2.3 AIR QUALITY MODELING SENSITIVITY TO PBL SCHEMES

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1. INTRODUCTION

The PSU/NCAR MM5 mesoscale meteorological model and the Community Multiscale Air Quality (CMAQ) photochemical model are the most popular air quality modeling suite adopted by EPA and other federal, state, and local agencies and universities for air quality research application and forecasting. This suite has been used extensively in the United States and other countries over the recent years (Byun and Ching, ed., 1999; Sakurai et al., 2003; Jun and Stein, 2004; Jimenez et al., 2005; Otte et al., 2005). Currently, there is a lack of assessment on how various PBL schemes in MM5 affect the results of CMAQ as both models are not run interactively. Once the MM5 data is judged satisfactory, CMAQ is executed with forcing meteorological conditions produced by a single configuration of MM5 (Grell et al., 1995).

This study attempts to explore MM5-CMAQ modeling sensitivity to five commonly used PBL schemes through a series of numerical experiments over a summer and a winter episode. The goals of the study are to quantify the model sensitivity and help develop strategies for reducing uncertainty in air quality simulations.

2. SENSITIVITY EXPERIMENT

2.1 MM5

The MM5 and CMAQ models were configured with two domains covering the continental U.S, and the southeast and central U.S., respectively. The horizontal resolution for both models was 36 km. There were 34 half-sigma layers in MM5 and 18 layers in CMAQ. Two 37-day episodes were selected for the simulations to represent summer and winter weather conditions. The summer episode comprised the month of July 2001 and included a seven-day ramp-up period beginning at 12Z on June 24, 2001. The winter episode comprised the month of January 2002 and included a seven-day ramp-up period beginning at 12Z on December 25, 2001. These month-long episodes were chosen for the simulations to represent a more objective and robust characterization of the variable meteorology and air quality that is typical during summer and winter months.

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Five modeling scenarios were configured for the MM5 simulations. These scenarios, referred to as Option-A through Option-E, were differentiated by the PBL and associated ground temperature (soil) schemes or land surface models (LSMs) (Table 1). The PBL scheme dictated the corresponding LSM for each scenario. Since no single LSM was applicable to all the PBL schemes, three LSMs were activated for the sensitivity experiments. Other model physics included mixed-phase for cloud microphysics, Grell's scheme for cumulus parameterization, and RRTM scheme for atmospheric radiation. No shallow convection was activated. The NCEP Eta analysis, NCEP ADP Global Upper Air Observations, and NCEP ADP Global Surface Observations were used for the initial and boundary conditions. The FDDA 3D and surface analysis nudging was applied to temperature, mixing ratio, and wind fields. The sole basis of distinguishing the scenarios by different PBL and their associated LSMs was to attempt to identify the most realistic simulation of land surface and PBL processes since they ultimately affect pollutant reactions and photochemical processes, which in turn, affect air quality.

Table 1. Matrix of MM5 PBL schemes and LSMs.

	Option - A	B	C	D	E
PBL scheme -					
Blackadar	x				
Mellor-Yamada		x			
Hong-Pan			x		
Gayno-Seaman				x	
Pleim-Xiu					x
Soil scheme -					
Five-layer LSM	x			x	
Noah LSM		x	x		
P-X LSM					x

2.2 Emissions

The SMOKE modeling system version 2.1 was used to prepare emissions for CMAQ over the summer and the winter episodes. Five different emission scenarios were produced for each episode with the only difference among the emission scenarios being the MCIP inputs created from the various MM5 data. Essentially, only the MCIP inputs were changed for each emissions scenario in order to determine the impact of different MM5 configurations on a static inventory.

