1.7 APPLICATION AND EVALUATION OF MM5 FOR NORTH CAROLINA WITH A 4-KM HORIZONTAL GRID SPACING

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1. INTRODUCTION

Odor, ammonia (NH_3), and other emissions from animal and poultry wastes in Southeast U.S., especially North Carolina (NC), have become a significant problem, owing to the enhanced pork and poultry industry. NH_3 emissions from livestock account for more than 80% of total NH_3 emissions in North Carolina (Wu et al., 2006). The goal of this study is to utilize the U.S. EPA Models-3 Community Multiscale Air Quality (CMAQ) modeling system to simulate the effect of hog and livestock sources in North Carolina on ambient air quality. Temperature, humidity, and the wind parameters are very important in any air quality study as they directly affect the transport and chemistry of species. Thus, accurate meteorological predictions are essential for accurate simulations of ambient air quality. In this study, the meteorological Penn State University /National Center for Atmospheric Research (PSU/NCAR) mesoscale model (known as MM5) model (version 3.7) (Grell et al., 1994) is used to provide the meteorological inputs to CMAQ. MM5 simulations can be conducted with various configurations such as different physical options, different horizontal grid spacing, and with or without nudging. The accuracy in MM5 predictions varies with configurations used. It is, therefore, of interest to test different configurations to identify an optimal setting that provides the most accurate meteorological predictions for a specific episode. This paper studies the influence of nudging and grid resolution on MM5 predictions. The MM5 results with 4- and 12-km horizontal spacing are analyzed and discussed. The 4-km results are based on Wu et al. (2005) and the 12-km results are obtained from the Visibility Improvement State and Tribal Association of the Southeast's (VISTAS) 2002 modeling program (http://www.vista-sesarm.org.asp).

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2. MODELING APPROACH

MM5 model (version 3.7) is a non-hydrostatic primitive equation model using a terrain-following sigma coordinate; it is designed to simulate mesoscale and regional-scale atmospheric circulation (Dudhia et al., 1993). It is widely used to provide the meteorological inputs to drive the air quality models such as the CMAQ model. Since the 12-km simulation results are used as the boundary conditions for the 4-km simulation, the model physics and other configurations for MM5 4-km simulation are kept to be identical to those described in the modeling protocol for the VISTAS Phase II regional haze modeling (Morris and Koo, 2004).

Figure 1 shows the modeling domain. It consists of over 90 sites covering nearly the entire state of North Carolina, and a small portion of several adjacent states such as South Carolina, Georgia, Tennessee, West Virginia, and Virginia. Most of the hog farms in North Carolina are located in the eastern North Carolina, i.e., the coastal plain southeast region of the state.

3. THE EFFECT OF NUDGING ON MM5 PREDICTIONS

3.1 Domain-Wide Analysis

Two simulations are carried out with 4-km grid spacing for August 2002. For the simulation with nudging, 3-D analysis nudging is performed for temperature and moisture aloft, and both 3-D and

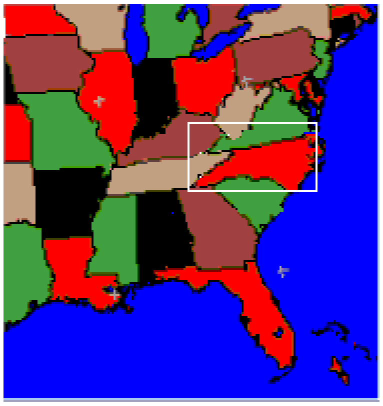

Figure 1. Nested modeling domain with 12- and 4-km horizontal grid spacings.

surface analysis nudging are conducted for wind fields. The observation datasets used in this evaluation are primarily from University Corporation for Atmospheric Research (UCAR)'s ds472.0 TDL archive (http://dss.ucar.edu/datasets/ds472.0/). In analyzing the results, the entire domain is further divided into coastal, rural, and urban regions based on the rural-urban continuum codes established by the Economic Research Service, the United States Department of Agriculture (USDA). Both domain-wide and area-specific statistics are calculated. While the domain-wide statistics give an overall model performance, the area-specific statistics provide insights into each area.

