Atmospheric Environment 44 (2010) 2116–2124

Contents lists available at ScienceDirect

Atmospheric Environment

journal homepage: www.elsevier.com/locate/atmosenv

Improving ozone modeling in complex terrain at a fine grid resolution – Part II: Influence of schemes in MM5 on daily maximum 8-h ozone concentrations and RRFs (Relative Reduction Factors) for SIPs in the non-attainment areas

Yunhee Kim, Joshua S. Fu*, Terry L. Miller

Department of Civil and Environmental Engineering, University of Tennessee, 223 Perkins Hall, Knoxville, TN 37996-2010, USA

ARTICLE INFO

Article history:
Received 27 April 2009
Received in revised form
11 February 2010
Accepted 26 February 2010

Keywords:
Model performance
CMAQ
Planetary boundary layer
SIPs
RRFs

ABSTRACT

Part II presents a comprehensive evaluation of CMAQ for August of 2002 on twenty-one sensitivity simulations (detailed in Part I) in MM5 to investigate the model performance for O_3 SIPs (State Implementation Plans) in the complex terrain. CMAQ performance was quite consistent with the results of MM5, meaning that accurate meteorological fields predicted in MM5 as an input resulted in good model performance of CMAQ. In this study, PBL scheme plays a more important role than its land surface models (LSMs) for the model performance of CMAQ. Our results have shown that the outputs of CMAQ on eighteen sensitivity simulations using two different nudging coefficients for winds (2.5 and 4.5 $\times$ 10^{-4} s^{-1}, respectively) tend to under predict daily maximum 8-h ozone concentrations at valley areas except the TKE PBL sensitivity simulations (ETA M-Y PBL scheme with Noah LSMs and 5-layer soil model and Gayno-Seaman PBL) using 6.0×10^{-4} s^{-1} with positive MB (Mean Bias). At mountain areas, none of the sensitivity simulations has presented over predictions for 8-h O_3, due to relatively poor meteorological model performance. When comparing 12-km and 4-km grid resolutions for the PX simulation in CMAQ statistics analysis, the CMAQ results at 12-km grid resolution consistently show under predictions of 8-h O_3 at both of valley and mountain areas and particularly, it shows relatively poor model performance with a 15.1% of NMB (Normalized Mean Bias). Based on our sensitivity simulations, the TKE PBL sensitivity simulations using a maximum value (6×10^{-4}) among other sensitivity simulations yielded better model performance of CMAQ at all areas in the complex terrain. As a result, the sensitivity of RRFs to the PBL scheme may be considerably significant with about 1–3 ppb in difference in determining whether the attainment test is passed or failed. Furthermore, we found that the result of CMAQ model performance depending on meteorological variations is affected on estimating RRFs for attainment demonstration, indicating that it is necessary to improve model performance. Overall, G_c (Gayo-Seaman PBL scheme) using the coefficient for winds, 6×10^{-4} s^{-1}, sensitivity simulation predicts daily maximum 8-h ozone concentration closer to observations during a typical summer period from May to September and provides generally low future design values (DVFs) at valley and mountain areas compared to other simulations.

1. Introduction

In April 2004, US EPA designated non-attainment areas for 8-h ozone NAAQS (National Ambient Air Quality Standard). The US EPA has set two NAAQS for O_3 from 1-h standard of 120 ppb to 8-h standard of 85 ppb. The 8-h ozone NAAQS was revised by US EPA in 1991 based on the 1-h NAAQS related to human health and welfare. The current 8-h NAAQS requires that the three-year average of the fourth highest daily maximum 8-h average ozone each year be less than or equal to 85 ppb at a given monitoring site. It is required more demanding than 1-h ozone NAAQS for protecting human health. The new NAAQS for 8-h O_3 was revised from 0.08 ppm to 0.075 ppm as of May 27 in 2008, expecting that this would result in more non-attainment areas in the United States.

Meteorological fields can influence the concentration of O_3 because it has direct impacts on air quality as an input to air quality models (Byun et al., 2007; Jimenez et al., 2005; Perez et al., 2006; Queen and Zhang, 2008; Zhang et al., 2006). Meteorological models such as MM5 (the Fifth Generation Pennsylvania State University, National Center for Atmospheric Research Mesoscale

---

* Corresponding author. Tel.: +1 865 974 2629.
E-mail address: jsfu@utk.edu (J.S. Fu).

1352-2310/$ – see front matter © 2010 Elsevier Ltd. All rights reserved.
doi:10.1016/j.atmosenv.2010.02.038

Model) have been broadly used to provide meteorological data into CMAQ or SMOKE (Sparse Matrix Operator Kernel Emissions) as inputs. Thus, the use of accuracy of the modeled meteorological fields can be important for demonstrating attainment for 8-h ozone NAAQS. Sistla et al. (2004) demonstrated that the choice of a photochemical grid modeling system could result in different conclusions on attainment. Arunachalam et al. (2006) indicated that the choice of grid resolution might bring in attainment or non-attainment and thus, also suggested that using RRFs (Relative Reduction Factors) and DVFs (Design Values for Future) resulted from 12-km grid resolution might be favorable for demonstrating future attainment. However, even though the DVFs from 12-km grid resolution meet the NAAQS for 8-h O_3, it may not provide valuable insights with local perspective associated with actual structure of atmospheric and control strategy for ozone.

Another issue is that most studies on model performance for MM5 or CMAQ were performed over a short time period, probably resulting in wrong decisions (Hogrefe et al., 2000). In particular, predicting RRFs for 8-h ozone in the non-attainment areas needs to simulate in sufficiently long time periods – at least during a typical summer season (May–September) – to calculate appropriately. In cases of Arunachalam et al. (2006) and Sistla et al. (2004), the simulation times for RRFs were only on 16 days and 14 days, respectively. One important criterion for calculating RRFs is to get a sufficient number of modeling days with daily maximum 8-h average modeled ozone more than 85 ppb at each monitoring site exceeding NAAQS in order to qualify the monitored attainment test. If the number of modeling days with 8-h ozone more than 70 ppb chosen is less than 5, then mean RRFs for the sites will get wrong (USEPA, 2007). According to US EPA guidance, a RRFs computed from a large number of days is more strong than an RRF from a small number of days. Therefore, in our studies, we simulated with a total of 120 days in order to compute appropriate RRFs for daily maximum 8-h ozone concentration.

We will present the results from CMAQ of each sensitivity simulation in Part II and discuss the influence of meteorological fields simulated with different physical options on air quality for 8-h O_3 SIPs on RRFs and DVFs in the complex terrain area of East Tennessee in determining whether the NAAQS is met or not. We will also discuss the contribution of MM5 on 12-km grid resolution and 4-km grid resolution for PX model in order to study the impacts of grid size resolutions on O_3 formation in the non-attainment area.

2. Description of the modeling systems

2.1. Description of the emission modeling

The SMOKE (Sparse Matrix Operator Kernel Emissions) modeling Version 2.1 was used to generate emissions for CMAQ required as inputs for the month of August. Twenty-one sensitivity simulations were selected in this study. For the base case, all source categories were included and are as follows: area, area-fire, fire, EGU (Electric Generating Unit), NEGU (Non-Electric Generating Unit), on-road, non-road and marine emissions. These emissions data were obtained from VISTAS 2002 Base G typical emissions (See http://www.vistas-sesarm.org/). It was necessary to generate biogenic emissions using BELD3 (Biogenic Emissions Landuse Database Version 3) data to the 4-km grid resolution. SMOKE was produced to use the Biogenic Emission Inventory System Version 3.09 to generate the biogenic components for each sensitivity simulation.

