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An Assessment of the Sensitivity and Reliability of the Relative Reduction Factor Approach in the Development of 8-hr Ozone Attainment Plans

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ABSTRACT

The updated regulatory framework for demonstrating that future 8-hr ozone (O_3) design values will be at or below the National Ambient Air Quality Standards (NAAQS) provides guidelines for the development of a State Implementation Plan (SIP) that includes methods based on photochemical modeling and analytical techniques. One of the suggested approaches is the relative reduction factor (RRF) for estimating the efficacy of emission reductions.

In this study, the sensitivity of model-predicted responses towards emission reductions to the choice of meteorology and chemical mechanisms was examined. While the different modeling simulations generally were found to be in agreement on whether predicted future-year design values would be above or below the NAAQS for 8-hr O_3 at a majority of the monitoring locations in the eastern United States, differences existed for a small percentage of monitors (~6.4%).

Another issue investigated was the ability of the attainment demonstration procedure to predict changes in monitored O_3 design values. A retrospective analysis was performed by comparing predicted O_3 design values from model simulations using emission estimates for 1996 and 2001 with monitored O_3 design values for 2001. Results indicated that an average gross error of ~5 ppb was present between modeled and observed design values and that, at ~27% of all sites, model-predicted and observed design values disagreed as to whether the design value was above or below the NAAQS. Retrospective analyses such as the one presented in this study can provide valuable insights into the strengths and limitations of modeling and analysis techniques used to predict future design values over time periods of a decade or more for the purpose of developing SIPs. Furthermore, such analyses could provide avenues for improvement and added confidence in the use of the RRF approach for addressing attainment of the NAAQS.

IMPLICATIONS

Application of photochemical models and analytical tools is a necessary step in the demonstration that an area will more than likely attain or maintain the NAAQS through the emission control programs identified in a SIP. This study shows that model-predicted responses to emission control strategies are fairly robust toward the choice of meteorological episodes and chemical mechanism, but that, at a small number of sites, the choice can lead to conflicting answers as to whether estimated future design values are above or below the level of the NAAQS. Furthermore, retrospective analysis presented in this study revealed differences between observed and predicted design values. Therefore, accounting for the model-to-model differences in the RRF and assessing a possible bias of future-year model predictions through a retrospective analysis should be undertaken as part of the SIP process to provide greater confidence in the use of photochemical modeling systems in the future air quality planning process.

INTRODUCTION

In 1997, the 1-hr ozone (O_3) National Ambient Air Quality Standard (NAAQS) was revised to that of an 8-hr standard in response to detrimental health and welfare effects resulting from extended periods of exposure to high O_3 concentrations. The U.S. Environmental Protection Agency (EPA) has issued draft modeling guidance[1] for the development of State Implementation Plans (SIPs) using

photochemical modeling techniques for evaluating control measures as a potential strategy for attaining and maintaining the NAAQS. An area is in nonattainment of the NAAQS if its current monitored design value (DVC) exceeds 84 ppb. As defined in 40CFR Part 50.10, Appendix I, paragraph 2.3, the DVC is calculated at each monitor by noting the fourth-highest 8-hr daily maximum concentration in each of three consecutive years and then computing the arithmetic mean of these three values. The form of the standard uses a 3-yr average as a means of reducing the DVC's dependence on short-term meteorological events. For areas whose DVC exceeds 75 ppb, the draft guidance outlines procedures for the estimation of future design values based on the DVC and O_3 concentrations predicted by grid-based photochemical models for base and future-year emission scenarios. In short, the guidance outlines a method in which the relative reduction factor (RRF) is calculated by computing the ratio between the modeled future-year and base-case 8-hr daily maximum O_3 concentrations at a given monitor both averaged over the simulation period. The future design value (DVF) then is calculated by multiplying the RRF with the DVC. The attainment test for a given monitor is passed if DVF is less than or equal to 84 ppb.

The draft modeling guidance does not identify any one photochemical modeling system for the calculation of the RRF; it outlines general criteria to be met when choosing a modeling system as well as the meteorological conditions to be used when applying models in developing the SIPs. Recent studies have investigated the robustness of the RRF to the choice of emission processors, modeling systems, and averaging time.[2,3] This study builds upon their findings, with the first objective of addressing the sensitivity of RRFs to the choice of input meteorology and chemical mechanisms. Toward this end, the model response to a specific set of emission reductions for two meteorological periods and two photochemical models was examined in terms of meeting the 8-hr O_3 NAAQS. In addition, the ability of the attainment demonstration methodology to predict changes in observed O_3 design values was investigated. To this end, a retrospective analysis was performed by simulating O_3 concentrations using emission estimates for 1996 and 2001 to assess whether the model-based changes in design values are consistent with those based on measurements.