Table 1 summarizes the mean observed and simulated values, and also the performance statistics in terms of the normalized mean bias (NMB) and the normalized mean error (NME) for four meteorological parameters: temperature (T), specific humidity (SH), wind speed (WSP), and wind direction (WDR), for the MM5 simulation with a 4-km grid spacing. The NMB and NME can be calculated using the formulae in Yu et al. (2003) as follows:

$$NMB = \frac{\sum_{i=1}^{N}(M_i - O_i)}{\sum_{i=1}^{N} O_i}.100\% \qquad (1)$$

$$NME = \frac{\sum_{i=1}^{N}|M_i - O_i|}{\sum_{i=1}^{N} O_i}.100\% \qquad (2)$$

where O_i and M_i are the observed and simulated values at a specific time and location i in a given time period or spatial location or both. N is the number of samples (by time and/or locations).

Compared to other variables, the model has a relatively poor performance for T, with underpredictions for both nudging and no-nudging settings (-13% and -14%, respectively). For SH, the model performance is the best among the four meteorological variables, with NMBs of 0.8% and 1.2% for simulations with and without nudging, respectively. For WSP, the nudging simulation gives slightly better predictions than the no-nudging simulation (7.4% vs. 9%). For WDR, the NMBs are -7.9% (nudging) and -11.0% (no-nudging). There is a caveat in the statistical calculation for wind direction. It is a vector; treating it as a scalar variable in its statistical calculation may give misleading results because the numeric differences between simulated and observed WDRs may exceed 180 º (Zhang et al., 2005). The statistics for the u- and v-component of the wind vectors is thus being calculated to evaluate the model predictions of wind fields.

Nudging is the technique that brings the predictions closer to the observations. The primary difference between nudging and no-nudging schemes is the nudging term in the prognostic equation. This term nudges the initial simulated values closer to the observed ones. In general, nudging helps improve the model predictions given dense observational data and an appropriate model grid resolution. For this particular episode, the data used for nudging are not sufficiently dense. This may explain the relatively small differences in overall statistics between simulations with and without nudging at a 4-km grid spacing for this particular episode.

3.2 Area-Specific Analysis

A more detailed analysis is performed by analyzing the statistics in each area type, i.e., coastal, rural, and completely urban for the 4-km simulations. Figure 2 shows the observed vs. simulated hourly temperatures with and without nudging for the month of August at Tri-County Airport, Ahoskie, NC. This site, being representative of the other sites in the rural area also shows the largest differences for temperature predictions. While the model simulations with and without nudging reproduce the peak T values on most days and the nighttime T values on August 4-6, 13, 14, 17, 22, 23, and 28-31. Both simulations fail to reproduce the nighttime T values on some days (e.g., August 7-11 and 19-22). The simulation with nudging gives an overall better agreement with observations on all days. . SH is underpredicted by both simulations especially during daytime, but larger underpredictions occur for the simulation with nudging, as compared with that without nudging. For Ahoskie, the underpredictions of SH occur from August 3 to 6 and on August 26. For WSP and WDR at Ahoskie, predictions by nudging seem to follow the observations better. For WDR, nudging is able to better reproduce the daytime observations, resulting in less underprediction as compared with the simulation with nudging.

Table 2 summarizes the area-specific statistics at the coastal areas, and rural, completely urban and other areas having USDA codes 8-9, 1-2, and 3-7, respectively. Nudging gives better results for WSP than no-nudging for SH (-4% vs. -5%), and WSP (7% vs. 13 %) at coastal sites; T (0.8% vs. 2.4%), WSP (23% vs. 28%), and WDR (-9.4% vs. -12.1%) at rural sites, and WDR (-6.6% to -11.2%) at urban sites. Compared with the domain-wide statistics, the differences in area-specific statistics between nudging and no-nudging are generally more pronounced for WSP in non-urban areas, WDR in urban areas, T in rural areas, and SH in coastal areas. The feedbacks between observations and predictions through nudging likely improve the predicted values in areas with denser observational dataset and better topographical details. These feedbacks affect the chemical predictions that depend on meteorological parameters.

A possible reason for the difference between the overall and area-specific sites is the averaging of the parameters over the complete domain, whereas in the area-specific domain, factors such as land-surface, topography, and proximity to the sea make a significant difference. This can be clearly shown in certain parameters and regions, e.g., SH in coastal areas. While the overall domain-wide SH is underpredicted by 1.2% and 0.8% by nudging and no-nudging respectively, it is underpredicted by 4% and 5%, respectively, for coastal areas.