For on-road, point combined EGU, NEGU and fire emissions, and biogenic sources, the emissions should be rerun by SMOKE because these source emissions are changed by meteorology. That is, these three source categories require meteorological data as an input in SMOKE. For each sensitivity simulation, those three source categories were rerun by SMOKE and then combined by other source categories that had already been done for the base case. The SMOKE CB-IV speciation profiles were used for CMAQ species in this study.

2.2. Description of the CMAQ modeling

CMAQ Version 4.5 was used for the simulation in this study. The initial and boundary information of the 4-km grids was extracted from VISTAS's 12-km grid resolution and obtained from VISTAS (VISTAS, 2004). Basically, the VISTAS's 36- and 12-km grid resolutions were simulated on the PX scheme (see details in Part I). The Carbon Bond-IV gas-phase chemistry mechanism, specifically cb4_ae4_aq mechanism, was selected for the ozone simulation. For all grid resolutions, 19 layers were utilized for SMOKE and CMAQ and then, the first layer (extended from the surface up to about 36 m) was extracted for analysis of CMAQ. For the ozone SIPs modeling, the sizes of the array of nearby cells around each monitoring site for daily maximum 8-h ozone values for the 4-km and 12-km grid resolutions are a 7 × 7 array and a 3 × 3 array, respectively, followed by the guidance (USEPA, 2007).

2.3. Description of the observational sites

The nested 4 km domain contains a total of seven monitor sites representing four valley sites (Anderson, Mildred, Rutledge, and Jefferson) and three mountain sites (Look Rock, Cove Mt., and Clingman's Dome) observed in this study (see Part I for details) to examine the performance of CMAQ and attainment demonstration of this non-attainment area at a local scale.

3. Model performance of CMAQ

3.1. Influence daily maximum 8-h ozone concentrations from CMAQ on all seven sensitivity simulations using default coefficients for winds

The NME (Normalized Mean Error), NMB (Normalized Mean Bias), MB (Mean Bias), UPA (Unpaired Peak Accuracy), and skill score were adopted to analyze the evaluation of CMAQ model performance from all seven sensitivity simulations for the whole month of August in 2002 at the 4-km domain at overall, valley, and mountain sites. A variety of statistical measures have been used to evaluate the model performance of air quality (Hogrefe et al., 2004; Tong and Mauzerall, 2006). Our evaluation focuses on the impact of meteorological fields such as winds, temperature, and PBL height on CMAQ for daily maximum 8-h ozone concentration at the

Table 1
Definition of statistical measures used in this study.

Measures	Definition
Mean Bias (MB)	$\frac{1}{ND}\sum_{i=1}^{N}\sum_{i=1}^{D}(P_i - O_i)$
Normalized Mean Bias (NMB)	$(\sum_{i=1}^{N}\sum_{i=1}^{D}(P_i - O_i))/(\sum_{i=1}^{N}\sum_{i=1}^{D}O_i)$
Normalized Mean Error (NME)	$(\sum_{i=1}^{N}\sum_{i=1}^{D}\lvert(P_i - O_i)\rvert)/(\sum_{i=1}^{N}\sum_{i=1}^{D}O_i)$
Mean Normalized Bias (MNB)	$\frac{1}{N}\sum_{i=1}^{N}((P_i - O_i)/O_i)$
Mean Normalized Gross Error (MNGE)	$\frac{1}{N}\sum_{i=1}^{N}(\lvert P_i - O_i\rvert/O_i)$
Root Mean Square Error (RMSE)	$[(1/\mathrm{ND})\sum_{i=1}^{N}\sum_{i=1}^{D}(P_i - O_i)^2]^{1/2}$
Mean Absolute Gross Error (MAGE)	$(1/\mathrm{ND})\sum_{i=1}^{N}\sum_{i=1}^{D}\lvert P_i - O_i\rvert$
Unpaired Peak Accuracy (UPA)	$(P - O_{peak})/(O_{peak})$
Skill Score	$(1/2)[1 - \lvert\mathrm{MB}/\mathrm{MAGE}\rvert + (\mathrm{MAGE\ RMSE})]$

Where *N* is the number of measurement sites, *D* is the number days when ozone was predicted and observed, *P* and *O* are the predicted and observed daily maximum 8-h ozone concentrations at each site, MB is mean bias, MAGE is mean absolute gross error, and RMSE is root mean square error, respectively.

surface. Statistical measures listed in Table 1 have been commonly and widely used in recent regional air quality model evaluations. Additionally, Mao et al. (2006) introduced the skill score using the equation based on RMSE (Root Mean Square Error), ABGE (Absolute Bias Gross Error) and MB (Mean Bias). The best model performance corresponds to high skill score. This skill score is formed to further enhance the assessment on model performance analysis (Mao et al., 2006). We therefore adopted this skill score to assess the model performance analysis of air quality on various meteorological sensitivities.

Model performance was calculated by the above statistics for the whole domain, valley, and mountain sites. Table 2 shows the summary of August 2002 CMAQ model performance statistics for daily maximum 8-h ozone concentrations at the 4-km domain (overall), valley, and mountain sites. All seven sensitivity simulations (using default coefficients for winds) under predict daily maximum 8-h ozone concentrations at all areas. In particular, the difference between observed and predicted O_3 was much larger at mountain sites than valley sites, corresponding to the meteorological conditions at valley sites are smaller in biases of winds and temperature than those of mountain sites.

Air quality performance of the PX scheme (A) which has been used primarily in the Southeast US (VISTAS, 2004) showed poor statistical model performance with −12%, −8.3%, and −16.8% for NMB, with −8.9 ppb, −6.2 ppb, and −12.6 ppb for MB, with 0.58, 0.65, and 0.53 for skill score at the entire domain (overall), valley, and mountain sites, respectively at a 4-km grid resolution due to the poor meteorological performance. Furthermore, the CMAQ performance on PX scheme, showed quite high wind speeds with MB of 0.71 $m\ s^{-1}$ and relatively lowest MB of temperature at mountain sites presented the largest MB of −12.6 ppb, the lowest skill score of 0.53, and the exceeded NMB of −17% over the values of ±5 to 15% suggested by US EPA, indicating again that the PX scheme is not an appropriate choice in predicting daily maximum 8-h ozone concentration in the complex terrain having mountain and valley areas for SIPs modeling as previously mentioned in Part I. However, the NME ranges from 14.2% to 15.7% for the PX simulation at both grid resolutions with regard to relatively lower RMSE (root mean square error) varying from 13.2 ppb to 13.9 ppb at valley sites when compared to other sensitivity simulations. This seems to suggest that the PX scheme is a better choice in simulating in a valley area. Additionally, the CMAQ results from 12-km grid resolution (PX) and 4-km grid resolution for PX scheme (A) also do not show significantly in difference even though the outputs from CMAQ at 12-km grid resolution give slightly better in statistical model performance than 4-km grid resolution like the results from the meteorological performance for PX (See details in Part I).

Table 2
Summary of August 2002 CMAQ model performance statistics for daily maximum 8-h ozone concentrations with 7 different sensitivity simulations on 4-km and PX PBL Scheme on 12-km grid resolution.

