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Improving ozone modeling in complex terrain at a fine grid resolution: Part I – examination of analysis nudging and all PBL schemes associated with LSMs in meteorological model

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Meteorological variables such as temperature, wind speed, wind directions, and Planetary Boundary Layer (PBL) heights have critical implications for air quality simulations. Sensitivity simulations with five different PBL schemes associated with three different Land Surface Models (LSMs) were conducted to examine the impact of meteorological variables on the predicted ozone concentrations using the Community Multiscale Air Quality (CMAQ) version 4.5 with local perspective. Additionally, the nudging analysis for winds was adopted with three different coefficients to improve the wind fields in the complex terrain at 4-km grid resolution. The simulations focus on complex terrain having valley and mountain areas at 4-km grid resolution. The ETA M–Y (Mellor–Yamada) and G–S (Gayno–Seaman) PBL schemes are identified as favorite options and promote O_3 formation causing the higher temperature, slower winds, and lower mixing height among sensitivity simulations in the area of study. It is found that PX (Pleim–Xiu) simulation does not always give optimal meteorological model performance. We also note that the PBL scheme plays a more important role in predicting daily maximum 8-h O_3 than land surface models. The results of nudging analysis for winds with three different increased coefficients' values (2.5, 4.5, and 6.0 $\times$ 10^{-4} s^{-1}) over seven sensitivity simulations show that the meteorological model performance was enhanced due to improved wind fields, indicating the FDDA nudging analysis can improve model performance considerably at 4-km grid resolution. Specifically, the sensitivity simulations with the coefficient value (6.0 $\times$ 10^{-4}) yielded more substantial improvements than with the other values (2.5 and 4.5 $\times$ 10^{-4}). Hence, choosing the nudging coefficient of 6.0 $\times$ 10^{-4} s^{-1} for winds in MM5 may be the best choice to improve wind fields as an input, as well as, better model performance of CMAQ in the complex terrain area. As a result, a finer grid resolution is necessary to evaluate and access of CMAQ results for giving a detailed representation of meteorological and chemical processes in the regulatory modeling. A recommendation of optimal scheme options for simulating meteorological variables in the complex terrain area is made.

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1. Introduction

The three-dimensional (3D) Air Quality Models (AQMs) for the State Implementation Plans (SIPs) of ozone (O_3) have been gaining increased attention because of playing an important role in guiding the development of regulatory modeling with the National Ambient Air Quality Standards (NAAQS) (Zhang et al., 2006). The non-attainment areas for the 8-h ozone designated by the U.S. Environmental Protection Agency (USEPA) must demonstrate the attainment using the 3D AQMs to see if the NAAQS for 8-h ozone does or does not meet a monitoring area of interest. Thus, each State having 8-h O_3 non-attainment areas are required to submit the SIPs to show for attainment of the 8-h NAAQS which currently meets less than 85 ppb at a localized monitoring area. Models generally tend to concentrate on how well models represent real values. However, there are many uncertainties in meteorological and photochemical models, and those responsibilities for decisions on control strategies need to use modeled scenarios without concern that inaccuracies and assumptions in the modeling may mislead them.

For the ozone SIPs modeling, air quality model performance at finer grid resolutions in the non-attainment areas is desirable because it is expected to propagate the actual structure of the atmosphere and show a more detailed representation of emissions, land-use, meteorological, and chemical processes as well as ozone control strategy. Thus, USEPA recommends that using 4 km

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horizontal grid may be desirable for urban and fine scales of nested regional grids (EPA, 2007). However, recent studies have presented the impacts of grid resolutions such as 36-, 12-, and 4-km for the evaluation of model performance. According to Mathur et al. (2005), 4-km simulation provided the most accurate and realistic ozone prediction while Arunachalam et al. (2006), Cohan et al. (2006), Queen and Zhang (2008), and Wu et al. (2008) found that 4-km grid resolution did not always produce the better model performance of meteorology and CMAQ (Byun and Schere, 2006). As a result, the 12-km grid simulation became more widely and properly chosen. In addition, for the Visibility Improvement State and Tribal Association of the Southeast (VISTAS)'s regional problem in the Southeast US was addressed by conducting the meteorological modeling at 36- and 12-km. Consequently, the PX PBL produced credible meteorological variables (VISTAS, 2004). As a result, the PX model was the preferred choice to provide meteorological inputs to AQMs. However, as indicated by Cohan et al. (2006), the results obtained from finer grid resolutions become necessary when localized variability is needed. Hence, sensitivity simulations from finer grid resolutions for ozone non-attainment areas would be necessary. This is critically important when CMAQ assessment and evaluation are performed in the regulatory modeling.

There are schemes and nudging analyses that may perform differently. Newtonian relaxation or nudging analysis is one method of four-dimensional data assimilation (FDDA). The nudging method described by Stauffer et al. (1991) and Stauffer and Seaman (1994) was found to be an effective and economical method for performing FDDA. In particular, some studies have shown that using nudging analysis in MM5 is considered valuable because it can provide improved wind fields (Bao and Errico, 1997; Barna and Lamb, 2000; Cohan et al., 2006). At the fine scale, selecting the appropriate nudging coefficients may have impacts on MM5 and CMAQ simulation. The magnitude of the impact of nudging coefficients in MM5 on the CMAQ simulations has not been quantified at a fine grid resolution. Determining the appropriate value of nudging in MM5 to the CMAQ simulation can be useful to improve model performance at a finer grid resolution for SIPs in the non-attainment areas. When nudging is used in MM5 to create inputs for CMAQ, it is expected that the improvements of wind fields, shown in MM5 with nudging, would also improve daily maximum 8-h ozone concentration in the CMAQ simulation.

The PBL height in meteorological models plays an important role for predicting and understanding ozone formation and other pollutants (Perez et al., 2006). The PBL has a thickness ranging from a hundred meters to a few kilometers and affects the dynamical and thermal forcing at the surface. Pollutants are emitted into the mixing layer (ML) and become gradually dispersed and mixed through the action of turbulence under convective (Seibert et al., 2000). Hence, the various PBL schemes in MM5 are needed to account for the influence of PBL or ML on ozone air quality during the typical ozone summer season in the complex terrain. CMAQ is then executed by forcing meteorological conditions as an input produced by a single configuration of MM5 (Mao et al., 2006). Some studies have shown how various PBL schemes affect the concentration of pollutants of CMAQ. Still, there is a lack of evaluation concerning how PBL schemes associated with LSMs affect CMAQ model performance at 4-km grid resolution.