Due to the difference between the projection plane used by VISTAS and the one used by this study, it was necessary to allocate gridding

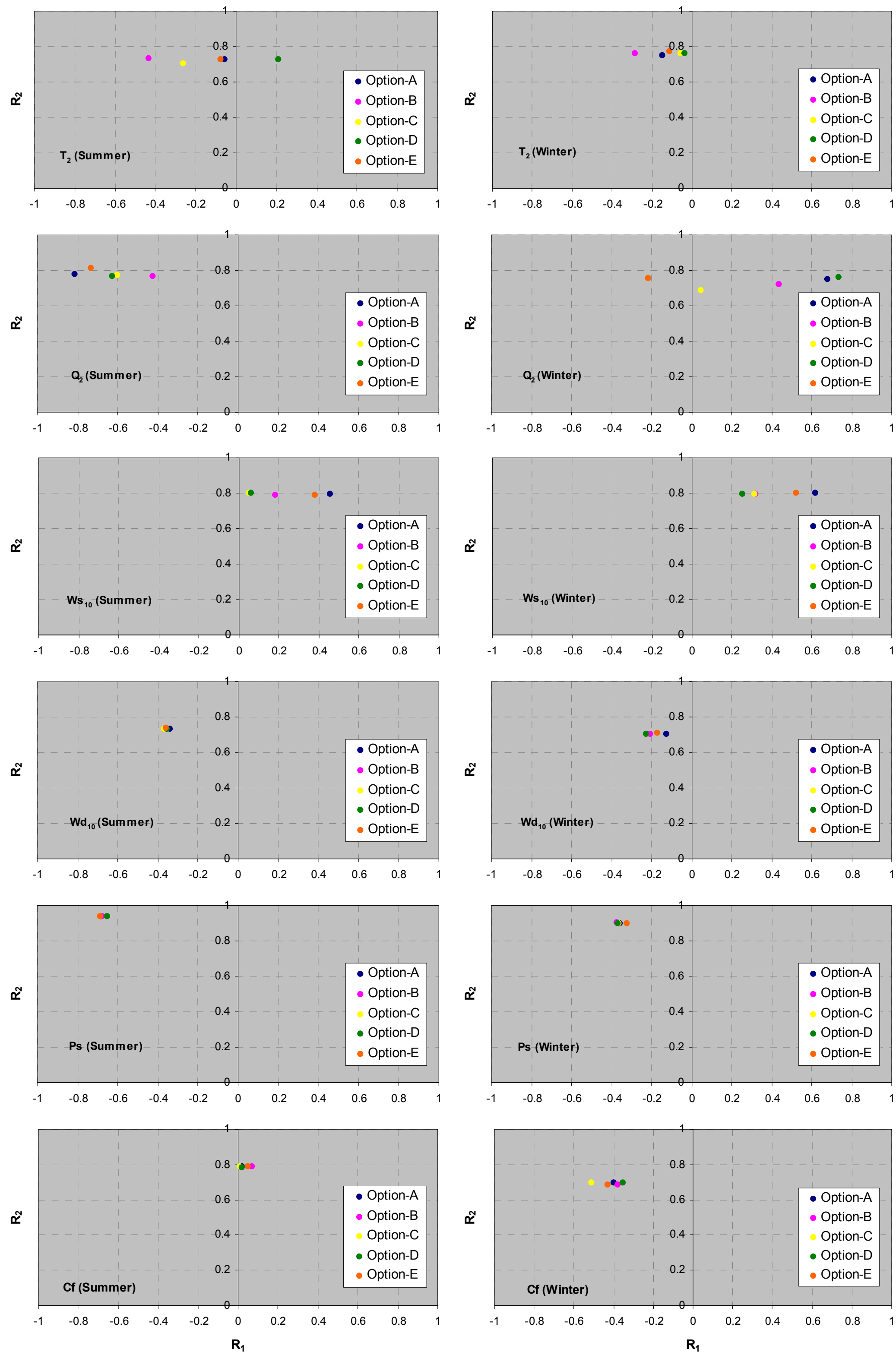

Fig. 1 Aspect ratios of error for MM5 surface variables (from top to bottom): 2-m temperature and mixing ratio, 10-m wind speed and direction, station pressure, and total cloud fraction. The summer period of 2001 is on the left and the winter period of 2002 is on the right.

surrogates and Biogenic Emissions Landuse Database version 3 (BELD3) data to the modeling domain. SMOKE was configured to use the Biogenic Emissions Inventory System version 3.09 to process the reallocated BELD3 data in order to produce the biogenic components that were used in each emissions scenario. Profiles, cross-references, and mobile source inputs were generally those supplied with the VISTAS files with only minor changes to handle the 2001/2002 inventory and episode differences. The SMOKE v2.1 CB-IV speciation profiles were used for inventory pollutant speciation to CMAQ-ready species.