Sensitivity	obs (ppb)	Mod (ppb)	MB (ppb)	NMB (%)	NME (%)	RMSE (ppb)	MAGE (ppb)	UPA (%)	Skill Score
A	74.4	65.5	−8.9	−12.0	18.0	16.0	13.4	−9.2	0.58
F	74.4	67.9	−6.6	−8.8	18.2	16.8	13.5	1.5	0.66
C	74.4	66.1	−8.3	−11.1	18.9	17.4	14.1	−9.3	0.61
E	74.4	64.8	−9.6	−13.0	20.0	18.5	14.9	−14.8	0.58
B	74.4	70.3	−4.2	−5.6	20.0	18.9	14.9	−0.1	0.75
D	74.4	69.7	−4.7	−6.3	19.5	18.6	14.5	0.4	0.73
G	74.4	70.0	−4.4	−6.0	18.0	17.2	13.4	−2.7	0.72
12-km	74.4	67.6	−6.8	−9.2	16.8	15.5	12.5	−1.3	0.63
Valley									
A	73.8	67.7	−6.2	−8.3	15.7	13.9	11.6	−11.6	0.65
F	73.8	69.7	−4.1	−5.6	16.3	14.7	12.0	1.5	0.74
C	73.8	68.1	−5.7	−7.8	17.5	16.1	12.9	−9.3	0.68
E	73.8	65.7	−8.1	−10.9	18.9	17.4	13.9	−14.8	0.61
B	73.8	73.2	−0.6	−0.8	20.2	18.9	14.9	−0.1	0.87
D	73.8	72.3	−1.5	−2.0	19.8	18.6	14.6	0.4	0.84
G	73.8	72.5	−1.3	−1.8	17.4	16.5	12.9	−2.7	0.84
12-km	73.8	70.4	−3.4	−4.6	14.2	13.2	10.5	−1.3	0.73
Mountain									
A	75.2	62.6	−12.6	−16.8	21.0	18.5	15.8	−6.3	0.53
F	75.2	65.4	−9.8	−13.0	20.7	19.2	15.6	−4.5	0.59
C	75.2	63.5	−11.7	−15.5	20.8	19.1	15.7	−18.8	0.54
E	75.2	63.5	−11.7	−15.6	21.6	19.9	16.3	−14.1	0.55
B	75.2	66.3	−8.9	−11.8	19.8	18.9	14.9	−11.7	0.59
D	75.2	66.2	−9.0	−12.0	19.1	18.7	14.4	−12.0	0.57
G	75.2	66.7	−8.6	−11.4	18.8	18.1	14.1	−9.0	0.59
12-km	75.2	63.9	−11.3	−15.1	20.2	18.2	15.2	1.4	0.54

CMAQ performance was quite consistent with the results of MM5. This means that accurate meteorological fields predicted in MM5 as an input resulted in good model performance of CMAQ. Overall, sensitivity B (ETA M-Y with Noah LSMs) had the best skill scores at overall, valley, and mountain sites and sensitivity G (G-S PBL) presented the good model performance of CMAQ with the lowest MB (Mean Bias), NME (Normalized Mean Error), and MAGE (Mean Absolute Gross Error) at mountain areas while sensitivity E (MRF with 5-soil layers) generally showed the worst statistics in our study area.

Sensitivity simulation B (ETA M-Y with Noah LSMs) and D (ETA M-Y with 5-soil layers) presented similar CMAQ performance statistics for daily maximum 8-h ozone concentration. The CMAQ model performance statistics of sensitivity simulation B and D, sensitivity simulation D and E, and sensitivity simulation A (PX) and F (Blackadar) achieved similar results. We can notice here that the difference between sensitivity simulation B and D, sensitivity simulation C and E, and sensitivity simulation A and F was simulated by only different land surface model (LSM) in MM5, indicating PBL schemes are more dominant than LSM at predicting daily maximum 8-h ozone concentration due to the meteorological input variables. As a result, we found in our study that the Noah land surface model showed the slightly better model performance of CMAQ than 5-layer soil model when compared with the same PBL scheme on different LSM while PX LSM showed the relatively poor model performance of CMAQ when compared to Blackadar PBL scheme on 5-layer soil model. It also consistently shows the same results as Han et al. (2008) demonstrating that the PX and Noah LSMs provide more realistic moisture process in soil moisture. Furthermore, the TKE (sensitivity simulation B, D, and G) schemes also presented better CMAQ model performance than that of non-local PBL schemes (sensitivity A, C, E, and F) as mentioned in meteorological statistics model performance. Therefore, it is noteworthy that the TKE schemes are better options to predict ozone concentrations in the complex terrain.

The difference in CMAQ statistical analysis for daily maximum 8-h ozone at the whole domain, valley, and mountain sites, respectively was 5.5 ppb, 7.5 ppb, and 4.1 ppb for MB, −7.4%, −10.1%, and −5.4% for NMB, 2.0%, 4.5%, and 2.8% for NME, 2.9 ppb, 5.0 ppb, and 1.8 ppb for RMSE, 1.5 ppb, 3.3 ppb, and 2.1 ppb for MAGE, −14.7%, −14.7%, and −14.3% for UPA, 0.2, 0.2, and 0.1 for skill score. These differences were bigger at valley than mountain areas. This suggests that the MM5 PBL schemes had significant impacts on the performance of CMAQ at valley areas while it had little effect at mountain areas. Based on the results, it is found that the MM5 PBL schemes had significant influences on CMAQ model performance, eventually resulting in determining attainment status for ozone SIPs. This yields totally opposite results from Mao et al. (2006) showing that no significant CMAQ sensitivity to any PBL schemes was observed. The results presented above indicated that the sensitivity B, D, and G were identified for favorite PBL schemes in complex terrain having valley and mountain areas at a finer grid resolution.

3.2. Influence daily maximum 8-h ozone concentrations on seven sensitivity simulations using three different nudging coefficients for winds

FDDA analysis nudging was used for both the surface and the 3D fields in all of the MM5 simulations. Three different nudging coefficients of 2.5, 4.5 and 6.0 × 10^{-4} s^{-1} (in FDDA analysis nudging with winds) were applied for all seven sensitivity simulations. Figs. 1–4 show NMB, NME, UPA, and skill score from 2002 August CMAQ sensitivity statistics performance with three different nudging coefficients for winds (a, b, and c, respectively) in daily maximum 8-h ozone concentrations. Table 3 also presents the summary of performance statistics derived from the 21 CMAQ simulations with three different nudging coefficients for winds (2.5, 4.5. 6.0 × 10^{-4} s^{-1}) at overall, valley, and mountain sites in August 2002.

The MB and the NMB are only positive for B_c (ETA M-Y PBL on Noah LSM with 6.0 × 10^{-4} s^{-1}), D_b (MRF PBL on 5-layer soil model with 4.5 × 10^{-4} s^{-1}), D_c (MRF PBL on 5-layer soil model with 6.0 × 10^{-4} s^{-1}), and G_c (Gayno-Seaman PBL on 5-layer soil model with 6.0 × 10^{-4} s^{-1}) at valley sites. It indicates that CMAQ generally underestimates surface daily maximum 8-h O_3. And this also indicates that CMAQ model performance shows better at valley sites than mountain sites showing underestimates with a larger bias.