Database

Monitored O_3 values used to calculate 8-hr O_3 design values for 1996 and 2001 were retrieved from the EPA Air Quality System (AQS) database, while most photochemical model simulations had been performed as part of previous studies. A brief overview of these simulations is provided, and the reader is referred to the relevant literature for more details. The photochemical models used in this study were the Community Model for Air Quality[4] (CMAQ) and the Comprehensive Air Quality Model with extensions[5] (CAMx). The meteorological fields for the CAMx simulation were based on RAMS3b,[6] while those used for the CMAQ simulation were prepared by applying MM5.[7] CAMx simulations were performed and evaluated by EPA in support of the proposed Interstate Air Quality Rule[13] for meteorological conditions during two 13-day periods in June and July of 1995 that have been described previously.[8] Additional details and a performance evaluation of the RAMS3b is provided in Hogrefe et al.[9] CMAQ simulations were performed for meteorological conditions during a 30-day period in July 1999. The setup and performance evaluation of the MM5 simulations for this period is described in Zhang et al.[10] The CMAQ simulations were performed with two different chemical mechanisms, namely, the CB4 mechanism[11] and the RADM2[12] mechanism, while only the CB4 mechanism was used for the CAMx simulations.

For the first objective of the study (i.e., the analysis of RRF differences caused by differences in meteorological regimes and chemical mechanisms), three different modeling systems (RAMS/CAMx-CB4, MM5/CMAQ-CB4, MM5/CMAQ-RADM2) were applied to simulate the effects of the emission reductions relative to 1996 that were proposed as part of the Clear Skies Act for 2010.[13] To address the second objective of the study (i.e., the comparison of observed and predicted changes in design values), observations and RAMS/CAMx simulations performed by EPA using 1995 meteorology and emission inventories for both 1996 and 2001 were utilized.[13,14] All emission inventories were processed by the Sparse Matrix Operator Kernel Emissions (SMOKE)[15] system, taking into account the meteorological fields and the chemical mechanism for each simulation. A summary of all simulations and the analysis for which they were used is provided in Table 1.

Before performing these analyses, model predictions for the respective base-case simulations (June and July 1995 meteorology with 1996 emissions for CAMx; July 1999 meteorology with 1996 emissions for CMAQ using both RADM2 and CB4 chemical mechanisms) were compared against O_3 observations for the time period corresponding to the meteorological fields used in the respective simulations. Visual comparison of the simulated daily 8-hr maximum O_3 fields (not shown) with measured data indicates similar spatial patterns for all days, although biases exist in some regions. CAMx utilizing the CB4 mechanism was able to predict 8-hr maximum O_3 better than the other two models, with mean biases of 2–4 ppb.

Table 1. Summary of model simulations used in analyses 1 and 2.

Simulation Period	Meteorological Model	Photochemical Model	Chemical Mechanism	Emission Inventory Base Case/Control Case	Used For
7/5/95–7/15/95 6/12/95–6/24/95	RAMS3b	CAMx	CB4	1996/2010	Analysis1
7/2/99–8/1/99	MM5	CMAQ	CB4	1996/2010	Analysis1
7/2/99–8/1/99	MM5	CMAQ	RADM2	1996/2010	Analysis1
7/5/95–7/15/95 6/12/95–6/24/95	RAMS3b	CAMx	CB4	1996/2001	Analysis2

CMAQ with CB4 or RADM2 chemical mechanisms tended to overpredict values in the Southeast, with biases often exceeding 8–12 ppb. The mean normalized bias and the mean normalized gross error were estimated for the 8-hr daily maximum concentrations over the entire episode for each monitoring location.