4. SENSITIVITY TO GRID RESOLUTIONS

To evaluate the effect of grid resolutions on model predictions, the model results with the 4- and 12-km horizontal grid spacings are compared and analyzed. Figure 3 (a) to (d) show observed and simulated daily-average T, SH, WSP, and WDR, respectively, at Ahoskie, NC. Due to errors in initialization for the first three days for the 12-km simulation, predictions from August 1-3 for both simulations are therefore not included in these Figures. The observed daily average T values are generally reproduced well with both simulations (within 6%). The model results with both 4- and 12-km grid spacings slightly underpredict the observational daily-average SH values for most days. For August 4-31, the predicted SH values with the 12-km grid spacing give better agreement with observations for 16 days, overpredicting it on August 20, and 24. The simulated values with a 4-km domain are lower than 12-km predictions for most days except August 5, 11, 15, 19, 21-22, 26-28, and 31. WSP is overpredicted by the simulation with the 12- and 4-km grid spacings on all days. The 12-km simulation compared with the 4-km prediction, overpredicts on all the days except August 8, 11, 13, 14, 16, 23, and 27-30. The significant difference between the observed values and predictions of WDR on August 10, 20, 23, 25, 29 could be due to the caveat in the calculation of the wind direction mentioned previously. For example, on August 29, when the observed WDR is around 350^o, the predicted values are in the range of 10^o-20^o. The numeric differences range from 330^o-340^o but the actual differences are 20^o-30^o.

Overall statistics and area-specific statistics at the two grid resolutions are calculated for further analyses. Table 3 compares the overall statistical performance of MM5 simulations with nudging and with both 12- and 4-km grid spacings. The wind parameters are better predicted with the 12-km simulation and T and SH are better predicted with the 4-km simulation. These differences can be attributed to several factors. First, 3-D and surface nudging of winds performs better at the 12-km resolution. This is likely because the observational winds are more suitable for 12-km resolution than for 4-km resolution. The observational T and SH used for their 3-D nudging, on the other hand, performs better with a finer resolution. Second, the meteorological schemes in MM5 may be sensitive to the grid resolution used. For example, Mass et al. (2002) showed that there is an apparent overprediction of wind parameters when the resolution increased from 12km to 4 km.

Table 4 compares the area-specific statistics at the coastal, rural, completely urban and other areas for the 12- and 4-km grid spacings. Note that the statistics for 4-km predictions with nudging in Table 4 are somewhat different from those in Table 1. This is due to the fact that the predictions from August 1-3 for both the 4- and 12-km simulations are not included for the statistical calculation in Table 4 (They are included in Table 1) for the reason mentioned previously. The temperatures are well predicted with both grid spacings, with a similar performance. For SH, the results from the 4-km simulation are slightly better for all areas that those from the 12-km simulation (with NMBs of 0 to -4% vs. -3.6 to -6%, respectively). For WSP, the model performance with a 4-km grid spacing is also generally better than that with a 12-km grid spacing except for other areas with the USDA code 3-7. The corresponding NMBs for 4-km vs. 12-km simulations are 14.0% vs. 15%, 23.9% vs. 30.4%, and 3.2% vs. 3.9%, for coastal, rural and urban areas, respectively. A more detailed topography structure is possible for the simulation with a 4-km resolution. This could be one factor for better predictions with a 4-km grid spacing as smaller scale feature-specific motions such as lee winds are incorporated in the model. Lacking of a complete meteorological dataset, however, could affect the statistical evaluation of the simulation with a 4-km grid spacing in a negative way. This would affect the analysis nudging scheme as well, where the difference between the observed and the simulated values on a grid is used to calculate the nudging term. The statistics for WDR suggest that the 12-km predictions give better results for all areas than the 4-km predictions, particularly in rural areas with NMB of 0.8% vs. –8.1%. This is because the number of days of overpredictions and underpredictions for the 12-km predictions is about the same (roughly 10 days each), resulting in a small net bias; whereas a consistent underprediction occurs for most days in the case of the 4-km simulation.

5. IMPACT ON AIR QUALITY MODEL

The impact of the meteorological predictions on modeling air quality is studied. The accuracy of predictions strongly depend on the accuracies of model inputs (e.g., emissions) and physics (e.g., meteorological schemes). Figure 4 shows the relation between the concentrations of black carbon (BC) and the values of WSPs predicted at a 4-km grid spacing at Asheville airport, NC. The 4-km simulation underpredicts observed BC concentrations by 25-50% on August 2, 7, 17, and 22 and underpredicts by 40% on August 12**.** A roughly anti-correlation between WSPs and the concentrations of BC exists; with the peaks in WSPs corresponding to the dips in BC concentrations. This is because BC is a primary PM species that is emitted from various sources; once emitted, it is affected primarily by meteorological and removal processes. At source regions, lower WSPs lead to an accumulation of the pollutant and an increase in its concentration, whereas higher WSPs transport the pollutants out of the region, thus resulting in the dips in BC concentrations.