The primary objective of this paper is to evaluate the performance of the meteorological model and CMAQ in the complex terrain at a 4-km grid resolution for ozone SIPs. We will also examine the impacts of nudging analysis for winds (and various PBL schemes associated with LSMs in MM5 on CMAQ simulation), to identify the most appropriate PBL schemes associated with LSMs and to determine the best nudging coefficient value for winds. We will present our results in two parts. Part I describes the influence of various nudging coefficients for winds, and five different PBL schemes associated with three different LSMs (21 sensitivity simulation scenarios) on meteorological fields at 4-km horizontal grid resolution to provide a better representation of the meteorology. It also presents impacts of meteorological fields on grid size resolutions of 12-km and 4-km with the PX PBL scheme. Part II focuses on daily maximum 8-h ozone concentrations from the 21 sensitivity simulation scenarios results of CMAQ.

Overall, the results of the study will provide a recommendation of the MM5 and CMAQ configurations for ozone SIP modeling exercises in the complex terrain areas. In addition, this study might provide thoughtful implications for giving a right decision that helps to improve the air quality management and their impacts on ozone SIPs to the State having 8-h O_3 non-attainment areas.

2. Methodology

2.1. Modeling components

The MM5–MCIP–SMOKE–CMAQ modeling system was used in this study. Version 3.7 of MM5 was used to generate meteorological fields for CMAQ as inputs. The output from MM5 was processed by MCIP (Meteorology Chemistry Interface Processor) version 3.1 (Byun and Ching, 1999). It was used and needed by SMOKE Version 2.1 (Houyoux et al., 2002) and CMAQ Version 4.5 as a proper format.

2.2. Episode selection

The 31-day episode was selected for the simulation to represent the typical summer condition. The summer episode is from 1 August to 31 August for the year of 2002 and included a 5-day spin-up period starting at 26 July 2002. The month of August was chosen for the simulation due to the fact that the model performance of the month of August showed generally poor conditions.

2.3. Description of the meteorological modeling

MM5 is a non-hydrostatic, prognostic, and mesoscale meteorological model developed by the Fifth Generation Pennsylvania State University, National Center for Atmospheric Research (Dudhia et al., 2004). The 4 km modeling domain covers East Tennessee, and a portion of several surrounding states including North Carolina (NC), South Carolina (SC), Georgia (GA), West Virginia (WV), and Alabama (AL). Fig. 1 and Table 1 show the Visibility Improvement State and Tribal Association of the Southeast (VISTAS)'s 36 km and 12 km domains, the nested 4 km domains, and all seven monitoring sites representing valley sites (Anderson, Mildred, Rutledge, and Jefferson) and for mountain sites (Look Rock, Cove Mt., and Clingman's Dome) observed in this study. The nested 4 km domain extracted VISTAS's 12 km outputs as its boundary and initial condition inputs. The 36 and 12 km model domains had 34 layers, performed with PX PBL scheme, Kain-Fritsch2 (KF2) cloud scheme, RRTM radiation scheme, and mixed-phase microphysics scheme in the current VISTAS's model configuration.

The INTERPPX is a new preprocessor used to initialize soil moisture, temperature, and canopy moisture from a previous run after NESTDOWN (Pleim and Chang, 1992). This method is only applied for PX model. The NESTDOWN is used to generate inputs for finer grid resolution MM5 run from the coarser resolution MM5 output. One-way NESTDOWN method was selected to generate inputs for the 4-km grid resolution MM5 run. This took output from MM5 run, together with TERRAIN output for a 4-km grid domain.

The 4-km grid resolution has 127 by 118 grids with 34 layers in MM5. The MM5 model was in Lambert conformal projection with true latitudes at 33° N and 45° N. The 4-km grid domain also

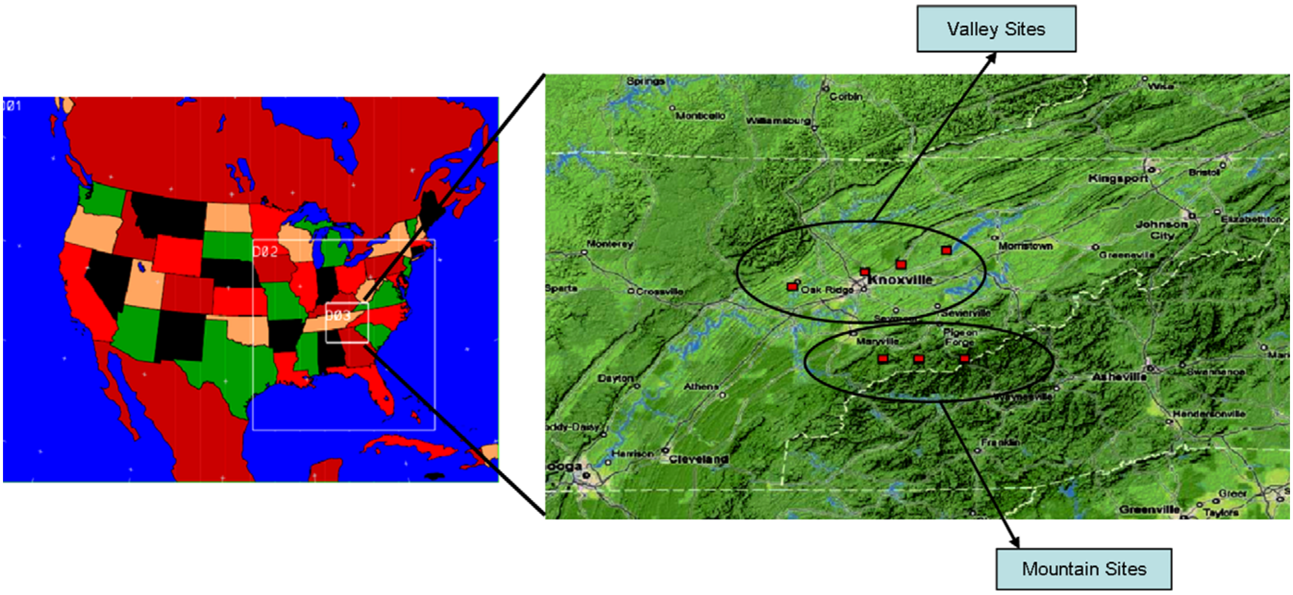

Fig. 1. The VISTAS's 36 (D01) and 12 km (D02) domains and nested 4 km (D03) domain for the East Tennessee and total seven monitor sites for valley sites (Anderson, Mildred, Rutledge, Jefferson) and for mountain sites (Look Rock, Cove Mt., and Clingman's Dome) observed in East Tennessee.

performed with Kain-Fritsch2 (KF2) cloud scheme, RRTM radiation scheme, and mixed-phase microphysics scheme, the same as 36-km and 12-km domains.