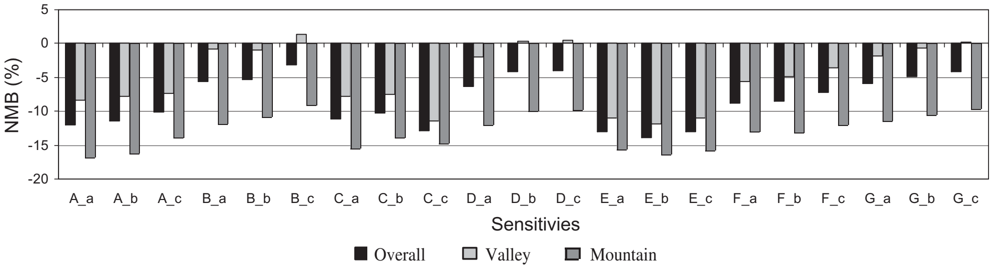

Fig. 1. NMB (Normalized Mean Bias) of daily Maximum 8-h Ozone Concentration in August 2002 at overall, valley, and mountain areas.

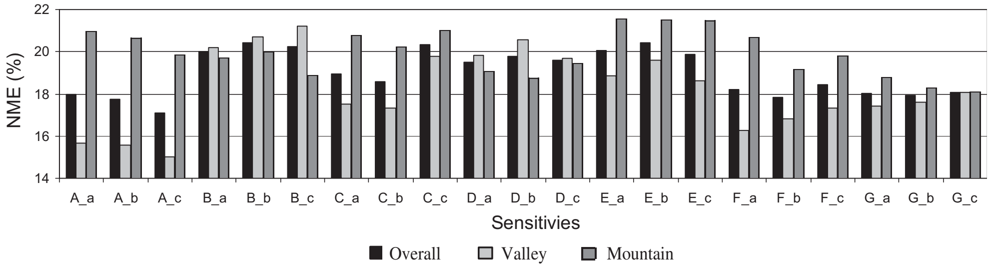

Fig. 2. NME (Normalized Mean Error) of daily Maximum 8-h Ozone Concentration in August 2002 at overall, valley, and mountain areas.

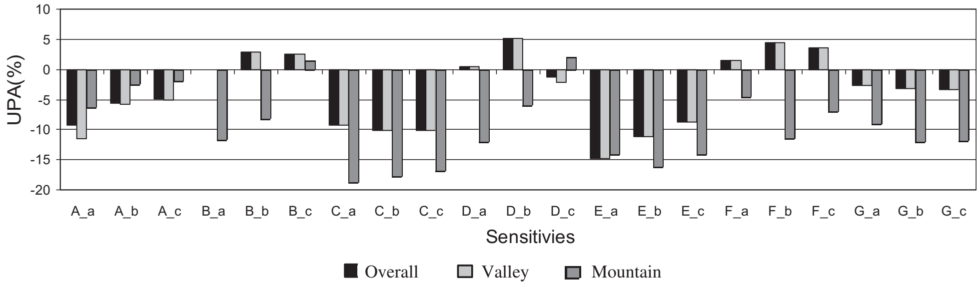

Fig. 3. UPA (Unpaired Peak Accuracy) of daily Maximum 8-h Ozone Concentration in August 2002 at overall, valley, and mountain areas.

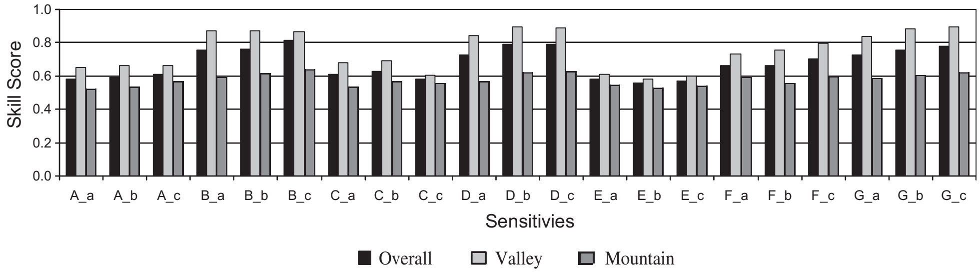

Fig. 4. Skill Score of daily Maximum 8-h Ozone Concentration in August 2002 at overall, valley, and mountain areas.

Table 3
Summary of performance statistics derived from the CMAQ simulations with three different nudging coefficients (a (2.5), b (4.5), and c (6.0×10^{-4} s^{-1})) at the whole domain (overall), valley, and mountain areas in August 2002.