As discussed in the guidance,[1] two of the criteria for establishing acceptable model performance for the base case are that the mean normalized gross error and mean normalized bias (see reference 16 for definitions) be less than 35% and within −15% to 15%, respectively. It should be noted that only 8-hr daily maxima that exceeded 40 ppb were included in these calculations. For CAMx utilizing the CB4 chemical mechanism, 80% of the monitoring sites fall within the ranges specified in EPA guidance for the mean normalized bias and mean normalized gross error criteria. For the simulation utilizing the CMAQ-CB4 modeling system, 78% of sites in the modeling domain fell within the EPA-recommended ranges, but the model failed to capture the magnitude of the measured O_3 levels over the Southeast portion of the domain. Of the three modeling systems studied, CMAQ utilizing the RADM2 chemical mechanism had the most difficulty in predicting 8-hr daily maxima, with only 45% of the sites falling in the acceptance range over the modeling domain and only 10% of the Southeastern sites falling in the level of acceptance. Though the level of performance of CMAQ/RADM2 would not meet the criteria set for its use in an actual SIP attainment process, the modeling system still was included in the subsequent analysis of the study to investigate the robustness of the RRF approach to predict future design values. Such an analysis could be useful to investigate the impact, if any, of a model's base-case performance on the estimation of the future design values in attainment demonstrations using the RRF approach.

RESULTS AND DISCUSSION

Sensitivity of the RRF to Meteorology and Chemical Mechanisms

As stated, the first objective of this study is to investigate the sensitivity of the RRFs to differences in meteorological episodes or chemical mechanisms used. This work is an extension of a recently published study by Sistla et al.,[3] who compared the RRFs predicted by different combinations of two emission processors and two photochemical models. For the purpose of this study, the RRF resulting from the emission reductions for the 2010 Clear Skies Act control case was computed using outputs from the modeling simulations marked as "Analysis 1" in Table 1. The spatial distributions of the estimated RRFs based on the three modeling systems are displayed in Figure 1. Areas for which RRFs could not be computed because of the screening criteria set forth in the draft guidance document[1] are left unshaded in Figure 1. On a spatial average basis, O_3 reductions, defined as [100% × (1 − RRF)], were

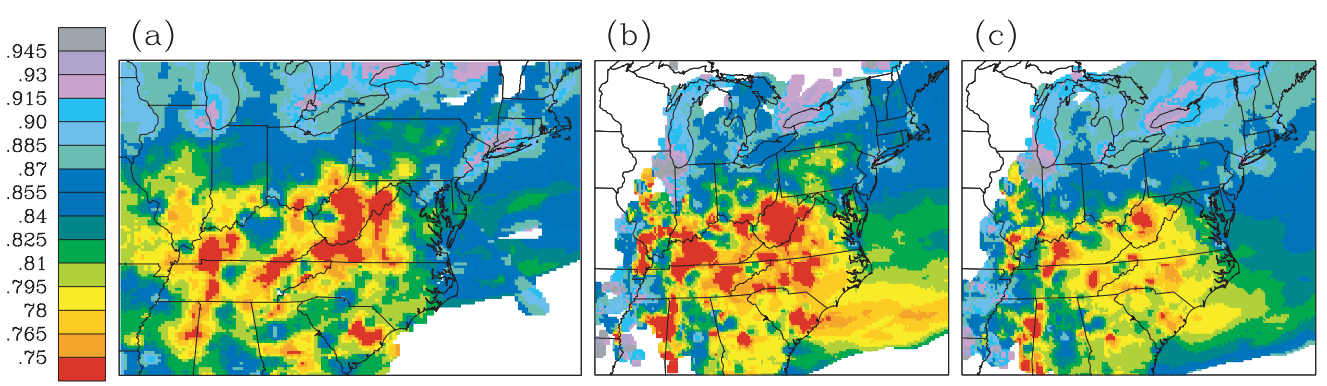

Figure 1. Maps of the RRFs simulated by three modeling systems as a result of the 2010 control case emissions relative to the 1996 base-case emissions as listed in Table 1. (a) RAMS3b/CAMx-CB4 using June/July 1995 meteorology; (b) MM5/CMAQ-CB4 using July 1999 meteorology; and (c) MM5/CMAQ-RADM2 using July 1999 meteorology.