3. MM5 sensitivity

3.1. Sensitivity to PBL schemes associated with land surface models

Meteorological fields of wind speeds, wind direction, temperature, and PBL have been examined on air quality for predicting ozone concentration because they have direct impacts on air quality through dispersion and transport. Thus, they are used as 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). A complex topography with valley and mountain areas in East Tennessee is a good example in this study. There, stagnant air traps air pollutants within the valley airshed. The generally low wind speeds, slow the dispersion and transport of pollutants out of the valley. In this area, the breezes and winds of mountain and valley induced have important impacts on the dispersion of the pollutants emitted (Miller and Fu, 2006). The pattern of winds in the complex area can be even more complicated due to the land-use and the types of vegetation (Perez et al., 2006). Some studies have shown that the MM5 tends to predict well for temperature while wind speed tends to over predict in terms of overall-wide statistics and area-specific statistics at a 4-km grid resolution (Wu et al., 2008; Zhang et al., 2006). Jang et al. (1995) and Jimenez et al. (2005) suggest that the modeling of photochemical pollution in complex terrains requires a high horizontal grid resolution and needs to evaluate the meteorological variables such as wind speed, temperature, and wind direction with respect to the overall-wide statistics and area-specific statistics to provide insights into a local area.

Seven PBL schemes are available in MM5 configuration. However, five PBL schemes among them are commonly used. Thus, the five PBL schemes were selected for the MM5 sensitivity simulations in this study. These PBL schemes used in the simulation are as follows: PX (Pleim and Chang, 1992), Noah ETA M–Y, Noah MRF (Medium Range Forecast) (Hong and Pan, 1996), Blackadar (Blackadar, 1979), and G–S (Gayno, 1994).

Each PBL scheme is coupled with one of three land surface models available in MM5 application. Due to their role of providing the surface boundary conditions to the atmosphere, the land surface processes are very important in influencing the PBL structure (Chen and Dudhia, 2001). The LSM options used are PX, Noah, and 5-layer soil model. The PX LSM (Xiu and Pleim, 2001) predicts soil temperature and moisture in two layers while the Noah LSM (Chen and Dudhia, 2001) predicts soil temperature, moisture, and snow cover in four layers. The 5-layer soil model (Dudhia, 1996) predicts soil temperature in five layers. The PX LSM can only work with PX PBL scheme while Noah LSM can be used with ETA M–Y and MRF schemes. The 5-layer soil model can be applicable with Blackadar, ETA M–Y, MRF, and G–S. The Blackadar scheme is suitable for high resolution. The ETA M–Y PBL scheme predicts Turbulent Kinetic Energy (TKE) and has local vertical mixing. The MRF PBL scheme (also known as Hong-Pan PBL), determines PBL depth from the critical bulk Richardson number. The G–S PBL scheme predicts TKE and allows for cloud-topped PBL processes. The G–S PBL scheme diagnoses the PBL height based on the vertical TKE profile. The PX PBL scheme is based on the Blackadar scheme

Table 1
Observed monitoring sites used in this study.

Observed monitoring sites	Valley sites				Mountain sites		
	Anderson	Mildred	Rutledge	Jefferson	Look rock	Cove Mt.,	Clingman's dome
Elevation (m MSL)	238	322	299	310	793	1243	2021
Latitude (deg N)	35.9650	36.0181	36.0847	36.1227	35.6331	35.6967	35.5619
Longitude (deg W)	84.2233	83.8761	83.7642	83.6002	83.9422	83.6086	83.4981

Table 2
MM5 model sensitivity scenarios used in the simulation.

MM5 sensitivity scenarios	A	B	C	D	E	F	G
PBL scheme	PX	Eta M–Y	MRF	Eta M–Y	MRF	Blackadar	Gayno–Seaman
LSM scheme	PX	Noah	Noah	5-Soil layer	5-Soil layer	5-Soil layer	5-Soil layer
Cloud microphysics	Mixed-phase	Mixed-phase	Mixed-phase	Mixed-phase	Mixed-phase	Mixed-phase	Mixed-phase
Cumulus parameterization	KF2	KF2	KF2	KF2	KF2	KF2	KF2
Atmospheric radiation	RRTM	RRTM	RRTM	RRTM	RRTM	RRTM	RRTM
Shallow convection	No	No	No	No	No	No	No

and Asymmetric convective model. The MRF and PX are non-local schemes while the ETA and G–S are local vertical TKE schemes. Table 2 shows the summary of PBL associated with LSM used in this study. The five different PBL schemes associated with LSM were examined to identify the most preferred PBL and LSM affecting ozone concentrations in the complex terrain at a 4-km horizontal grid resolution.

3.2. *Sensitivity to analysis nudging*

Stauffer et al., 1991 indicated that the technique of Newtonian relaxation or nudging, was found to be an effective and economical method for performing Four-Dimensional Data Assimilation. Nudging technique (Stauffer and Seaman, 1994; Stauffer et al., 1991) is known to be a method of FDDA relaxing the model state toward the observed state by adding artificial forcing terms to the model equations based on the difference between the two states weighed by nudging coefficients in MM5. The nudging toward gridded analysis (based on the model's time step as a simple method nudging FDDA) was used in this study. The gridded analysis nudging is well-known as a relatively flexible method to insert FDDA into the model (Otte, 2008). Basically, the numerical coefficient is related with the numerical stability because it is applied at every time step. If the nudging coefficient is increased, the observed state will have more impacts on the model state. On the other hand, if the nudging coefficient is decreased, the observation will have smaller effects on the model state (Dudhia et al., 2004). However, if the nudging term is greater than 1/time step, the model will become undesirable because it is numerically unstable. Therefore, choosing appropriate nudging coefficients is important to get better model performance as well as numerical stability.