Sensitivity	obs (ppb)	Mod (ppb)	MB (ppb)	NMB (%) (±5 to 15)	NME (%) (30–35)	RMSE (ppb)	MAGE (ppb)	UPA (%) (±15 to 20)	Skill Score
Overall									
A_a	74.4	65.5	−8.9	−12.0	18.0	16.0	13.4	−9.2	0.58
A_b	74.4	65.9	−8.5	−11.4	17.8	15.9	13.2	−5.6	0.59
A_c	74.4	66.9	−7.6	−10.2	17.1	15.6	12.7	−4.9	0.61
B_a	74.4	70.3	−4.2	−5.6	20.0	18.9	14.9	−0.1	0.75
B_b	74.4	70.5	−3.9	−5.3	20.4	19.3	15.2	2.9	0.76
B_c	74.4	72.1	−2.4	−3.2	20.2	19.2	15.0	2.5	0.81
C_a	74.4	66.1	−8.3	−11.1	18.9	17.4	14.1	−9.3	0.61
C_b	74.4	66.8	−7.6	−10.3	18.6	17.0	13.8	−10.1	0.63
C_c	74.4	64.9	−9.5	−12.8	20.3	19.0	15.1	−10.2	0.58
D_a	74.4	69.7	−4.7	−6.3	19.5	18.6	14.5	0.4	0.73
D_b	74.4	71.4	−3.1	−4.1	19.8	18.7	14.7	5.1	0.79
D_c	74.4	71.4	−3.0	−4.0	19.6	18.5	14.6	−1.2	0.79
E_a	74.4	64.8	−9.6	−13.0	20.0	18.5	14.9	−14.8	0.58
E_b	74.4	64.1	−10.3	−13.9	20.4	19.1	15.2	−11.2	0.56
E_c	74.4	64.7	−9.7	−13.1	19.9	18.5	14.8	−8.7	0.57
F_a	74.4	67.9	−6.6	−8.8	18.2	16.8	13.5	1.5	0.66
F_b	74.4	68.1	−6.3	−8.4	17.9	16.7	13.3	4.5	0.66
F_c	74.4	69.0	−5.4	−7.3	18.4	17.2	13.7	3.5	0.70
G_a	74.4	70.0	−4.4	−6.0	18.0	17.2	13.4	−2.7	0.72
G_b	74.4	70.8	−3.6	−4.9	17.9	16.9	13.3	−3.1	0.76
G_c	74.4	71.4	−3.1	−4.1	18.1	17.1	13.5	−3.4	0.78
Valley									
A_a	73.8	67.7	−6.2	−8.3	15.7	13.9	11.6	−11.6	0.65
A_b	73.8	68.1	−5.8	−7.8	15.6	13.9	11.5	−5.8	0.66
A_c	73.8	68.4	−5.4	−7.3	15.0	13.6	11.1	−5.1	0.66
B_a	73.8	73.2	−0.6	−0.8	20.2	18.9	14.9	−0.1	0.87
B_b	73.8	73.1	−0.8	−1.0	20.7	19.1	15.3	2.9	0.87
B_c	73.8	74.8	1.0	1.4	21.2	19.6	15.7	2.5	0.87
C_a	73.8	68.1	−5.7	−7.8	17.5	16.1	12.9	−9.3	0.68
C_b	73.8	68.3	−5.6	−7.5	17.3	15.7	12.8	−10.1	0.69
C_c	73.8	65.4	−8.4	−11.4	19.8	18.8	14.6	−10.2	0.60
D_a	73.8	72.3	−1.5	−2.0	19.8	18.6	14.6	0.4	0.84
D_b	73.8	74.0	0.2	0.3	20.6	18.8	15.2	5.1	0.90
D_c	73.8	74.2	0.3	0.5	19.7	18.2	14.5	−2.2	0.89
E_a	73.8	65.7	−8.1	−10.9	18.9	17.4	13.9	−14.8	0.61
E_b	73.8	65.0	−8.8	−11.9	19.6	18.6	14.5	−11.2	0.58
E_c	73.8	65.7	−8.1	−11.0	18.6	17.5	13.7	−8.7	0.60
F_a	73.8	69.7	−4.1	−5.6	16.3	14.7	12.0	1.5	0.74
F_b	73.8	70.2	−3.6	−4.8	16.8	15.7	12.4	4.5	0.75
F_c	73.8	71.1	−2.7	−3.6	17.3	16.0	12.8	3.5	0.80
G_a	73.8	72.5	−1.3	−1.8	17.4	16.5	12.9	−2.7	0.84
G_b	73.8	73.4	−0.4	−0.6	17.6	16.3	13.0	−3.1	0.88
G_c	73.8	73.9	0.1	0.2	18.1	16.7	13.3	−3.4	0.90
Mountain									
A_a	75.2	62.6	−12.6	−16.8	21.0	18.5	15.8	−6.3	0.53
A_b	75.2	63.1	−12.2	−16.2	20.7	18.3	15.5	−2.6	0.53
A_c	75.2	64.8	−10.4	−13.9	19.9	17.9	14.9	−1.9	0.57
B_a	75.2	66.3	−8.9	−11.8	19.8	18.9	14.9	−11.7	0.59
B_b	75.2	67.1	−8.1	−10.8	20.0	19.6	15.0	−8.2	0.61
B_c	75.2	68.4	−6.8	−9.1	18.9	18.7	14.2	1.5	0.64
C_a	75.2	63.5	−11.7	−15.5	20.8	19.1	15.7	−18.8	0.54
C_b	75.2	64.8	−10.4	−13.8	20.2	18.6	15.2	−17.7	0.57
C_c	75.2	64.1	−11.1	−14.7	21.0	19.3	15.8	−16.9	0.56
D_a	75.2	66.2	−9.0	−12.0	19.1	18.7	14.4	−12.0	0.57
D_b	75.2	67.8	−7.5	−9.9	18.8	18.4	14.1	−5.9	0.62
D_c	75.2	67.8	−7.4	−9.9	19.4	19.0	14.6	2.0	0.63
E_a	75.2	63.5	−11.7	−15.6	21.6	19.9	16.3	−14.1	0.55
E_b	75.2	62.9	−12.3	−16.4	21.5	19.8	16.2	−16.1	0.53
E_c	75.2	63.4	−11.9	−15.8	21.5	19.9	16.2	−14.1	0.54
F_a	75.2	65.4	−9.8	−13.0	20.7	19.2	15.6	−4.5	0.59
F_b	75.2	65.3	−9.9	−13.2	19.2	18.0	14.4	−11.4	0.56
F_c	75.2	66.2	−9.0	−12.0	19.8	18.6	14.9	−7.0	0.60
G_a	75.2	66.7	−8.6	−11.4	18.8	18.1	14.1	−9.0	0.59
G_b	75.2	67.3	−7.9	−10.5	18.3	17.7	13.8	−11.9	0.60
G_c	75.2	67.9	−7.3	−9.7	18.1	17.6	13.6	−11.9	0.62

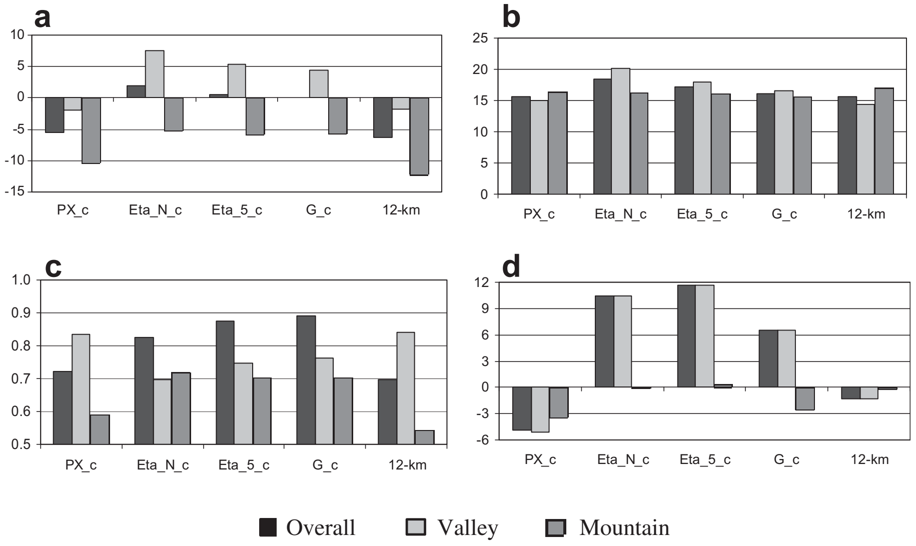

Fig. 5. NMB (a), NME (b), skill score (c), and UPA (d) of daily maximum 8-h ozone concentration at overall, valley, and mountain areas.

The results presented above suggest that using the FDDA nudging analysis for winds with the strongest value (6.0×10^{-4} s^{-1}) generally affected CMAQ performance significantly and improved statistics model performance.

US EPA has recommended that criteria for regulatory modeling are ±5 to 15% for NMB, 30–35% for NME, ±15 to ±20% for UPA (Russell and Dennis, 2000). The criteria are met at overall and valley sites except mountain sites. At mountain areas, PX PBL scheme with 2.5 and 4.5×10^{-4} s^{-1} (nudging coefficients for winds), MRF PBL scheme with 2.5×10^{-4} on Noah LSM and MRF PBL scheme with 2.5, 4.5, and 6.0×10^{-4} on 5-layer soil model are not met by the criteria for NMB indicating the larger differences between observed and predicted mean biases. Furthermore, All PBL schemes with increased nudging coefficients except MRF PBL scheme showed better model performance in CMAQ statistical analysis at the whole domain, valley and mountain areas. Our results demonstrate that Noah ETA M-Y PBL with 6.0×10^{-4} (B_c), 5-layer ETA PBL with 6.0×10^{-4} (D_c), and Gayno-Seaman with 6.0×10^{-4} (G_c) yielded the best CMAQ model performance for daily maximum 8-h O_3 at overall, valley, and mountain sites. It means that applying nudging analysis using a strong coefficient value (6.0×10^{-4}) for winds is helpful to improve CMAQ model performance at any site and also shows again that these PBL schemes are favorable options in the complex terrain at a finer grid resolution and identified.