6. SUMMARY

The MM5 simulation results for August 2002 with 4- and 12-km with and without nudging are evaluated. The analyses of hourly and daily predictions show that the MM5 simulation with nudging gives better agreement for nighttime temperature predictions at all locations throughout the simulation period, although the simulation without nudging give a slightly better overall prediction in terms of NMB. The SH predictions between nudge and no-nudging simulations over the whole domain are similar. Both WSP and WDR are slightly better predicted with nudging . The differences in overall domain-wide statistics in MM5 predictions with and without nudging are relatively small (up to 3% in NMBs) but the differences in the area-specific statistics may be as high as 6%. Nudging may help improve model predictions of some meteorological variables such as wind speed, wind direction, and specific humidity in coastal area, wind speed/direction and temperature in rural area, wind speed/directions and humidity in coastal area.

The model simulation with a 4-km grid spacing generally gives better results than those with a 12-km grid spacing except for wind direction in the coastal and rural areas and temperature in coastal area. The overall results show that 12-km simulation gives better results for the wind parameters, whereas the 4-km T and SH predictions are closer to the observed values.

The predictions of several key air pollutants such as BC, CO, O_3, and $PM_{2.5}$ with 4- and 12-km grid spacings will be compared to assess the sensitivity of CMAQ to different grid resolutions. The CMAQ predictions will be analyzed to investigate the influence of meteorological parameters on the formation and transport of NH_3 in North Carolina. In addition, a MM5 simulation with a time resolution less than one-hour will be conducted. The results will be analyzed to study the effect of the time resolution on the model meteorological and chemical predictions.

7. ACKNOWLEDGEMENTS

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Table 1. Overall model performance statistics for the August 2002 simulations with a 4-km grid spacing.

Overall	T		SH		WSP		WDR	
	Nudge	No Nudge	Nudge	No Nudge	Nudge	No Nudge	Nudge	No Nudge
Obs	25.3	25.3	14.4	14.4	3.1	3.1	152.7	152.7
Sim	21.8	22	14.3	14.3	3.3	3.3	140.6	136.2
Data pair	62898	62898	56872	56872	38826	38826	38826	38826
NMB,%	-14.0	-13.0	-1.2	-0.8	7.4	9.0	-7.9	-11.0
NME,%	19.0	22.0	10.6	10.2	35.0	37.0	35.0	38.0

Table 2. Area-specific model performance statistics for the August 2002 simulations with a 4-km grid spacing.

	T		SH		WSP		WDR	
Coastal	Nudge	No Nudge	Nudge	No Nudge	Nudge	No Nudge	Nudge	No Nudge
Obs	27.4	27.4	16.1	16.1	3.8	3.8	151	151
Sim	26.9	27.2	15.5	15.3	4.1	4.3	145.8	146.4
Data pair	5129	5129	5127	5127	4184	4184	4183	4183
NMB,%	-2.0	-1.0	-4.0	-5.0	7.0	13.0	-3.4	-3.1
NME,%	5.7	6.6	9.4	9.4	34.0	37.0	27.8	30.6
Rural								
Obs	24.6	24.6	14.2	14.2	2.4	2.4	174.4	174.4
Sim	24.8	25.2	13.6	13.6	3	3.1	158	153.3
Data pair	3247	3247	2947	2947	1149	1149	1149	1149
NMB,%	0.8	2.4	-4.1	-3.7	23.0	28.0	-9.4	-12.1
NME,%	7.3	8.4	11.2	11.1	45.0	48.0	37.3	39.9
Urban								
Obs	26.6	26.6	14.4	14.4	3.3	3.3	148	148
Sim	26.5	26.7	14.3	14.4	3.2	3.3	138.2	131.4
Data pair	18379	18379	17613	17613	11635	11635	11635	11635
NMB,%	0.0	0.1	-0.4	0.4	-2.0	-1.0	-6.6	-11.2
NME,%	5.9	7.7	10.6	9.9	31.0	33.0	36.3	39.4
Other								
Obs	30.4	30.4	14.3	14.3	2.9	2.9	155.3	155.3
Sim	30.4	30.7	14.1	14.2	3.2	3.2	143.1	138.9
Data pair	35379	35379	30442	30442	21289	21289	21289	21289
NMB,%	0.0	0.8	-1.1	-0.7	7.5	9.7	-7.9	-10.5
NME,%	5.2	6.8	11.0	10.5	34.7	36.9	35.0	37.3

Table 3. Overall model performance comparison statistics for the August 2002 simulations with 12- and 4-km grid spacings.

