normalized mean bias (NMB) is used as a normalization to facilitate a range of concentration magnitudes. This statistic averages the difference (model - observed) over the sum of observed values. NMB is a useful model performance indicator because it avoids over inflating the observed range of values, especially at low concentrations. Normalized mean bias is defined as:

$$\text{NMB} = \frac{\sum_{1}^{n}(P-O)}{\sum_{1}^{n}(O)} * 100, \text{ where P = predicted concentrations and O = observed}$$

Normalized mean error (NME) is also similar to NMB, where the performance statistic is used as a normalization of the mean error. NME calculates the absolute value of the difference (model - observed) over the sum of observed values. Normalized mean error is defined as:

$$\text{NME} = \frac{\sum_{1}^{n}|P-O|}{\sum_{1}^{n}(O)} * 100, \text{ where P = predicted concentrations and O = observed}$$

Fractional bias is defined as:

$$\text{FB} = \frac{1}{n}\left(\frac{\sum_{1}^{n}(P-O)}{\sum_{1}^{n}\left(\frac{(P+O)}{2}\right)}\right) * 100, \text{ where P = predicted concentrations and O = observed}$$

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MA, MD, ME, NH, NJ, NY, PA, RI, and VT; Southeast is AL, FL, GA, KY, MS, NC, SC, TN, VA, and WV; Central is AR, IA, KS, LA, MN, MO, NE, OK, and TX; West is CA, OR, WA, AZ, NM, CO, UT, WY, SD, ND, MT, ID, and NV.

[20] See: U.S. Environmental Protection Agency; Technical Support Document for the Final Clean Air Interstate Rule: Air Quality Modeling; Office of Air Quality Planning and Standards; RTP, NC; March 2005 (CAIR Docket OAR-2005-0053-2149); and U.S. Environmental Protection Agency, 2006. Technical Support Document for the Final PM NAAQS Rule: Office of Air Quality Planning and Standards, Research Triangle Park, NC

FB is a useful model performance indicator because it has the advantage of equally weighting positive and negative bias estimates. The single largest disadvantage in this estimate of model performance is that the estimated concentration (i.e., prediction, P) is found in both the numerator and denominator.

Fractional error (FE) is similar to fractional bias except the absolute value of the difference is used so that the error is always positive. Fractional error is defined as:

$$\mathrm{FE} = \frac{1}{n}\left(\frac{\sum_{1}^{n}|P-O|}{\sum_{1}^{n}\left(\frac{(P+O)}{2}\right)}\right)*100,$$ where P = predicted concentrations and O = observed

Overall, the bias and error statistics shown in Table II-3, II-4, and II-5 below indicate that the base case model ozone and $PM_{2.5}$ concentrations are within the range or close to that found in recent OAQPS applications. The CMAQ model performance results give us confidence that our applications of CMAQ using this 2002 Platform provide a scientifically credible approach for assessing ozone and $PM_{2.5}$ concentrations for the purposes of the Ozone NAAQS Final Rule. A detailed summary of the CMAQ model performance evaluation is available in the docket for this rulemaking[21]. A summary of the $PM_{2.5}$ and ozone evaluation is presented here.

*1. Ozone:* The ozone evaluation focuses on the observed and predicted hourly ozone concentrations and eight-hour daily maximum ozone concentrations using a (observation) threshold of 40 ppb. This ozone model performance was limited to the period used in the calculation of projected design values within the analysis, that is: May, June, July, August, and September. Ozone ambient measurements for 2002 were obtained from the Air Quality System (AQS) Aerometric Information Retrieval System (AIRS). A total of 1178 ozone measurement sites were included for evaluation. These ozone data were measured and reported on an hourly basis.

Table II-3 and II-4 provides hourly and eight-hour daily maximum ozone model performance statistics, respectively, calculated for a threshold of 40 ppb of observed and modeled concentrations, restricted to the ozone season modeled for the 12-km Eastern and Western U.S. domain and the five subregions. Generally, hourly and eight-hour ozone model performance are under-predicted in both the 12-km EUS and WUS when applying a threshold of 40 ppb for the modeled ozone season (May-September). For the 12-km EUS and WUS domain, the bias and error statistics are comparable for the aggregate of the ozone season and for each individual ozone month modeled.