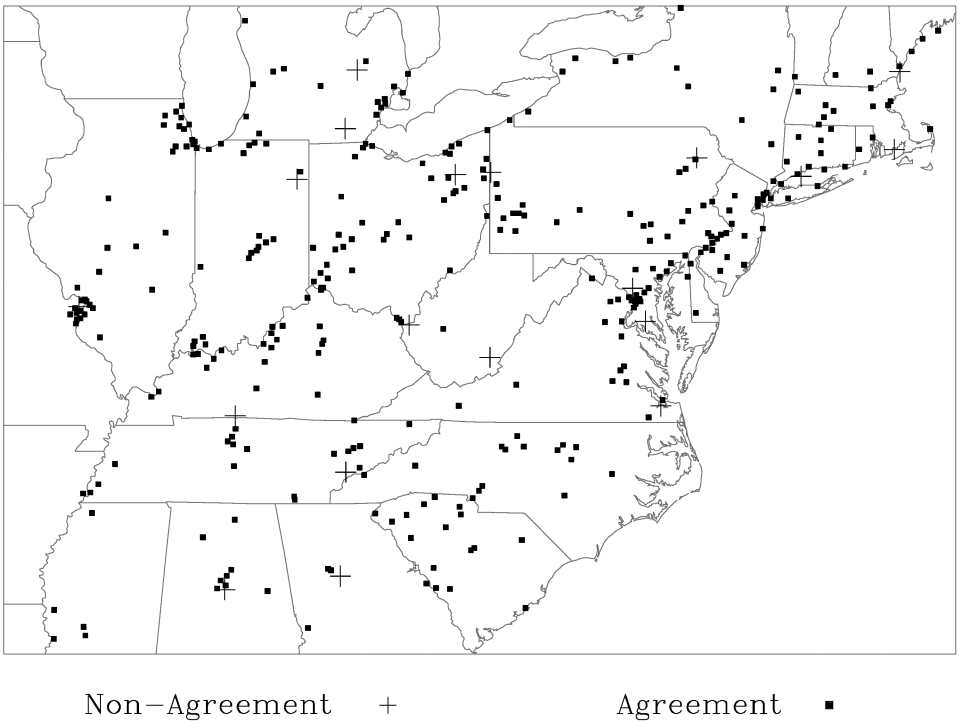

Figure 2. Location of the O_3 monitors that show model-to-model agreement or nonagreement as to whether the predicted future design value for 2010 is above or below the NAAQS.

found to be 14–16% over the entire domain depending on the modeling system, while the three modeling systems predicted average reductions of 11–13% over the Northeast and 16–18% over the Southeast. Although the general spatial patterns of the RRF agree between the modeling systems, the magnitude of predicted O_3 reductions are generally higher for CMAQ/CB4 than for CAMx/CB4. As a measure of uncertainty, the mean and SD of the RRF for each grid cell for the three modeling systems was calculated as discussed in Sistla et al.[3] The RRF standard deviation ranged from 0.015 to 0.035 over the modeling domain, which would translate to DVF uncertainties in the 2–4 ppb range for measured 8-hr design values occurring in the 75–100 ppb range. These results are similar to those reported in Sistla et al.,[3] who estimated the RRF uncertainty introduced by using different emission processors and photochemical models.

While model-to-model differences of the DVF derived from the RRF generally are smaller than model-to-model differences in predicted absolute base and control-case O_3 concentrations,[17] it is nevertheless possible that even small model-to-model RRF differences may lead to opposite answers in determining whether DVF is above or below the NAAQS at a given monitor. To illustrate this, a hypothetical attainment demonstration was performed according to the EPA draft modeling guidance[1] using the observed design values for the 1996 base-case and the model-predicted RRF values for all monitoring sites within the modeling domain. For each site, it was determined whether the DVF was above or below the 8-hr NAAQS for each of the modeling systems. Sites for which the three modeling systems are not in agreement if DVF is either above or below the NAAQS are marked with a + in Figure 2, while sites for which all modeling systems agree upon whether DVF is above or below the NAAQS are marked with a ■. Of the 358 sites in the modeling domain, all models agreed at 92.7% of these sites. However, in an actual SIP attainment demonstration, the pass/fail of the modeled attainment test for a nonattainment area comprised of Metropolitan Statistical Areas (MSAs) or Consolidated Metropolitan Statistical Areas (CMSAs) would be based on the DVF of an individual monitor that fails the attainment test, even if all other monitors in the area pass the test. Thus, the model-to-model differences in DVF even at a single monitor might have important implications as to whether a given control strategy is predicted to lead to future NAAQS compliance of the area.

Visual examination of Figure 2 shows that there is no spatial pattern in the models' agreement or disagreement in predicting future NAAQS compliance/noncompliance. Furthermore, the analysis was repeated for each pairwise combination of the modeling systems (CMAQ-CB4/CMAQ-RADM2, CMAQ-CB4/CAMx-CB4, CMAQ-RADM2/CAMx-CB4). This pairwise analysis revealed that no one modeling system's behavior was fundamentally different from the others in predicting DVF above or below the NAAQS

throughout the modeling domain. In this respect, it is particularly interesting to note that the pass/fail status of the modeled attainment test based on the CMAQ/RADM2 modeling system (which had a poor base case performance) is quite similar to that based on the other two modeling systems at most monitors. While this implies that a model's performance in predicting base-case concentrations may not have a pronounced effect on its prediction of the DVF under the RRF approach, it is critical that further detailed assessment of this issue is performed to provide confidence in this result and its implications for assessing model performance under the SIP process.