2.3 CMAQ

CMAQ version 4.4, which was released in October 2004, was used for the sensitivity modeling in this study. Aerosol processes and aqueous chemistry were activated. The computationally efficient Euler backward iterative solver was selected for the Carbon Bond-IV gas-phase chemistry mechanism (i.e., cb4_ae3_aq mechanism). The initial concentrations and boundary conditions were created from output concentration files from the VISTAS Phase 1 Regional Haze Modeling. Corresponding meteorological conditions processed by MCIP and the emissions inventories processed by SMOKE were used in each simulation with a seven-day ramp-up period.

2.4 Assessment

The MM5-CMAQ modeling sensitivity to various PBL schemes was assessed through two objective evaluations within the CMAQ domain. The first evaluation compared MM5 model results with observed meteorological data from 50 surface and 21 upper air sounding stations. The second evaluation compared CMAQ modeling results with observed air quality measurements from 2217 monitoring sites. Evaluations were performed for both episodes. A 3-2-1 statistical analysis approach was developed for the sensitivity assessment. It included three basic statistical measures (i.e., bias, absolute error, and root-mean-square error), two aspect ratios of error (i.e., the ratio of bias to absolute error R_1 and the ratio of absolute error to root-mean-square error R_2), and one skill score (i.e., $S = \left(1 - \left| R_1 \right| + R_2\right)/2$). In addition, a fractional bias and a fractional absolute error were introduced in the CMAQ sensitivity analysis.

3. RESULTS

The aspect ratios of error for the 2-m temperature (T_2) and mixing ratio (Q_2), 10-m wind speed (Ws_{10}) and direction (Wd_{10}), station pressure (P_s), and total cloud fraction (C_f) over the summer and winter periods are shown in Fig. 1. There were very little variations of R_2 for T_2. It appeared the Blackadar scheme performed the best in the summer while the Gayno-Seaman scheme did the best in the winter period. Q_2 had the largest spread of R_1 compared with the rest of the variables. The R_2 for Q_2 was around 0.8, and R_1 varied from -0.4 in Mellor-Yamada to -0.8 in Blackadar during the summer period, suggesting that MM5 was relatively dry near the surface with all five PBL schemes. A different performance was observed in Q_2 during the winter period when all the simulations showed a positive R_1 except for the P-X scheme. Although the Hong-Pan scheme resulted in the smallest R_1, it had the lowest R_2, suggesting it had more extreme errors than the other schemes during the winter time. MM5 had a similar performance for 10-m wind speed with all five PBL schemes during the summer and the winter periods. For 10-m wind direction, surface pressure, and total cloud fraction, there were very small differences among all the simulations during each period. The spread of the aspect ratios of error is limited across all five PBL schemes.

A skill score averaged over different variables was calculated to assess the relative model performance (Fig. 2). For the surface variables, it ranged from 0.70 to 0.73 in the summer and 0.69 to 0.75 in the winter - a three percent and a six percent difference between the highest and the lowest scores, respectively. Likewise, the skill score for the 850 mb variables ranged from 0.68 to 0.70 in the summer and 0.72 to 0.74 in the winter, a two percent difference between the highest and the lowest scores. No single PBL scheme led to an extremely good or extremely poor model performance.

Summary of domain-wide CMAQ performance statistics for selected gaseous species O_3, NO_2, NO_x, and SO_2 during the July 2001 period is provided in Table 2. It shows that CMAQ performance was fairly consistent across Option-A through Option-E for each species. For example, the difference between the maximum and minimum performance statistics for O_3 was 2.6 ppb for BIAS, 0.06 for fractional BIAS, 1.42 ppb for ABSE, 0.03 for fractional ABSE, and 1.65 ppb for RMSE. These differences were even smaller during the winter period (not shown). Similar results were also observed for NO_2, NO_x, and SO_2. There was no single PBL scheme in MM5 that resulted in extremely good or poor CMAQ model performance. The skill scores for each species were without significant differences. These were also true for $PM_{2.5}$ (not shown). This suggests the MM5 PBL schemes had little effect on the performance of CMAQ.