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[21] Technical Support Document: 2002 CMAQ Model Performance Evaluation for Ozone and Particulate Matter, January 2008. This file is available in the docket for this rulemaking.

**Table II-3. Summary of CMAQ 2002 hourly ozone model performance statistics.**

| CMAQ 2002 Hourly Ozone: Threshold of 40 ppb | | No. of Obs. | NMB (%) | NME (%) | FB (%) | FE (%) |
|---|---|---|---|---|---|---|
| **May** | 12-km EUS | 241185 | -0.7 | 15.9 | -2.0 | 17.1 |
| | 12-km WUS | 124931 | -3.7 | 15.9 | -5.0 | 17.3 |
| | Northeast | 51055 | 1.2 | 17.1 | -0.3 | 18.2 |
| | Midwest | 55859 | 3.3 | 16.2 | 2.4 | 16.9 |
| | Southeast | 69073 | -2.5 | 14.1 | -3.1 | 14.8 |
| | Central | 41728 | -6.4 | 17.3 | -9.2 | 20.3 |
| | West | 111385 | -3.9 | 16.1 | -5.2 | 17.6 |
| **June** | 12-km EUS | 256263 | -7.5 | 16.8 | -9.0 | 18.6 |
| | 12-km WUS | 125662 | -8.37 | 17.7 | -9.3 | 19.1 |
| | Northeast | 61354 | -8.46 | 17.3 | -9.9 | 19.1 |
| | Midwest | 54515 | -7.19 | 17.9 | -8.3 | 19.6 |
| | Southeast | 67867 | -7.2 | 15.3 | -7.6 | 16.3 |
| | Central | 46026 | -10.0 | 17.5 | -13.5 | 21.2 |
| | West | 109157 | -8.8 | 18.2 | -9.9 | 19.7 |
| **July** | 12-km EUS | 257076 | -5.3 | 17.7 | -6.6 | 19.2 |
| | 12-km WUS | 116785 | -12.0 | 21.5 | -14.9 | 24.3 |
| | Northeast | 66774 | -3.9 | 17.0 | -4.8 | 18.0 |
| | Midwest | 59360 | -10.5 | 19.4 | -12.3 | 21.7 |
| | Southeast | 68619 | -3.6 | 16.5 | -3.9 | 17.2 |
| | Central | 36021 | -3.6 | 18.7 | -6.3 | 21.1 |
| | West | 104321 | -13.6 | 21.8 | -16.8 | 24.9 |
| **August** | 12-km EUS | 235090 | -8.7 | 17.8 | -10.2 | 19.7 |
| | 12-km WUS | 125575 | -7.91 | 20.1 | -10.2 | 22.1 |
| | Northeast | 53837 | -6.4 | 16.7 | -7.4 | 18.0 |
| | Midwest | 54179 | -10.8 | 19.1 | -12.4 | 21.4 |
| | Southeast | 62506 | -9.4 | 17.3 | -9.9 | 18.5 |
| | Central | 41456 | -9.3 | 18.7 | -12.8 | 22.4 |
| | West | 110225 | -8.5 | 20.6 | -11.1 | 22.8 |
| **September** | 12-km EUS | 179156 | -9.9 | 17.2 | -11.8 | 19.5 |
| | 12-km WUS | 99710 | -10.7 | 19.0 | -12.7 | 21.1 |
| | Northeast | 44678 | -8.7 | 16.3 | -10.6 | 18.4 |
| | Midwest | 34285 | -11.4 | 18.5 | -12.9 | 20.4 |
| | Southeast | 41627 | -8.2 | 16.5 | -9.0 | 17.8 |
| | Central | 41549 | -12.8 | 18.8 | -16.6 | 22.8 |
| | West | 83921 | -11.7 | 20.0 | -13.8 | 22.1 |
| **Seasonal Aggregate** | 12-km EUS | 1168770 | -6.4 | 17.1 | -7.7 | 18.8 |
| | 12-km WUS | 592663 | -8.4 | 18.8 | -10.3 | 20.7 |
| | Northeast | 277698 | -5.4 | 16.9 | -6.5 | 18.4 |
| | Midwest | 258198 | -7.3 | 18.3 | -8.4 | 20.0 |