The PX, Blackadar (BK), and Gayno-Seaman (G-S) PBL schemes with increasing nudging coefficients for winds were affected greatly on CMAQ model performance while the ETA M-Y (ETA) and MRF PBL schemes had little impact on CMAQ simulations at overall, valley, and mountain sites. MRF PBL (sensitivities C and E) schemes presented the lowest skill score, highest UPA values, larger MB, and NMB consistently at all sites while ETA M-Y (sensitivity B and D) and G-S (sensitivity G) were consistent with observed data in magnitude as well as high skill score, smaller NMB, and UPA values at all sites. Since the TKE (sensitivity simulation B, D, and G) and non-local schemes (A, C, E, and F) had displayed similar patterns and results with MB, NMB, and skill score each other as shown in Table 2, these two schemes with increasing nudging coefficients for winds also presented slightly more improved results for statistical analysis of CMAQ than using with default (2.5×10^{-4} s^{-1}) nudging coefficients for winds. Hence, one can find an interesting fact indicating that the non-local scheme and TKE scheme have shown different results for statistical analysis due to the different methods in the diagnosis to predict the PBL height. From our results, the TKE schemes (ETA M-Y and G-S PBL schemes) with strong nudging coefficients (6×10^{-4} sec^{-1}) for winds predicting vertical TKE (Turbulent Kinetic Energy) show better model performance with good agreement at all areas than that of non-local schemes (PX and MRF PBL schemes) with increasing nudging coefficients for winds.

4. Attainment demonstration

4.1. Model performance evaluation from CMAQ

In the modeling conducted to estimate more appropriate DVF (Design Value for the Future year) and RRFs (Relative Reduction Factors) in the O_3 non-attainment areas in East Tennessee, we performed 120 days during typical summer seasons (May to September) of 2002 and 2008 as a base-case year and a future-year, respectively, using MM5 from three sensitivity simulations (ETA PBL schemes associated with Noah LSMs and 5-layer soil model and

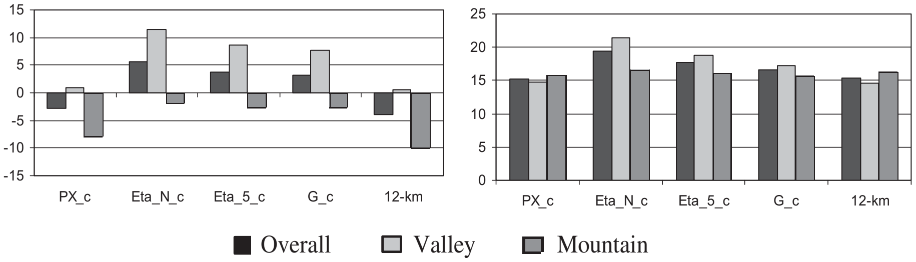

Fig. 6. Mean normalized bias (MNB (%)) (left) and mean normalized gross error (MNGE (%)) (right) for 8-h O_3 at overall, valley, and mountain areas.

Gayno-Seaman PBL scheme) with a strong value of nudging coefficient for winds (already evaluated in Part I), SMOKE, and CMAQ modeling system.

As a result of our extended CMAQ model performance, Fig. 5 shows the normalized mean bias (NMB), the normalized mean error (NME), the skill score, and unpaired peak accuracy (UPA) for 8-h O_3 computed on PX_c (PX with $6 \times 10^{-4}\ s^{-1}$) which is the base case, ETA_N_c (ETA PBL on Noah LSM with $6 \times 10^{-4}\ s^{-1}$), ETA-5_c (ETA PBL on 5-layer soil model with $6 \times 10^{-4}\ s^{-1}$), G_c (Gayno-Seaman PBL with $6 \times 10^{-4}\ s^{-1}$), and 12-km grid resolution (PX) at overall, valley, and mountain sites in East Tennessee. The daily maximum 8-h O_3 mean biases on the TKE schemes (ETA M-Y on Noah, 5-layer soil, and Gayno-Seaman PBL schemes) achieved for 120 days are positive at all sites except mountain areas while the PX at both of 12-km and 4-km grid resolutions shows negative values with a larger MB ranging from −1.3 ppb to −8.8 ppb at all areas. This overall negative mean bias on the PX simulation may suggest that the O_3 formation in the complex topography (particularly at mountain areas) is not sufficiently efficient.

As shown in Fig. 6, all four sensitivity simulations (PX_c, ETA_N_c, ETA_5_c, and G-c) at 4-km grid resolution and the PX at 12-km grid resolution are well within the statistical measures of MNB (±5 to 15%) and MNGE (30–35%) as a suite of metrics for evaluating model performance. However, the TKE simulations at 4-km grid resolution generally show over predictions with the positive bias at overall and valley sites (except mountain areas) while the PX model at 12-km and 4-km grid resolution presents under predictions with negative bias at all areas (except valley areas). The statistical model performance from the PX at both of 12- and 4-km grid resolutions in the extended period (4-month period) at the valley also shows consistently lower MNB and MNGE than those of the TKE sensitivity simulations at 4-km grid resolution whereas it produces higher MNB and MNGE at mountain areas as mentioned in Section 3.1. In addition, we also compared the observed 8-h ozone concentrations using 60 ppb cutoff to 8-h modeled ozone concentrations with 60 ppb cutoff, giving more precise evaluation of the model's capability due to the closer predictions to the 8-h NAAQS and decreasing model errors at low observations (USEPA, 1991). The MNB and MNGE using 60 ppb cutoff for 8-h ozone computed from the TKE sensitivity simulations at 4-km grid resolution as well as the PX at 4-and 12-km grid simulation as shown in Fig. 7 yielded relatively smaller bias and errors than the PX at both of grid resolutions, illustrating that the models simulated at 4-km grid resolution tend to produce much higher ozone formations at valley and mountain sites and generally show better model performance in comparison with higher observations than the PX sensitivity simulation. With the purpose of attainment demonstration, this result seems to be more helpful to evaluate the capability of the model and reduce model errors by predicting concentrations closer to the NAAQS.

Overall, the sensitivity simulation G_c (Gayno-Seaman PBL scheme with $6 \times 10^{-4}\ s^{-1}$) presents significantly small bias and errors among them for a 4-month period at all areas in the East Tennessee.

Table 4
Summary of results of the TKE sensitivity simulations at 4-km grid resolution and PX at 12- and 4-km grid resolution for DVCs, RRF, and DVFs at overall, valley, and mountain areas.

Sensitivity	DVCs	RRFs	2008DVFs
Overall			
PX_c	90.9	0.86	78.6
Eta_N_c	90.9	0.87	78.7
Eta_5_c	90.9	0.87	78.7
G_c	90.9	0.85	77.3
12-km	90.9	0.85	77.1
Valley			
PX_c	89.8	0.87	78.1
Eta_N_c	89.8	0.89	79.9
Eta_5_c	89.8	0.89	79.8
G_c	89.8	0.86	77.4
12-km	89.8	0.85	76.0
Mountain			
PX_c	92.4	0.86	79.4
Eta_N_c	92.4	0.83	77.1
Eta_5_c	92.4	0.84	77.3
G_c	92.4	0.83	77.1
12-km	92.4	0.85	78.5

4.2. *Modeling system for DVF (Design Values for Future year) and RRFs (Relative Reduction Factors)*

The DVCs (Current Design Values) were calculated based on the average annual, fourth highest, daily maximum 8-h ozone concentration, measured from each monitoring site over a three consecutive year period from 2000 to 2005. The US EPA guidance outlines a procedure to derive RRFs (Relative Reduction Factors) that are computed by calculating the ratio between base-case daily maximum 8-h ozone concentrations and future-year modeled concentrations at each given monitor. The future-year design values (DVFs) are then calculated by multiplying the RRFs and the DVCs. Finally, the modeled attainment test is passed if the DVFs are less than and equal to 84 ppb (NAAQS for 8-h O_3) at a given monitor. We performed future-year (DVFs) simulations for 2008 emissions that were obtained from VISTAS (the Visibility Improvement State and Tribal Association of the Southeast).