Analyses of O_3 and $PM_{2.5}$ were also performed on an urban scale to better understand modeling sensitivity. Fig. 3 shows the simulated and observed hourly O_3 concentrations for Nashville, Tennessee from July 22 through July 24, 2001. The highest O_3 concentration of the month was recorded on July 23. All five simulations reproduced the observed O_3

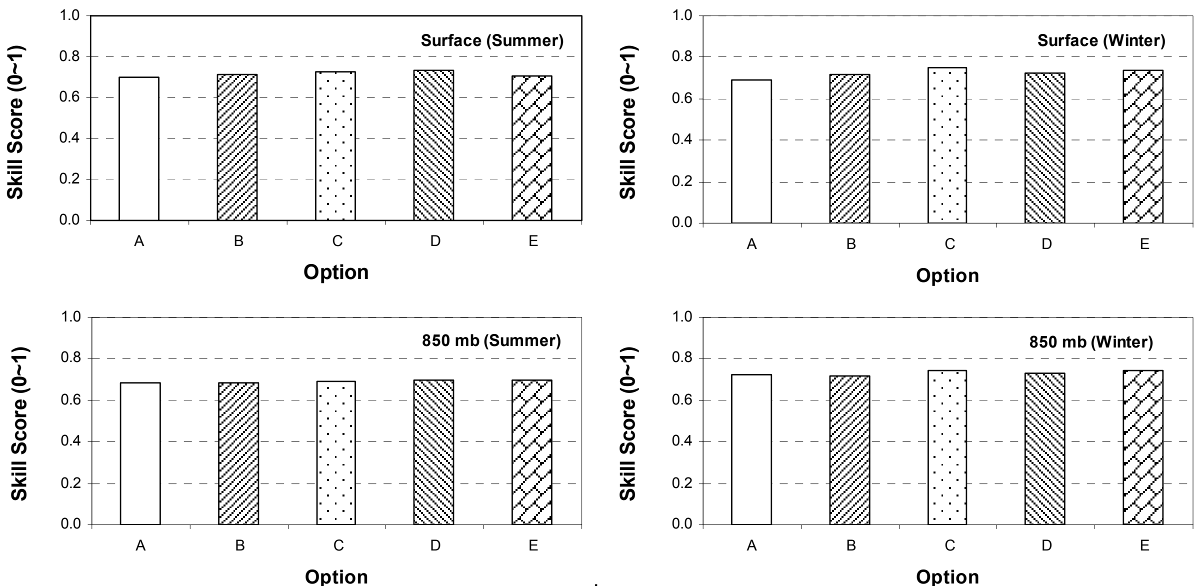

Fig. 2 Average skill scores for the MM5 surface variables during the summer (top left) and the winter (top right), and for the 850 mb variables during the summer (bottom left) and the winter (bottom right).

Table 2. Summary of July 2001 CMAQ performance statistics for hourly average gases species.