**Table II-4. Summary of CMAQ 2002 eight-hour daily maximum ozone model performance statistics.**

| CMAQ 2002 Eight-Hour Maximum Ozone: Threshold of 40 ppb | | No. of Obs. | NMB (%) | NME (%) | FB (%) | FE (%) |
|---|---|---|---|---|---|---|
| **May** | 12-km EUS | 19172 | 3.9 | 12.7 | 4.3 | 12.6 |
| | 12-km WUS | 9223 | 0.2 | 12.6 | 0.6 | 12.8 |
| | Northeast | 4255 | 6.7 | 14.3 | 6.8 | 14.2 |
| | Midwest | 4198 | 7.8 | 13.7 | 8.2 | 13.5 |
| | Southeast | 5470 | 0.6 | 10.9 | 1.1 | 11.0 |
| | Central | 3379 | 0.3 | 12.3 | 0.7 | 12.4 |
| | West | 8155 | -0.1 | 12.8 | 0.3 | 12.9 |
| **June** | 12-km EUS | 19462 | -3.9 | 12.3 | -3.3 | 12.4 |
| | 12-km WUS | 9029 | -4.9 | 14.1 | -4.2 | 14.2 |
| | Northeast | 4608 | -5.3 | 12.5 | -4.7 | 12.7 |
| | Midwest | 4104 | -3.2 | 12.7 | -2.2 | 12.8 |
| | Southeast | 5110 | -4.8 | 11.8 | -4.1 | 11.9 |
| | Central | 3603 | -4.5 | 12.2 | -4.4 | 12.7 |
| | West | 7818 | -5.3 | 14.5 | -4.7 | 14.7 |
| **July** | 12-km EUS | 20565 | -1.6 | 13.5 | -1.0 | 13.6 |
| | 12-km WUS | 8809 | -7.4 | 17.1 | -8.1 | 18.0 |
| | Northeast | 5380 | -0.7 | 13.0 | -0.2 | 12.9 |
| | Midwest | 4368 | -6.5 | 14.2 | -5.8 | 14.4 |
| | Southeast | 5633 | -0.9 | 13.0 | -0.1 | 13.0 |
| | Central | 3114 | 1.3 | 14.4 | 1.2 | 14.7 |
| | West | 7784 | -9.0 | 17.2 | -9.9 | 18.2 |
| **August** | 12-km EUS | 19260 | -5.1 | 13.2 | -4.4 | 13.4 |
| | 12-km WUS | 9551 | -2.8 | 15.8 | -3.1 | 16.1 |
| | Northeast | 4667 | -2.9 | 12.4 | -2.2 | 12.4 |
| | Midwest | 4012 | -8.1 | 13.9 | -7.5 | 14.2 |
| | Southeast | 5067 | -6.4 | 13.4 | -5.4 | 13.4 |
| | Central | 3543 | -4.0 | 13.5 | -3.9 | 14.1 |
| | West | 8311 | -3.2 | 16.1 | -3.6 | 16.5 |
| **September** | 12-km EUS | 15865 | -6.2 | 12.6 | -5.9 | 12.9 |
| | 12-km WUS | 8185 | -6.7 | 15.0 | -6.9 | 15.5 |
| | Northeast | 4074 | -6.0 | 11.8 | -6.0 | 12.3 |
| | Midwest | 3120 | -7.2 | 13.3 | -6.5 | 13.3 |
| | Southeast | 3671 | -4.5 | 12.6 | -3.8 | 12.7 |
| | Central | 3492 | -8.5 | 13.8 | -8.7 | 14.5 |
| | West | 6911 | -7.3 | 15.9 | -7.6 | 16.4 |
| **Seasonal Aggregate** | 12-km EUS | 94324 | -2.6 | 12.9 | -1.9 | 13.0 |
| | 12-km WUS | 44797 | -4.3 | 14.9 | -4.2 | 15.3 |
| | Northeast | 22984 | -1.9 | 12.8 | -1.2 | 12.9 |
| | Midwest | 19802 | -3.6 | 13.6 | -2.5 | 13.7 |