To facilitate comparisons, Table 4 summarizes the results of the TKE sensitivity simulations (ETA_N_c, ETA_5_c, and G_c) at 4-km grid resolutions and the PX simulation at 12- and 4-km grid resolutions for RRFs and 2008 DVFs, and the corresponding DVCs at overall, valley, and mountain sites. The difference of RRFs between 12-km and 4-km grid size for the PX sensitivity simulation is shown as 1.7% at overall, 2.3% at valley, and 1.0% at mountain sites. These differences in RRFs correspond to DVFs differences on average 0.9–2.1 ppb

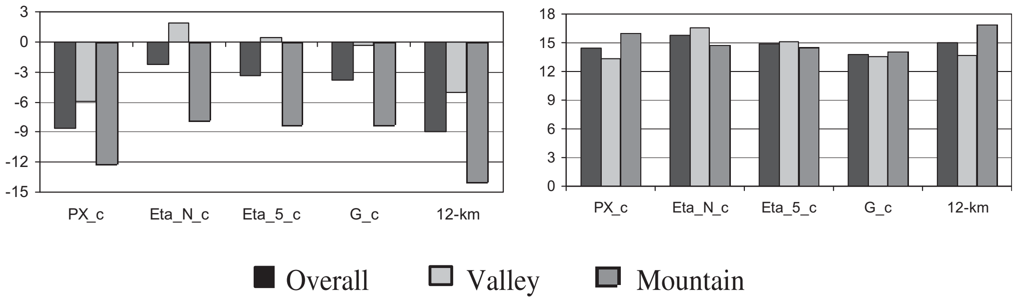

Fig. 7. Mean normalized bias (MNB (%)) (left) and mean normalized gross error (MNGE (%)) (right) using 60 ppb cutoffs for 8-h O_3 at overall, valley, and mountain areas.

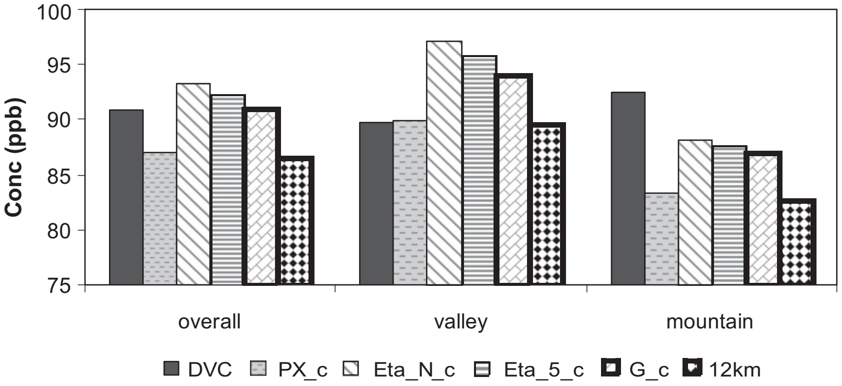

Fig. 8. Comparison of DVCs with base-case modeled O_3 for the TKE sensitivity simulations at 4-km and PX at 12- and 4-km grid resolutions at overall, valley, and mountain areas.

between 12- and 4-km grid resolutions for the PX simulation at valley and mountain sites. These results are quite similar to the findings by Arunachalam et al. (2006), Jones et al. (2005) that presented the DVFs in differences estimating the RRFs uncertainties about 1–3 ppb in modeling options. It is noteworthy that the difference of the DVFs computed from the RRFs at mountain areas is generally smaller than at valley sites when comparing 12–4-km outputs for the PX simulation due to the relatively poorer meteorological model performance of the PX sensitivity at mountain than valley sites, which indicates the sensitivity of the DVFs computed from RRFs to the meteorological conditions modeled. Even when comparing among these TKE sensitivity simulations (ETA_N_c, ETA_5_c, and G_c) at a 4-km grid resolution, the differences of DVFs based on RRFs are obvious. This seems to indicate again that estimating the RRFs and then DVFs at a given monitor site is dependent upon the meteorological model performance at a given grid resolution. Since the G_c (Gayno-Seaman with 6×10^{-4} s^{-1} for winds) sensitivity simulation produced quite good model performance in meteorological and CMAQ statistical analysis than other sensitivity simulations, the RRFs and DVFs from G_c simulation also were computed with a consistent average value of 77.3 ppb.

Fig. 8 shows the comparison of current design values (DVCs) with modeled base-case predictions for 8-h O_3 at each area at the TKE sensitivity simulations at 4-km and the PX at 12- and 4-km grid resolutions. Daily maximum 8-h ozone predictions modeled from the TKE sensitivity simulations of 4-km grid resolution at valley (except PX simulation at 12- and 4-km grid resolutions) tend to over predict whereas all sensitivity simulations including 12-km grid resolution always have tendencies to under predict at mountain. Specifically, the PX sensitivity simulation shows more under prediction with larger differences at mountain and the ETA_N_c and ETA_5_c simulations present over predictions at valley, resulting in higher DVFs and RRFs. Hence, it is believed that computing RRFs and then DVFs are dependent upon how well the modeling predicts at a given monitoring site.

As reported in Jones et al. (2005), RRFs differences may give opposite answers to determine if DVFs is met 8-h NAAQS or not. Based on our results, the 2008 DVFs at all areas for all sensitivity simulations (including 12-km grid resolution) all met the 8-h NAAQS. We also found that the result of model performance is affected by estimating RRFs for attainment demonstration, indicating that it is necessary to improve model performance. As a result, G_c (Gayo-Seaman PBL scheme) sensitivity simulation predicts daily maximum 8-h ozone concentration closer to observations at all areas during typical summer period and provides consistently low DVFs at valley and mountain areas than other simulations.

5. Conclusions

Our results show that all seven sensitivity simulations underestimated observed daily maximum 8-h ozone concentrations at valley sites with MB ranging from −8.1 ppb to −0.6 ppb, NMB ranging from −11% to −1%, NME ranging from 16% to 20%, UPA ranging from −14.8% to 1.5%, and skill score ranging from 0.61 to 0.87 and also under predicted it at mountain areas with MB ranging from −12.6 ppb to −8.6 ppb, NMB ranging from −17% to −11%, NME ranging from 19% to 22% UPA ranging from −18.8% to −4.5%, and skill score ranging from 0.53 to 0.59. The CMAQ statistical performance across seven sensitivity simulations is quite consistent with the results of MM5 performance, indicating that accurate meteorological fields predicted in MM5 as an input resulted in good model performance of CMAQ. As previously mentioned in the meteorological analysis, sensitivity B (ETA PBL with Noah LSMs), D (ETA PBL with 5-layer soil), and G (G-S PBL with 5-layer soil) from the results of CMAQ showed better model performance than other sensitivity simulations. This supports the idea that the meteorological fields such as wind speed, temperature, and PBL heights as inputs have critical impacts on air quality modeling. In this study, PBL scheme plays a more important role than its land surface models (LSMs) for the model performance of CMAQ.