The NCEP (National Centers for Environmental Prediction) final analysis data for REGRID and NCEP ADP Upper Air Observations and NCEP ADP Surface Observations for the surface FDDA were used. The time step used was 30 s. The FDDA 3D and surface analysis nudging is available in MM5 application and known to be useful to improve wind fields (Bao and Errico, 1997; Barna and Lamb, 2000; Cohan et al., 2006). The nudging term is weighted by a selected coefficient. Typically, the nudging coefficients range from 2.5×10^{-4} to 6.0×10^{-4} s^{-1} in the analysis nudging method. That is, the model approaches the observations with an e-folding term, which is about 0.5–1.1 h for the nudging terms of 2.5×10^{-4} to 6.0×10^{-4} s^{-1} (Dudhia et al., 2004). This assumes frequency insertions of the observed data into the model. The FDDA 3D and surface analysis nudging was applied for temperature, winds, and mixing ratio. The nudging coefficients were 2.5×10^{-4} for temperature and 1.0×10^{-5} for mixing ratio used at each sensitivity simulation. According to Bao and Errico (1997), nudging winds were more effective and dominant than temperature. Hence, we applied the nudging winds with increasing nudging coefficients that could produce better results than using the nudging coefficients for winds with a default value of 2.5×10^{-4} s^{-1}.

In this study, the nudging coefficients for winds of 2.5×10^{-4}, 4.0×10^{-4}, and 6.0×10^{-4} s^{-1} were utilized at each sensitivity simulation.

Table 3
Summary of the meteorological performance statistics of seven sensitivity scenarios used default nudging coefficient (2.5×10^{-4} s^{-1}) for wind speeds at overall, valley, and mountain areas.

Sensitivity	Wind speed				Wind direction		Temperature	
	Bias (m s^{-1})	RMSE (m s^{-1})	Benchmark bias (m s^{-1})	Benchmark RMSE (m s^{-1})	Bias (deg)	Benchmark bias (deg)	Bias (K)	Benchmark bias (K)
Overall								
A	0.62	1.63	≤±0.5	≤2	5.6	≤±10	0.28	≤±0.5
B	0.15	1.52	≤±0.5	≤2	3.4	≤±10	0.56	≤±0.5
C	0.45	1.68	≤±0.5	≤2	6.0	≤±10	0.98	≤±0.5
D	0.16	1.53	≤±0.5	≤2	3.1	≤±10	0.57	≤±0.5
E	0.47	1.73	≤±0.5	≤2	5.4	≤±10	0.77	≤±0.5
F	0.63	1.82	≤±0.5	≤2	4.2	≤±10	0.62	≤±0.5
G	0.34	1.86	≤±0.5	≤2	5.1	≤±10	1.12	≤±0.5
Valley								
A	−0.18	1.10	≤±0.5	≤2	4.7	≤±10	0.39	≤±0.5
B	−0.45	1.14	≤±0.5	≤2	5.4	≤±10	−0.03	≤±0.5
C	−0.10	1.14	≤±0.5	≤2	9.3	≤±10	0.41	≤±0.5
D	−0.40	1.14	≤±0.5	≤2	5.7	≤±10	0.27	≤±0.5
E	−0.10	1.16	≤±0.5	≤2	4.9	≤±10	0.43	≤±0.5
F	−0.13	1.15	≤±0.5	≤2	7.1	≤±10	0.35	≤±0.5
G	−0.35	1.30	≤±0.5	≤2	8.1	≤±10	0.88	≤±0.5
Mountain								
A	0.71	1.78	≤±0.5	≤2	5.5	≤±10	2.03	≤±0.5
B	0.26	1.76	≤±0.5	≤2	6.3	≤±10	2.89	≤±0.5
C	0.62	1.68	≤±0.5	≤2	7.4	≤±10	3.12	≤±0.5
D	0.33	1.56	≤±0.5	≤2	4.8	≤±10	3.00	≤±0.5
E	0.66	1.74	≤±0.5	≤2	7.5	≤±10	2.91	≤±0.5
F	0.83	1.81	≤±0.5	≤2	6.1	≤±10	2.83	≤±0.5
G	0.49	1.64	≤±0.5	≤2	5.3	≤±10	3.32	≤±0.5

4. Results and discussions

4.1. Statistics for meteorology to PBL schemes

The meteorological performance statistics of seven sensitivity simulations are shown in Table 3. The statistical measures of wind speed, wind direction, and temperature at the surface were calculated by METSTAT program (METSTAT, 2005). The METSTAT program reads predicted temperature at 2-m heights and predicted winds at 10-m heights (Louis, 1979). The observed temperature, wind speed, and wind direction at the valley, mountain sites, and entire 4-km domain (overall) was compared with predicted temperature, wind speed, and wind direction. The meteorological model performance statistics of all seven simulations were computed hourly and evaluated for mean bias (MB) and Root Mean Square Error (RMSE) with a benchmark of MB and RMSE. For the temperature, all schemes tend to over predict the surface temperature, as shown in the positive bias except sensitivity B (ETA M–Y PBL with Noah LSM) showed the lowest mean bias at valley sites. Sensitivity A (PX) showed the lower mean bias at overall and mountain sites while sensitivity G (5-layer soil model with Gayno–Seaman PBL) showed the over prediction with the higher mean bias at overall, valley, and mountain areas. The PX sensitivity simulation tends to predict better at overall and valley areas (except mountain areas) than other schemes. Especially, the PX model from 4-km grid resolution presents relatively smaller mean bias in predicting temperature than 12-km resolution. Because the interactions between surface characterization and PBL schemes are strongly associated, vertical transport is one of the most important keys of air quality modeling due to the boundary layer turbulence (Mao et al., 2006). Figs. 2–4 show the mean bias of temperature at 2 m and mean bias of wind speed at 10 m for the overall domain of the study, valley, and mountain areas and RMSE simulated by MM5 with 7 different sensitivity simulation scenarios (shown in Table 3) from 1 August through 31 August of Year 2002.

All seven sensitivity simulation scenarios for wind speed resulted in positive biases for overall and mountain sites except for valley sites where negative biases were shown. Interestingly, sensitivity B (ETA M–Y PBL with Noah LSM) and D (ETA M–Y PBL with 5-layer soil model), A (PX) and F (Blackadar with 5-layer soil model), and C (MRF PBL with Noah LSM) and E (MRF PBL with 5-layer soil model) show similar results for wind speed due to the same PBL scheme used with different LSM. This means that the PBL scheme selected, influences wind speeds more than LSM. Only sensitivity simulation B, D, and G can meet the benchmark of bias (0.5 m s^{-1}) for wind speed at the whole domain (overall), valley, and mountain sites. The ETA M–Y PBL schemes with Noah LSM and 5-layer soil model show the lowest bias and RMSE for wind speed.