| CMAQ 2002 Eight-Hour Maximum Ozone: Threshold of 40 ppb | | No. of Obs. | NMB (%) | NME (%) | FB (%) | FE (%) |
|---|---|---|---|---|---|---|
| | Southeast | 24951 | -3.1 | 12.4 | -2.3 | 12.4 |
| | Central | 17131 | -3.3 | 13.2 | -3.1 | 13.7 |
| | West | 38979 | -4.9 | 15.3 | -5.0 | 15.7 |

*2. $PM_{2.5}$:* The $PM_{2.5}$ evaluation focuses on $PM_{2.5}$ total mass and its components including sulfate ($SO_4$), nitrate ($NO_3$), total nitrate ($TNO_3=NO_3+HNO_3$), ammonium ($NH_4$), elemental carbon (EC), and organic carbon (OC). The $PM_{2.5}$ performance statistics were calculated for each month and season individually and for the entire year, as a whole. Seasons were defined as: winter (December-January-February), spring (March-April-May), summer (June-July-August), and fall (September-October-November). $PM_{2.5}$ ambient measurements for 2002 were obtained from the following networks for model evaluation: **S**peciation **T**rends **N**etwork (STN- total of 199 sites), **I**nteragency **M**onitoring of **PRO**tected **V**isual **E**nvironments (IMPROVE- total of 150), and **C**lean **A**ir **S**tatus and **T**rends **Net**work (CASTNet- total of 83). For $PM_{2.5}$ species that are measured by more than one network, we calculated separate sets of statistics for each network. For brevity, Table II-5 provides annual model performance statistics for $PM_{2.5}$ and its component species for the 12-km Eastern domain, 12-km Western domain, and five subregions defined above (Midwest, Northeast, Southeast, Central, and West U.S.).