Comparison of Model-Predicted and Observed Design Values through Retrospective Analysis

To address the second objective of this study, a retrospective analysis was conducted to investigate the ability of the attainment demonstration methodology to predict changes in monitored DVCs for 8-hr O_3 from 1996 to 2001. For the purpose of this analysis, two RAMS/CAMx simulations with 1996 and 2001 emissions inventories that had been performed by EPA in support of the proposed Interstate Air Quality Rule were utilized.[14] These simulations are marked as "Analysis 2" in Table 1. As discussed in the EPA technical support document,[14] the 2001 emission inventory used in these simulations was based largely on projected 1996 emissions rather than the actual 2001 National Emission Inventory that had not yet been available for all source categories. In other words, this set of simulations provides a data set for assessing the uncertainties created by projecting future-year emissions similar to the process followed in developing a SIP.

Visual examination of a scatter plot (not shown) of both the observed and predicted (by multiplying the 1996 observed DVC with the model-derived RRF) design values for 2001 versus the observed 1996 design values indicates that in general the model overpredicted O_3 reductions for sites that had 1996 observed design values greater than 95 ppb and underpredicted O_3 reductions for sites that had 1996 observed design values less than 85 ppb. Comparison between 2001 observed and predicted (based on 1996 observations and RRF) design values over the modeling domain revealed a spatially averaged gross absolute error of ~5 ppb in the predicted design values. The spatially averaged difference between observed and predicted changes in design values was 1.3 ppb, with the model-estimated design values exhibiting an average decrease of 2.4 ppb and the observations revealing an average decrease of 1.1 ppb. Note that, if the change in design values were underpredicted by 4 ppb at one site and overpredicted by 4 ppb at another site, the average gross absolute error of the predicted RRF would be 4 ppb, while the average difference would be zero. In terms of sub-regional differences, the model was unable to capture the directionality of the design value change for the southern states; the model predicted an average decrease of ~2.6 ppb, while observations showed an average increase of 0.2 ppb from 1996 to 2001. The average model-estimated design values decreased by 2.3 and 2.1 ppb in the Northeast and the Midwest, respectively, while average measured design values decreased by 1.7 and 2.8 ppb, respectively.

Subsequently, it was determined whether the observed and predicted 2001 design values were above or below the 8-hr O_3 NAAQS of 84 ppb. Figure 3 displays sites labeled as "false pass" for which the model-predicted design values were at or below 84 ppb while the observed design value was greater than 84 ppb, and those labeled as "false fail" for which the model-predicted design values were above 84 ppb while the observed design value was at or below 84 ppb. It should be noted that sites for which the model correctly predicted whether the 2001 design value was above or below 84 ppb were not included in the figure. Of the 358 sites included in the modeling domain, 73% were correctly predicted as being either in or out of attainment by the model, while this percentage was only 66% for sites in the Southeast.

There are several possible contributors to the differences in observed and predicted design values. First, the 2001 emissions projected from the 1996 base-year inventory as described by EPA[14] may not reflect the actual emissions during the years 1999–2001, over which the observed 2001 design value was calculated. This problem is likely to be encountered in SIP applications as well when future-year emissions are projected over a time period of a decade or more. Second, although observed design values are derived from 3 years of observations, and although RRFs are fairly robust toward the choice of meteorological episodes as long as simulations are performed for a sufficient number of days, the approach of using the same meteorological conditions to simulate both the base-case and the control-case scenario also may contribute to the differences. The assumption of "static" meteorology actually might be of some concern in the SIP process because it is conceivable that changes in land use and regional climate that would alter meteorological conditions could occur over the same time horizon for which emission projections are made. Finally, it is entirely conceivable that the parameterizations and formulations in the photochemical modeling system are not well suited to predict the exact response of observed design values to changes in emissions. Consequently, further