Species	Run	BIAS (ppb)	Fractional BIAS	ABSE (ppb)	Fractional ABSE	RMSE (ppb)	Skill Score
O_3	A	8.55	0.34	14.64	0.51	18.56	0.60
O_3	B	7.95	0.32	15.28	0.52	19.56	0.63
O_3	C	8.27	0.32	14.89	0.52	19.01	0.61
O_3	D	8.43	0.33	14.83	0.52	18.93	0.61
O_3	E	10.55	0.38	16.06	0.54	20.21	0.57
NO_2	A	-0.66	-0.04	6.86	0.75	10.14	0.79
NO_2	B	0.31	0.07	7.00	0.72	10.32	0.82
NO_2	C	0.39	0.04	7.28	0.74	10.92	0.81
NO_2	D	-0.11	0.02	6.90	0.73	10.22	0.83
NO_2	E	0.04	-0.01	7.24	0.76	10.81	0.83
NO_X	A	-2.71	-0.05	10.10	0.78	18.64	0.64
NO_X	B	-1.36	0.06	10.49	0.76	19.17	0.71
NO_X	C	-1.39	0.02	10.70	0.78	19.45	0.71
NO_X	D	-2.10	-0.01	10.22	0.77	18.75	0.67
NO_X	E	-2.03	-0.04	10.56	0.80	19.32	0.68
SO_2	A	-0.41	0.42	3.91	1.06	8.62	0.67
SO_2	B	-0.50	0.42	3.89	1.06	8.65	0.66
SO_2	C	-0.43	0.42	3.92	1.06	8.65	0.67
SO_2	D	-0.18	0.47	3.98	1.06	8.62	0.71
SO_2	E	-0.33	0.44	3.96	1.06	8.68	0.69

diurnal cycles reasonably well. The maximum daily O_3 concentrations were simulated better than the nighttime minimums. In fact, CMAQ was persistently positively biased during the night throughout the entire month of July. Perhaps, the most interesting phenomenon was seen in the deviations among the simulations during peak ozone times. For example, for the simulated daily afternoon maximum O_3 concentrations, the largest differences were more than 22 ppb between Option-C and Option-D on July 22, and 14 ppb between Option-B and Option-A on July 23. Fig. 4 shows the time series of simulated and observed daily average $PM_{2.5}$ for Nashville, Tennessee during January 2002. Model behaviors in all five simulations looked similar during the month.

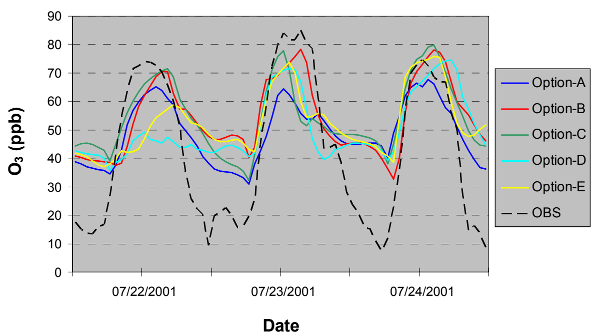

Fig. 3 Simulated and observed hourly ozone values for Nashville, Tennessee during July 22 through July 24, 2001.

4. CONCLUSIONS

Assessment and evaluation of MM5-CMAQ results indicated that both models did not appear to be very sensitive to the five PBL schemes examined in this study. The performances of the models were fairly consistent across all the simulations during the summer and the winter periods. No significant CMAQ sensitivity to the five PBL schemes was observed on domain-wide average for O_3, NO_2, NO_x, SO_2, and $PM_{2.5}$. However, CMAQ did show different responses to the PBLs on an urban scale. Differences in O_3 and $PM_{2.5}$ across the CMAQ simulations were considerable, but no favorable PBL scheme was identified. These results suggest that efforts to improve CMAQ performance solely through investigation of alternative PBL schemes for MM5 are unlikely to be successful and that effort could be more productively directed toward improving other components of the air quality modeling system.

5. ACKNOWLEDGMENTS

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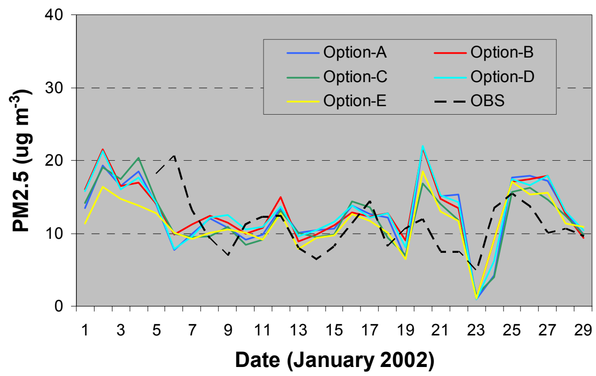

Fig. 4 Simulated and observed daily average $PM_{2.5}$ for Nashville, Tennessee during January 2002.

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