**Table II-5. Summary of 2002 CMAQ annual $PM_{2.5}$ species model performance statistics.**

| CMAQ 2002 Annual | | | No. of Obs. | NMB (%) | NME (%) | FB (%) | FE (%) |
|---|---|---|---|---|---|---|---|
| $PM_{2.5}$ Total Mass | STN | 12-km EUS | 10307 | 10.8 | 42.8 | 5.4 | 42.6 |
| | | 12-km WUS | 3000 | -5.8 | 46.9 | -3.1 | 45.0 |
| | | Northeast | 1516 | 14.9 | 35.6 | 13.2 | 34.4 |
| | | Midwest | 2780 | 20.5 | 48.2 | 16.6 | 42.6 |
| | | Southeast | 2554 | -3.9 | 36.0 | -10.0 | 39.7 |
| | | Central | 2738 | 14.5 | 49.1 | 6.0 | 49.4 |
| | | West | 2487 | -7.4 | 46.8 | -4.5 | 44.8 |
| | IMPROVE | 12-km EUS | 8436 | -2.3 | 49.0 | -5.7 | 51.4 |
| | | 12-km WUS | 10123 | -26.4 | 53.5 | -26.3 | 57.5 |
| | | Northeast | 592 | 8.6 | 41.5 | 2.4 | 41.0 |
| | | Midwest | 2060 | 21.0 | 59.4 | 17.4 | 51.6 |
| | | Southeast | 1803 | -13.1 | 41.2 | -19.8 | 49.9 |
| | | Central | 1624 | -13.1 | 49.4 | -17.6 | 57.0 |
| | | West | 9543 | -27.8 | 53.1 | -27.1 | 57.2 |
| Sulfate | STN | 12-km EUS | 10157 | -3.9 | 33.6 | -9.7 | 38.4 |
| | | 12-km WUS | 2926 | -20.6 | 41.9 | -12.2 | 43.5 |
| | | Northeast | 1487 | 3.6 | 34.9 | -2.9 | 36.2 |
| | | Midwest | 2730 | -4.3 | 29.1 | -8.8 | 33.6 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | Southeast | 2541 | -7.6 | 33.4 | -16.3 | 38.8 |
| | | Central | 2686 | -3.2 | 39.2 | -7.2 | 44.3 |
| | | West | 2446 | -26.1 | 44.9 | -15.8 | 44.8 |
| | IMPROVE | 12-km EUS | 8532 | -10.8 | 33.0 | -7.2 | 40.6 |
| | | 12-km WUS | 10232 | -7.5 | 42.4 | 7.6 | 45.7 |
| | | Northeast | 597 | -4.9 | 29.9 | -10.0 | 35.7 |
| | | Midwest | 2070 | -12.3 | 30.1 | -9.9 | 36.1 |
| | | Southeast | 1805 | -9.5 | 32.9 | -16.8 | 40.5 |
| | | Central | 1671 | -16.1 | 35.0 | -16.0 | 42.4 |
| | | West | 9645 | -5.5 | 43.5 | 8.6 | 45.9 |
| | CASTNet | 12-km EUS | 3173 | -11.3 | 20.5 | -16.3 | 26.1 |
| | | 12-km WUS | 1158 | -21.3 | 34.6 | -11.2 | 35.9 |
| | | Northeast | 663 | -8.3 | 19.3 | -16.3 | 24.3 |
| | | Midwest | 839 | -12.3 | 17.9 | -15.6 | 21.6 |
| | | Southeast | 1085 | -11.2 | 21.5 | -17.8 | 27.2 |
| | | Central | 229 | -20.7 | 27.3 | -27.4 | 33.6 |
| | | West | 1118 | -20.4 | 35.3 | -10.7 | 36.1 |
| Nitrate | STN | 12-km EUS | 8770 | 18.3 | 65.9 | -29.1 | 84.5 |
| | | 12-km WUS | 2726 | -45.0 | 63.1 | -70.6 | 95.0 |
| | | Northeast | 1488 | 17.4 | 59.1 | -5.0 | 67.3 |
| | | Midwest | 2731 | 32.7 | 70.4 | -10.9 | 78.1 |
| | | Southeast | 2540 | 8.6 | 84.6 | -64.7 | 107.5 |
| | | Central | 1298 | 12.7 | 52.5 | -13.4 | 69.1 |
| | | West | 2446 | -47.5 | 62.8 | -73.8 | 95.4 |
| | IMPROVE | 12-km EUS | 8514 | 48.4 | 106.8 | -52.8 | 116.4 |
| | | 12-km WUS | 10110 | -34.8 | 80.67 | -101.0 | 130.0 |
| | | Northeast | 597 | 43.0 | 86.0 | -37.0 | 102.8 |
| | | Midwest | 2069 | 122.2 | 153.8 | 3.5 | 107.5 |
| | | Southeast | 1803 | 33.5 | 112.2 | -78.5 | 130.8 |
| | | Central | 1672 | 18.1 | 81.0 | -59.6 | 114.1 |
| | | West | 9522 | -39.6 | 81.1 | -104.0 | 131.1 |
| Total Nitrate ($NO_3$+$HNO_3$) | CASTNet | 12-km EUS | 3171 | 24.4 | 37.3 | 16.8 | 35.1 |
| | | 12-km WUS | 1157 | -19.5 | 44.2 | -12.0 | 46.0 |
| | | Northeast | 662 | 20.5 | 29.4 | 16.3 | 25.3 |
| | | Midwest | 839 | 39.1 | 46.5 | 29.0 | 39.7 |
| | | Southeast | 1085 | 22.9 | 39.5 | 15.8 | 37.2 |
| | | Central | 229 | 6.2 | 35.6 | 0.6 | 36.2 |
| | | West | 1117 | -20.4 | 45.8 | -12.1 | 46.6 |
| Ammonium | STN | 12-km EUS | 10157 | 11.9 | 40.6 | 14.4 | 45.2 |
| | | 12-km WUS | 2926 | -23.6 | 55.7 | 7.2 | 58.1 |
| | | Northeast | 1488 | 16.0 | 39.6 | 21.8 | 42.8 |