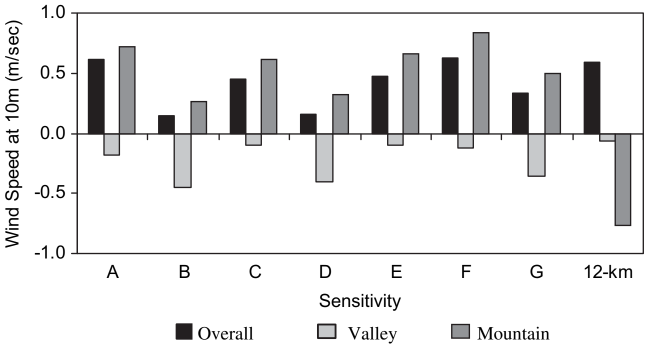

Fig. 2. Mean Bias of MM5 for wind speed at 10 m with 7 different sensitivity simulations on 4-km and PX PBL scheme on 12-km grid resolution for August in 2002.

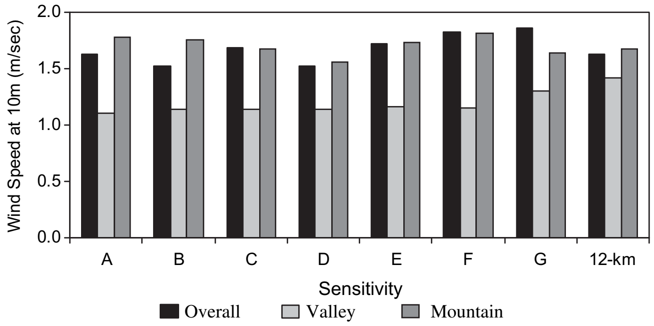

Fig. 3. RMSE of MM5 for Wind Speed at 10 m with 7 different sensitivity simulations on 4-km and PX PBL scheme on 12-km grid resolution for August in 2002.

For the wind direction, all seven sensitivity simulations meet the benchmark of bias, which is 10° in bias. However, as indicated in Han et al, 2008, the comparison for wind direction might be unreasonable due to the wind direction is a vector while in order to compare with observed values, it is a scalar, thus when wind direction is around is 0° or 360°.

It is noteworthy that the PX scheme used primarily in the Southeast US (VISTAS, 2004), does not always give good meteorological model performance. When even comparing 12-km grid resolution to sensitivity simulations at 4-km grid resolution used PX scheme in order to study the impact of grid resolution on meteorological fields, as seen in Figs. 2–4, the PX simulation at 4-km grid resolution for wind speed in bias shows over prediction at mountain areas whereas 12-km grid simulation present many under predictions. At valley areas, both of 4-km and 12-km grid resolution, generally show for wind speeds good model performance with small mean bias (−0.18 and −0.07 m s^{-1}, respectively) even though 4-km grid resolution give much lower RMSE (Root Mean Square Error) with 1.1 m s^{-1} than that of 12 km grid resolution with 1.42 m s^{-1}. Overall (valley and mountain areas), the impact of grid resolutions on meteorological variations in our local area is also not showing a significant difference, as indicated in Cohan et al. (2006) and Wu et al. (2008).

Figs. 5 and 6 show the diurnal variations in the PBL height with all seven sensitivity simulations modeled at valley and mountain sites on 5 August 2002, which was shown as one of high ozone days. It is interesting that all sensitivity simulations show a similar variation pattern in PBL height during the daytime and nighttime at valley and mountain areas. Generally, as shown in Figs. 5 and 6, all sensitivity simulations show higher in predicting PBL heights at valley areas during the daytime than at mountain areas. In particular, A consistently produced the highest mixing depths while B, D, and G schemes showed relatively lower mixing depths than other simulations over the valley and mountain areas. With our

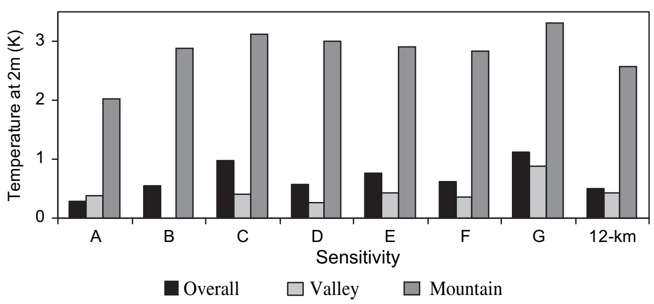

Fig. 4. Mean Bias of MM5 for Temperature at 2 m with 7 different sensitivity simulations on 4-km and PX PBL scheme on 12-km grid resolution for August in 2002.

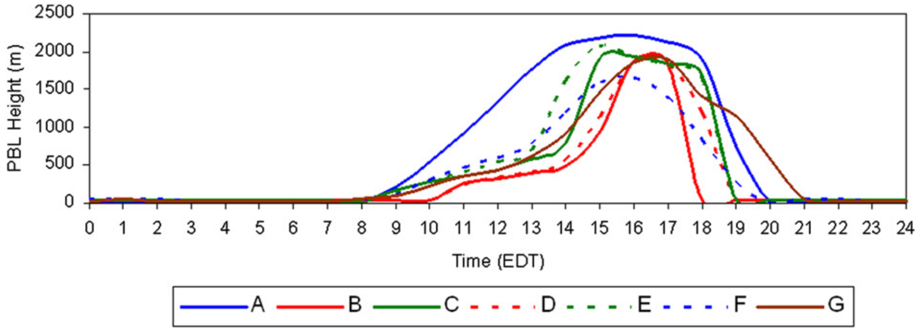

Fig. 5. Diurnal variations in the PBL height with seven scenarios at valley site on August 5, 2002 (EDT).

attentions, these schemes (ETA M–Y and G–S schemes) consistently produced relatively lower mixing depths at any areas than other schemes, as found in Han et al, 2008. C and E scenarios with Noah and 5-layer soil model showed similar pattern and somehow differences in the mixing depths and B and D scenarios with Noah and 5-layer soil model looked similar as mentioned previously. Surprisingly, for cases of B and C using the same LSMs (Noah) and D and E using the same LSMs (5-layer soil model), they showed much significant differences in the diurnal variations of PBL heights than those of using the same PBL but different LSMs. It seems to indicate that PBL schemes give more significant contributions in the diurnal variations of PBL heights. We can also notice that the pattern of the PBL prediction from the TKE PBL schemes such as ETA M–Y and G–S are alike while that of the non-local schemes such as PX and MRF are similar. As indicated in Han et al., 2008, the PBL schemes are more associated with the PBL height prediction. Based on the results of the above analyses, the TKE scheme (B, D, and G scenarios) shows better model performance while the non-local scheme (A, C, E, and F scenarios) shows somewhat poor model performance in our study area. It is noted that the TKE schemes compute the mixing depths using the turbulent energy of the surface mixing layer (depending on the situation of convection) whereas Blackadar and PX schemes predict the PBL heights from potential temporal profile. Additionally, the mixing height in MRF scheme is determined by a critical bulk Richardson number at the top of PBL and near surface (Perez et al., 2006), resulting in considerable difference in PBL height computation.