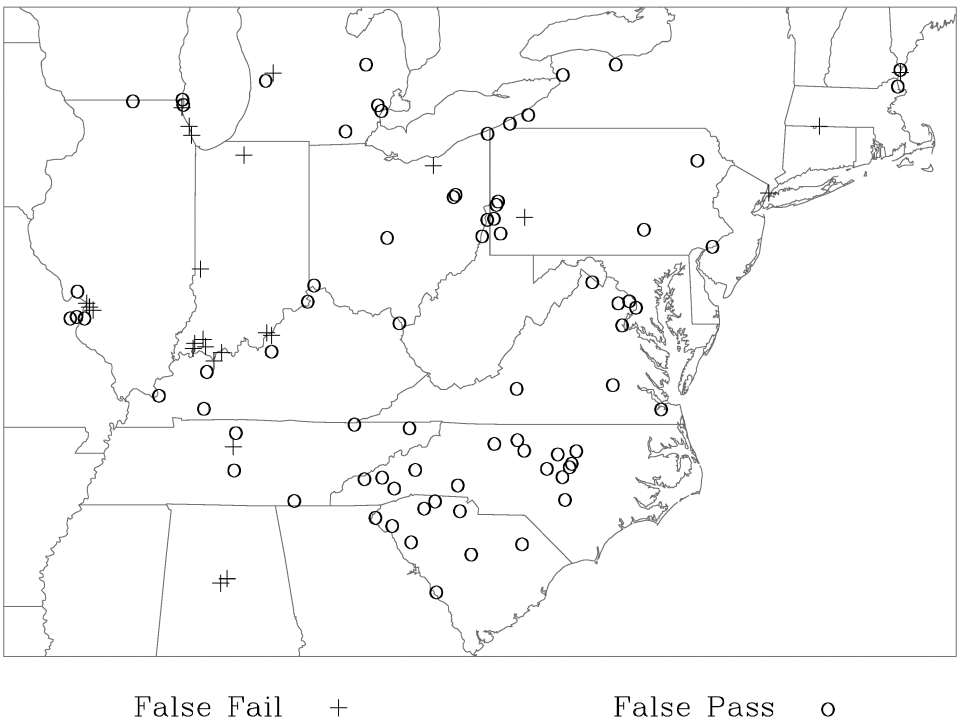

Figure 3. Comparison of the observed and predicted 2001 8-hr O_3 design values. The figure displays sites labeled as "false pass" for which the model-predicted design values were at or below 84 ppb while the observed design value was greater than 84 ppb, and those labeled as "false fail" for which the model-predicted design values were above 84 ppb while the observed design value was at or below 84 ppb. Sites for which the model correctly predicted whether the 2001 design value was above or below 84 ppb are not included in the figure.

retrospective-type analyses such as the one performed in this study should be performed to address the utility and validity of the current attainment demonstration approach when estimating design values over extended periods of time.

CONCLUSIONS

The first objective of the present study was to examine the response of three modeling systems based upon different photochemical models, meteorology, and chemical mechanisms to reductions in O_3 precursor emissions. While model-to-model differences in the RRF were generally small, it was found that these differences nevertheless could lead to different answers as to whether a predicted future-year design value is above or below the 8-hr O_3 NAAQS for a given monitor depending on the modeling system used. In general, the relatively small differences among the RRFs from different model applications is encouraging, and this analysis suggests use of a combination of model applications as an approach for determining uncertainty and determining the optimal set of control measures. It also was found that base-case model performance had little impact on the predicted RRF and, consequently, future-year design values. This result needs further confirmation.

In the second part of the study, a retrospective analysis was performed to compare model-predicted design values with monitored design values. This analysis was based on RAMS/CAMx simulations using both 1996 emissions and emissions projected to 2001 from the 1996 base case. The spatial average gross absolute error between predicted and observed 2001 design values was found to be ~5 ppb, while the spatially averaged difference between observed and predicted changes in design values was 1.3 ppb, with the model-estimated design values exhibiting an average decrease of 2.4 ppb and the observations revealing an average decrease of 1.1 ppb from 1996 to 2001. These differences caused an incorrect prediction as to whether a given site had a design value above or below the NAAQS at 27% of all sites. Potential contributors to the differences in predicted and observed design values are uncertainties in projecting emission inventories for the control year, the assumption that the effect of inter-annual meteorological variability on design values is eliminated by the current attainment demonstration procedure, or inherent limitations in the formulations of photochemical modeling systems. It is, therefore, important to perform retrospective-type analyses such as the one presented in this study to address the validity of the current attainment demonstration approach when predicting design values over time periods of a decade or more. Such analyses could provide avenues for improvement and added confidence in the use of the RRF approach for addressing attainment of the NAAQS.

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