|  |  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|---|
|  |  | Midwest | 2731 | 12.3 | 38.4 | 19.2 | 42.4 |
|  |  | Southeast | 2540 | 7.3 | 38.4 | 6.0 | 41.8 |
|  |  | Central | 2685 | 15.0 | 46.6 | 14.3 | 52.1 |
|  |  | West | 2446 | -30.6 | 56.7 | 2.9 | 59.7 |
|  | CASTNet | 12-km EUS | 3166 | 5.3 | 30.8 | 2.7 | 31.6 |
|  |  | 12-km WUS | 1156 | -16.8 | 42.5 | -13.0 | 41.1 |
|  |  | Northeast | 661 | 15.3 | 27.6 | 13.6 | 25.2 |
|  |  | Midwest | 837 | 9.8 | 34.7 | 11.9 | 33.9 |
|  |  | Southeast | 1085 | -7.7 | 30.1 | -9.7 | 33.6 |
|  |  | Central | 229 | 7.4 | 33.1 | 3.0 | 35.6 |
|  |  | West | 1116 | -21.1 | 43.5 | -14.4 | 41.4 |
| Elemental Carbon | STN | 12-km EUS | 10031 | 45.0 | 78.9 | 22.1 | 56.9 |
|  |  | 12-km WUS | 2975 | 43.1 | 82.6 | 18.2 | 61.3 |
|  |  | Northeast | 1498 | 37.1 | 58.9 | 24.5 | 48.3 |
|  |  | Midwest | 2744 | 53.1 | 76.7 | 26.3 | 54.7 |
|  |  | Southeast | 2506 | 16.9 | 66.0 | 7.2 | 51.7 |
|  |  | Central | 2570 | 91.7 | 118.0 | 41.0 | 68.1 |
|  |  | West | 2475 | 49.0 | 86.2 | 17.1 | 62.7 |
|  | IMPROVE | 12-km EUS | 8282 | -15.0 | 49.2 | -23.4 | 52.8 |
|  |  | 12-km WUS | 10069 | -14.1 | 67.2 | -29.5 | 62.1 |
|  |  | Northeast | 599 | -22.6 | 37.5 | -27.4 | 46.5 |
|  |  | Midwest | 2056 | 11.6 | 57.5 | 0.5 | 50.8 |
|  |  | Southeast | 1795 | -32.4 | 44.6 | -42.0 | 55.6 |
|  |  | Central | 1532 | -24.3 | 47.6 | -29.8 | 55.9 |
|  |  | West | 9493 | -15.5 | 67.8 | -31.3 | 62.7 |
| Organic Carbon | STN | 12-km EUS | 9726 | -39.9 | 58.0 | -41.1 | 70.5 |
|  |  | 12-km WUS | 2903 | -37.6 | 60.3 | -40.4 | 69.3 |
|  |  | Northeast | 1447 | -45.2 | 60.9 | -41.6 | 73.1 |
|  |  | Midwest | 2641 | -26.5 | 61.7 | -19.7 | 67.6 |
|  |  | Southeast | 2474 | -47.4 | 55.3 | -53.7 | 70.7 |
|  |  | Central | 2504 | -43.6 | 54.0 | -51.3 | 69.7 |
|  |  | West | 2408 | -36.3 | 61.4 | -37.9 | 70.2 |
|  | IMPROVE | 12-km EUS | 8287 | -32.4 | 60.5 | -37.1 | 67.9 |
|  |  | 12-km WUS | 10082 | -34.8 | 60.0 | -31.2 | 63.0 |
|  |  | Northeast | 598 | -42.4 | 54.8 | -40.2 | 63.8 |
|  |  | Midwest | 2057 | -6.4 | 68.2 | -0.7 | 60.8 |
|  |  | Southeast | 1800 | -46.1 | 58.4 | -69.7 | 81.3 |
|  |  | Central | 1531 | -47.9 | 61.6 | -61.2 | 79.6 |
|  |  | West | 9508 | -34.5 | 59.6 | -29.7 | 61.9 |

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