4.2. Statistics for meteorology to nudging analysis

MM5 has two nudging methods that can be used commonly for improving meteorological variables such as winds, temperature, and mixing ratio. One is for gridded analysis and the other one is observational nudging. FDDA analysis nudging (gridded analysis) was used for both 3D and surface fields in all twenty-one sensitivity MM5 simulations. It supports air quality studies and has been of greater benefit to these variables (Mao et al., 2006).

Figs. 7–9 show the results from MM5 using three different nudging coefficients (2.5, 4.5, and 6.0 $\times$ 10^{-4} s^{-1}) over seven sensitivity simulations at the whole domain, valley, and mountain areas. As increased with nudging coefficients for winds in MM5, wind speeds were decreased gradually at valley and mountain areas. All seven sensitivity simulations with three different nudging coefficients showed improved wind speed in mean bias and RMSE and no significant difference in temperature. Sensitivity simulation scenarios B and D with 6.0 $\times$ 10^{-4} had the slowest wind speed and scenario G with 6.0 $\times$ 10^{-4} also showed the second slowest wind speed. As a result, using 6.0 $\times$ 10^{-4} s^{-1} for winds in MM5 is a good option to improve wind speed in complex terrain at a fine grid resolution.

Table 4 also shows the summary of meteorological model performance of statistics among all sensitivity simulations used with three different nudging coefficients for winds at 4-km grid resolution. As already mentioned above, these TKE PBL schemes (scenarios B, D, and G) with high nudging coefficient (6 $\times$ 10^{-4} s^{-1}) for winds produce better model performance of MM5 in statistics for wind speed with smaller mean bias than with other nudging coefficients. It can be explained due to the addition of artificial forcing terms to the model equation. Only A scenario with three nudging coefficients for winds meet the benchmark of bias for temperature at overall areas, however, all sensitivity simulation scenarios with the three nudging coefficients [except G scenario] reach the biases of temperature and wind speeds at valley sites. At mountain areas, only the TKE schemes with increased nudging coefficients for winds are somewhat superior to other schemes in predicting wind speeds. Instead, none of the schemes meets the benchmark of temperature. Obviously, all sensitivity simulations for the model performance of meteorology at valley sites yield

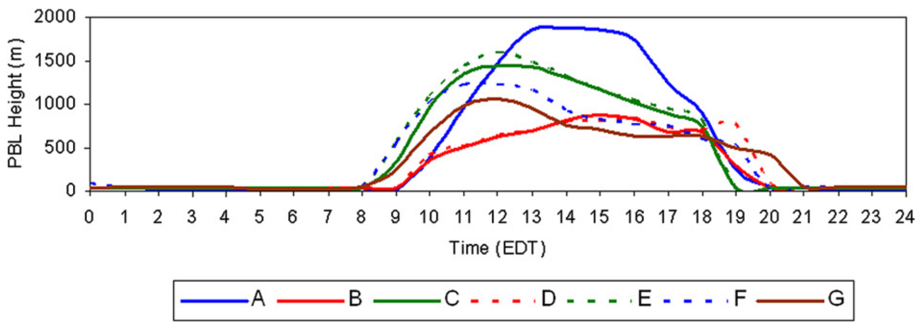

Fig. 6. Diurnal variations in the PBL height with seven scenarios at mountain site on August 5, 2002 (EDT).

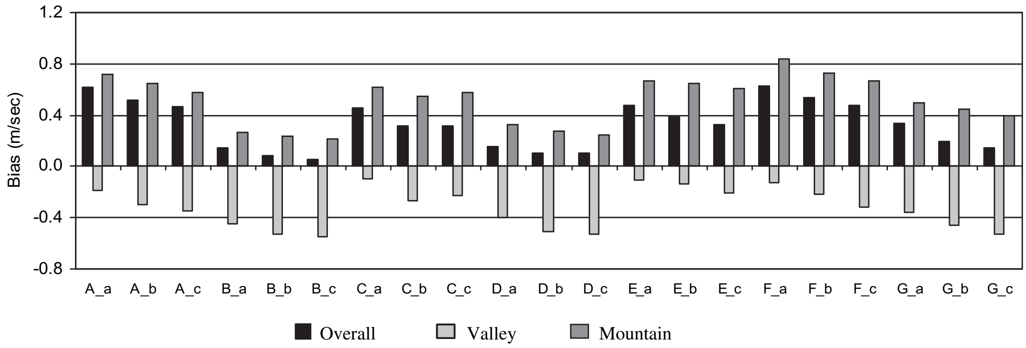

Fig. 7. Plots of bias for wind speed on seven scenario simulations with three different nudging coefficients (a (2.5), b (4.5), and c (6×10^{-4} s^{-1})) at the whole domain, valley, and mountain areas.

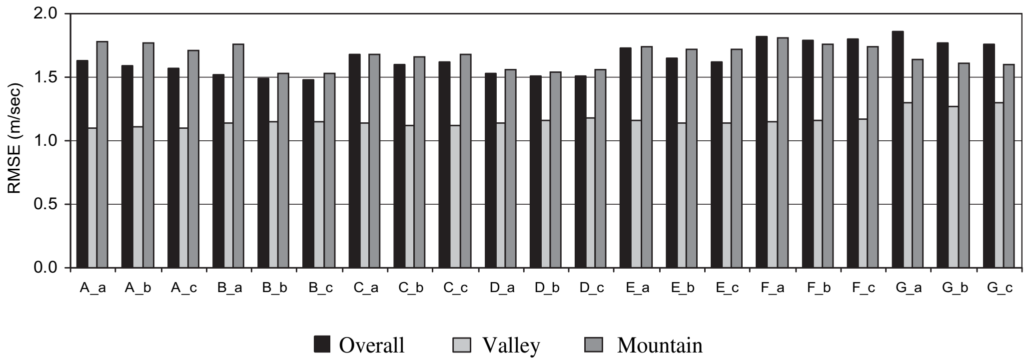

Fig. 8. Plots of RMSE for wind speed on seven scenario simulations with three different nudging coefficients (a (2.5), b (4.5), and c (6×10^{-4} s^{-1})) at the whole domain, valley, and mountain areas.