Assessment of CMAQ results with nudging analysis showed that the sensitivity simulations that used the strongest nudging coefficient value (6.0×10^{-4}) showed slightly better model performance than those of lower values, indicating that it is helpful to improve CMAQ model performance at any area and also shows that using the highest value of nudging coefficient for winds might be a good choice in the complex terrain at a finer grid resolution. For regulatory modeling, the criteria suggested by US EPA are met except sensitivity A (PX), C (MRF PBL with Noah LSMs), and E (MRF PBL with 5-soil layer model) used nudging coefficient of 2.5 and 4.5×10^{-4} at mountain sites. However, among of these sensitivity simulations used with nudging coefficients of 6.0×10^{-4} are met by the criteria for NMB, which is within ±5 to 15% except E (MRF PBL scheme).

The impacts of various PBL schemes associated with three different LSMs (Land Surface Models) and FDDA nudging analysis for winds in MM5 as inputs for the complex terrain at a 4-km grid resolution have been investigated for daily maximum 8-h ozone. As a result, we found that the ETA M-Y PBL scheme associated with Noah LSMs and G-S (Gayno-Seaman) PBL schemes were identified as favorite PBL schemes as well as 6.0×10^{-4} of the nudging coefficient for winds was the best option to improve wind fields in MM5. Because these ETA M-Y and G-S PBL schemes tend to predict higher temperature, lower mixing height, and lower wind speeds in the area of study, they promote O_3 formation and improve the statistical results at all locations.

The MNB and MNGE using 60 ppb cutoff for 8-h ozone computed from the TKE sensitivity simulations at 4-km grid resolution yielded relatively smaller bias and errors than the PX at 12- and 4-km grid resolutions, illustrating that the TKE models simulated at 4-km grid resolution tend to produce much higher ozone formations at valley and mountain sites and show generally better model performance in comparison with higher observations than PX at 12- and 4-km grid resolutions. However, the results from PX sensitivity simulation at both grid resolutions are generally produced by good model performance in CMAQ statistical analysis. This seems to suggest that the PX scheme is a better choice in simulating in a valley area. Additionally, no significant differences are shown to the grid size sensitivity between 12- and 4-km grid resolutions for the PX simulation in the CMAQ analysis. Based on our results, the sensitivity simulation G_c (Gayno-Seaman PBL scheme using 6.0×10^{-4} per sec) at 4-km grid resolution presents significantly small bias and errors among them for a 4-month period at all areas in East Tennessee.

In our study, DVFs differences were shown with about 1–3 ppb among sensitivity simulations which may yield opposite responses in determining if the NAAQS for 8-h is meet or not. Hence, it is believed that computing RRFs and then DVFs are depending on how well the modeling predicts at a given monitoring site that indicates the sensitivity of the DVFs computed from RRFs to meteorological condition modeled at a given monitoring area. Overall, using RRFs and DVFs computed from G_c (Gayno-Seaman PBL scheme) at 4-km grid resolution may be appropriate options for the future attainment demonstrations because generally the G_c sensitivity simulation shows consistent model performance at most areas in the complex terrain having mountain and valley areas.

Acknowledgments

This work was supported by the TDEC (Tennessee Department of Environment and Conservation) project. We also thank VISTAS (Visibility Improvement State and Tribal Association of the Southeast) for offering inputs of BCs (Boundary Conditions) and ICs (Initial Conditions) from 12-km grid domain.

References

Arunachalam, S., Holland, A., Do, B., Abraczinskas, M., 2006. A quantitative assessment of the influence of grid resolution on predictions of future-year air quality in North Carolina. Atmospheric Environment 40 (26), 5010–5026.

Byun, D.W., Kim, S.T., Kim, S.B., 2007. Evaluation of air quality models for the simulation of a high ozone episode in the Houston metropolitan area. Atmospheric Environment 41 (4), 837–853.

Han, Z.W., Ueda, H., An, J.L., 2008. Evaluation and intercomparison of meteorological predictions by five MM5-PBL parameterizations in combination with three land-surface models. Atmospheric Environment 42 (2), 233–249.

Hogrefe, C., Rao, S.T., Zurbenko, I.G., Porter, P.S., 2000. Interpreting the information in ozone observations and model predictions relevant to regulatory policies in the Eastern United States. Bulletin of the American Meteorological Society 81 (9), 2083–2106.

Hogrefe, C., et al., 2004. Simulating regional-scale ozone climatology over the eastern United States: model evaluation results. Atmospheric Environment 38 (17), 2627–2638.

Jimenez, P., Jorba, O., Parra, R., Baldasano, J.M., 2005. Influence of high-model grid resolution on photochemical modelling in very complex terrains, pp. 180–200.

Jones, J.M., Hogrefe, C., Henry, R.F., Ku, J.Y., Sistla, G., 2005. An assessment of the sensitivity and reliability of the relative reduction factor approach in the development of 8-hr ozone attainment plans. Journal of the Air & Waste Management Association 55 (1), 13–19.

Mao, Q., et al., 2006. Numerical experiments on MM5-CMAQ sensitivity to various PBL schemes. Atmospheric Environment 40 (17), 3092–3110.

Perez, C., Jimenez, P., Jorba, O., Sicard, M., Baldasano, J.M., 2006. Influence of the PBL scheme on high-resolution photochemical simulations in an urban coastal area over the Western Mediterranean. Atmospheric Environment 40 (27), 5274–5297.

Queen, A., Zhang, Y., 2008. Examining the sensitivity of MM5-CMAQ predictions to explicit microphysics schemes and horizontal grid resolutions, part III – the impact of horizontal grid resolution. Atmospheric Environment 42 (16), 3869–3881.

Russell, A., Dennis, R., 2000. NARSTO critical review of photochemical models and modeling. Atmospheric Environment 34 (12–14), 2283–2324.

Sistla, G., et al., 2004. An operational assessment of the application of the relative reduction factors in the demonstration of attainment of the 8-hr ozone national ambient air quality standard. Journal of the Air & Waste Management Association 54 (8), 950–959.

Tong, D.Q., Mauzerall, D.L., 2006. Spatial variability of summertime tropospheric ozone over the continental United States: implications of an evaluation of the CMAQ model. Atmospheric Environment 40 (17), 3041–3056.

USEPA, 1991. Guideline for Regulatory Application of the Urban Airshed Model. Office of Air Quality Planning and Standards. EPA-450/R-91–013. USEPA, Research Triangle Park, NC.

USEPA, 2007. Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, $PM_{2.5.}$ and Regional Haze. EPA-454/B-07–002. USEPA.

VISTAS, 2004. Documentation of 2002 Meteorological Modeling. VISTAS.

Zhang, Y., Liu, P., Pun, B. and Seigneur, C., 2006. A comprehensive performance evaluation of MM5-CMAQ for the Summer 1999 Southern Oxidants Study episode – Part I: Evaluation protocols, databases, and meteorological predictions, pp. 4825–4838.