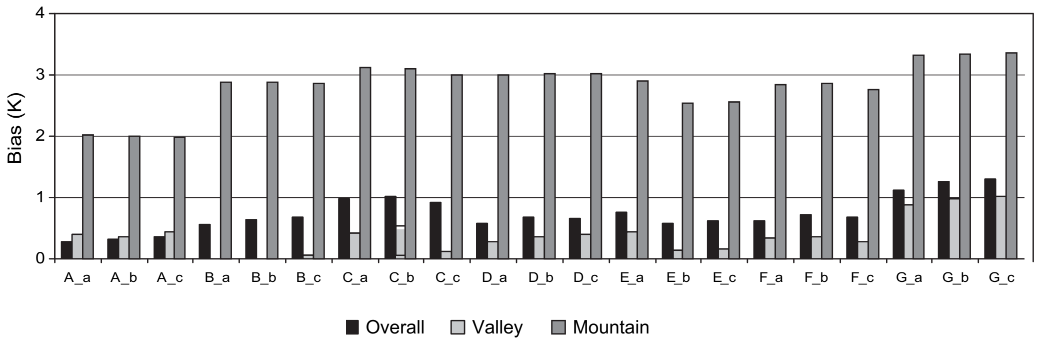

Fig. 9. Plots of Bias for temperature on seven scenario simulations with three different nudging coefficients (a (2.5), b (4.5), and c (6×10^{-4} s^{-1})) at the whole domain, valley, and mountain area.

better model performance with mean bias and RMSE than at mountain. With the view of overall points, modelers should be able to choose optimally with good agreement of model performance at any area. Therefore, these TKE PBL schemes at 4-km grid resolution generally predicted better at overall, valley, and mountain areas than other grid resolution in our results.

5. Conclusions

Twenty-one sensitivity simulations were conducted over a 31-day period of August 2002 to various PBL schemes with three different LSM and three different nudging coefficients for winds used in MM5 in the complex terrain at a 4-km grid resolution. We evaluated the model performance to show which PBL schemes associated with LSMs are favorite options in the complex terrain and determined the best nudging coefficients for winds to use in MM5 at a 4-km grid resolution.

The meteorological model performance statistics of all seven PBL simulations were computed hourly and evaluated for bias and RMSE with benchmark of mean bias and RMSE. All seven PBL sensitivity simulations at 4-km grid resolution tend to under predict the wind speed at valley sites and over predict it at mountain sites. For temperature, all simulations overestimate except sensitivity scenario B at all areas. Sensitivity scenario A showed the lowest bias for temperature at overall and mountain sites while sensitivity scenario G showed the over prediction with the highest bias at all locations, making higher mixing height estimation due to the warmer surface temperature. Planetary

Table 4
Summary of meteorological model performance statistics of twenty-one sensitivity scenarios used three different nudging coefficients (2.5, 4.5, and 6 $\times$ 10^{-4} s^{-1}, respectively), for wind speeds at overall, valley, and mountain areas.

	Wind speed				Wind direction		Temperature	
	Bias	RMSE	Benchmark bias (m s^{-1})	Benchmark RMSE (m s^{-1})	Bias	Benchmark bias (deg)	Bias	Benchmark bias (K)
Overall								
A_2.5	0.62	1.63	≤±0.5	≤2	5.6	≤±10	0.28	≤±0.5
A_4.5	0.52	1.59	≤±0.5	≤2	5.2	≤±10	0.33	≤±0.5
A_6	0.46	1.57	≤±0.5	≤2	5.0	≤±10	0.36	≤±0.5
B_2.5	0.15	1.52	≤±0.5	≤2	3.4	≤±10	0.56	≤±0.5
B_4.5	0.09	1.49	≤±0.5	≤2	3.3	≤±10	0.63	≤±0.5
B_6	0.05	1.48	≤±0.5	≤2	3.8	≤±10	0.69	≤±0.5
C_2.5	0.45	1.68	≤±0.5	≤2	6.0	≤±10	0.98	≤±0.5
C_4.5	0.31	1.60	≤±0.5	≤2	5.0	≤±10	1.03	≤±0.5
C_6	0.31	1.62	≤±0.5	≤2	5.0	≤±10	0.91	≤±0.5
D_2.5	0.16	1.53	≤±0.5	≤2	3.1	≤±10	0.57	≤±0.5
D_4.5	0.10	1.51	≤±0.5	≤2	3.0	≤±10	0.67	≤±0.5
D_6	0.11	1.51	≤±0.5	≤2	3.0	≤±10	0.66	≤±0.5
E_2.5	0.47	1.73	≤±0.5	≤2	5.4	≤±10	0.77	≤±0.5
E_4.5	0.38	1.65	≤±0.5	≤2	5.6	≤±10	0.59	≤±0.5
E_6	0.32	1.62	≤±0.5	≤2	5.2	≤±10	0.62	≤±0.5
F_2.5	0.63	1.82	≤±0.5	≤2	4.2	≤±10	0.62	≤±0.5
F_4.5	0.53	1.79	≤±0.5	≤2	4.5	≤±10	0.72	≤±0.5
F_6	0.47	1.80	≤±0.5	≤2	4.6	≤±10	0.67	≤±0.5
G_2.5	0.34	1.86	≤±0.5	≤2	5.1	≤±10	1.12	≤±0.5
G_4.5	0.20	1.77	≤±0.5	≤2	5.5	≤±10	1.25	≤±0.5
G_6	0.14	1.76	≤±0.5	≤2	4.8	≤±10	1.30	≤±0.5
Valley								
A_2.5	−0.18	1.10	≤±0.5	≤2	4.7	≤±10	0.39	≤±0.5
A_4.5	−0.30	1.11	≤±0.5	≤2	8.5	≤±10	0.36	≤±0.5
A_6	−0.35	1.10	≤±0.5	≤2	4.3	≤±10	0.43	≤±0.5
B_2.5	−0.45	1.14	≤±0.5	≤2	5.4	≤±10	−0.03	≤±0.5
B_4.5	−0.52	1.15	≤±0.5	≤2	5.4	≤±10	0.01	≤±0.5
B_6	−0.55	1.15	≤±0.5	≤2	6.2	≤±10	0.07	≤±0.5
C_2.5	−0.10	1.14	≤±0.5	≤2	9.3	≤±10	0.41	≤±0.5
C_4.5	−0.27	1.12	≤±0.5	≤2	7.5	≤±10	0.47	≤±0.5
C_6	−0.23	1.12	≤±0.5	≤2	5.5	≤±10	0.12	≤±0.5
D_2.5	−0.40	1.14	≤±0.5	≤2	5.7	≤±10	0.27	≤±0.5
D_4.5	−0.51	1.16	≤±0.5	≤2	5.8	≤±10	0.36	≤±0.5
D_6	−0.53	1.18	≤±0.5	≤2	9.1	≤±10	0.40	≤±0.5
E_2.5	−0.10	1.16	≤±0.5	≤2	4.9	≤±10	0.43	≤±0.5
E_4.5	−0.14	1.14	≤±0.5	≤2	12.2	≤±10	0.14	≤±0.5
E_6	−0.21	1.14	≤±0.5	≤2	9.6	≤±10	0.15	≤±0.5
F_2.5	−0.13	1.15	≤±0.5	≤2	7.1	≤±10	0.35	≤±0.5
F_4.5	−0.22	1.16	≤±0.5	≤2	7.8	≤±10	0.36	≤±0.5
F_6	−0.32	1.17	≤±0.5	≤2	8.8	≤±10	0.28	≤±0.5
G_2.5	−0.35	1.30	≤±0.5	≤2	8.1	≤±10	0.88	≤±0.5
G_4.5	−0.46	1.27	≤±0.5	≤2	11.2	≤±10	0.98	≤±0.5
G_6	−0.53	1.30	≤±0.5	≤2	9.7	≤±10	1.01	≤±0.5
Mountain								
A_2.5	0.71	1.78	≤±0.5	≤2	5.5	≤±10	2.03	≤±0.5
A_4.5	0.65	1.77	≤±0.5	≤2	5.9	≤±10	2.01	≤±0.5
A_6	0.58	1.71	≤±0.5	≤2	7.1	≤±10	1.98	≤±0.5
B_2.5	0.26	1.76	≤±0.5	≤2	6.3	≤±10	2.89	≤±0.5
B_4.5	0.24	1.53	≤±0.5	≤2	6.4	≤±10	2.89	≤±0.5
B_6	0.21	1.53	≤±0.5	≤2	5.6	≤±10	2.87	≤±0.5
C_2.5	0.62	1.68	≤±0.5	≤2	7.4	≤±10	3.12	≤±0.5
C_4.5	0.55	1.66	≤±0.5	≤2	6.7	≤±10	3.11	≤±0.5
C_6	0.57	1.68	≤±0.5	≤2	3.0	≤±10	3.00	≤±0.5
D_2.5	0.33	1.56	≤±0.5	≤2	4.8	≤±10	3.00	≤±0.5
D_4.5	0.27	1.54	≤±0.5	≤2	4.8	≤±10	3.02	≤±0.5
D_6	0.25	1.56	≤±0.5	≤2	5.7	≤±10	3.02	≤±0.5
E_2.5	0.66	1.74	≤±0.5	≤2	7.5	≤±10	2.91	≤±0.5
E_4.5	0.65	1.72	≤±0.5	≤2	5.0	≤±10	2.54	≤±0.5
E_6	0.61	1.72	≤±0.5	≤2	4.8	≤±10	2.55	≤±0.5
F_2.5	0.83	1.81	≤±0.5	≤2	6.1	≤±10	2.83	≤±0.5
F_4.5	0.72	1.76	≤±0.5	≤2	7.2	≤±10	2.86	≤±0.5
F_6	0.67	1.74	≤±0.5	≤2	7.0	≤±10	2.77	≤±0.5
G_2.5	0.49	1.64	≤±0.5	≤2	5.3	≤±10	3.32	≤±0.5
G_4.5	0.44	1.61	≤±0.5	≤2	6.3	≤±10	3.35	≤±0.5
G_6	0.39	1.60	≤±0.5	≤2	5.6	≤±10	3.36	≤±0.5

boundary layers have a critical parameter for air quality simulations (Byun et al., 2007; Perez et al., 2006; Queen and Zhang, 2008; Zhang et al., 2006). The MRF and PX are non-local schemes while ETA and G–S are local vertical TKE schemes. Our MM5 results present that sensitivity simulation scenarios B, D, and G called the TKE PBL schemes produced better model performance for winds than non-local schemes (PX and MRF). These local vertical TKE schemes (scenarios B, D, and G) show more underestimation of wind speed than the other non-local schemes at all areas. The weaker winds in the local schemes can be explained by producing more O_3 formation at valley and mountain sites. In addition, these three local schemes also present the lowest PBL heights and highest surface temperatures, which produce an enhanced O_3 formation at valley and mountain sites. It indicates that predicting local TKE in PBL yields relatively better meteorological model performance than non-local scheme based on Rib number method in the complex terrain at 4-km grid resolution. Since the impact of meteorological variations on grid size resolution in our local area does not show a significant difference, the non-local scheme in lower grid resolution also would produce relatively poor model performance than local TKE scheme.

The results of nudging analysis for winds with three different increased coefficient values (2.5, 4.5, and $6.0 \times 10^{-4}\ s^{-1}$) over seven sensitivity simulations show that the meteorological model performance was enhanced slightly due to improved wind fields, indicating the FDDA nudging analysis can improve model performance considerably at 4-km grid resolution. More specifically, the sensitivity simulations with the highest coefficient value (6.0×10^{-4}) generally gave more substantial improvements than with the other values (2.5 and 4.5×10^{-4}).

Comparing the 12-km grid resolution to 4-km grid resolution in PX simulation in the meteorological model performance of statistics, there was no significant difference. Generally speaking, PX simulation showed the tendencies to predict temperature well at most areas whereas Blackadar simulation had tendencies to present very poor model performance with large bias of wind speeds at mountain areas. We also found that the PX sensitivity simulation recommended by USEPA did not produce optimal meteorological conditions in our study area. As previously mentioned in the introduction, ozone SIPs modeling, unlike global or regional modeling, should be more focused on local areas to observe the actual atmospheric structure and evaluate the control strategy for O_3. We also noticed that it is very important to find appropriate PBL schemes associated with direct influence on meteorological conditions at local areas of interest for ozone SIPs in a finer grid resolution due to the dependence on MM5 as inputs into the air quality model (e.g., CMAQ). Based on our results, the TKE PBL schemes on 4-km grid resolution gave significant contributions for SIPs modeling in the complex terrain areas with local perspective.

We will present the effects of the seven sensitivity simulations used with the best value of nudging coefficient for winds based on the results of this study on CMAQ and RRFs (Relative Response Factors) for SIPs in the non-attainment areas as well as the contributions of 4-km grid resolution on CMAQ model in Part II of this paper.

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