Overall	T		SH		WSP		WDR	
	12-km	4-km	12-km	4-km	12-km	4-km	12-km	4-km
Obs	24.8	24.8	14.3	14.3	3.1	3.1	155.2	155.2
Sim	25.1	24.9	13.8	14.3	3.3	3.3	152.3	143.7
Data pair	38678	38678	50500	50500	35370	35370	35369	35369
NMB,%	1.3	0.4	-4.0	-0.6	7.0	8.8	-1.8	-7.4
NME,%	6.5	7.9	11.9	10.2	35.5	35.8	35.0	34.6

Table 4. Area-specific statistics of the meteorological predictions for the August 2002 simulations with 4- and 12-km grid spacings.

Coastal	T		SH		WSP		WDR	
	12-km	4-km	12-km	4-km	12-km	4-km	12-km	4-km
Obs	26.2	26.2	16.1	16.1	3.7	3.7	153.8	153.8
Sim	25.9	25.8	15.3	15.5	4.3	4.2	151.7	148.8
Data pair	4622	4622	4622	4622	3858	3858	3858	3858
NMB,%	-1.0	-2.0	-5.0	-4.0	15.0	14.0	-1.0	-3.0
NME,%	6.0	6.0	10.0	9.0	38.0	37.0	31.0	27.0
Rural								
Obs	23.4	23.4	14	14	2.4	2.4	175.2	175.2
Sim	23.6	23.5	13.1	13.5	3.2	3	176.6	161
Data pair	2887	2887	2587	2587	1053	1053	1053	1053
NMB,%	0.8	0.5	-6.0	-4.0	30.4	23.9	0.8	-8.1
NME,%	7.1	7.6	12.0	10.9	50.0	45.1	40.3	36.9
Urban								
Obs	26.6	26.6	14.3	14.3	3.1	3.1	149.2	149.2
Sim	27.6	26.4	13.7	14.3	3.2	3.2	147.5	142
Data pair	16603	16603	15912	15912	10719	10719	10719	10719
NMB,%	0.1	0.0	-4.2	0.0	3.9	3.2	-1.1	-4.8
NME,%	0.6	0.5	12.0	10.4	33.9	33.0	36.6	34.5
Other								
Obs	24.7	24.7	14.1	14.1	3	3	157.6	157.6
Sim	25.2	24.7	13.6	14.1	3.1	3.2	153.7	147.3
Data pair	31170	31170	27383	27383	19740	19740	19740	19740
NMB,%	1.7	-0.2	-3.6	-0.3	5.6	7.6	-2.5	-6.5
NME,%	6.5	6.4	12.1	10.8	35.2	34.7	34.7	33.9

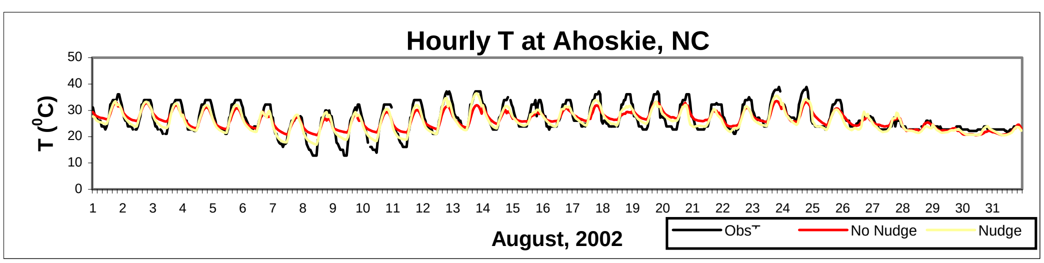

Figure 2. Observed vs. simulated hourly T at a 4-km grid spacing with and without nudging at Tri-County, Ahoskie, NC, during August 2002.

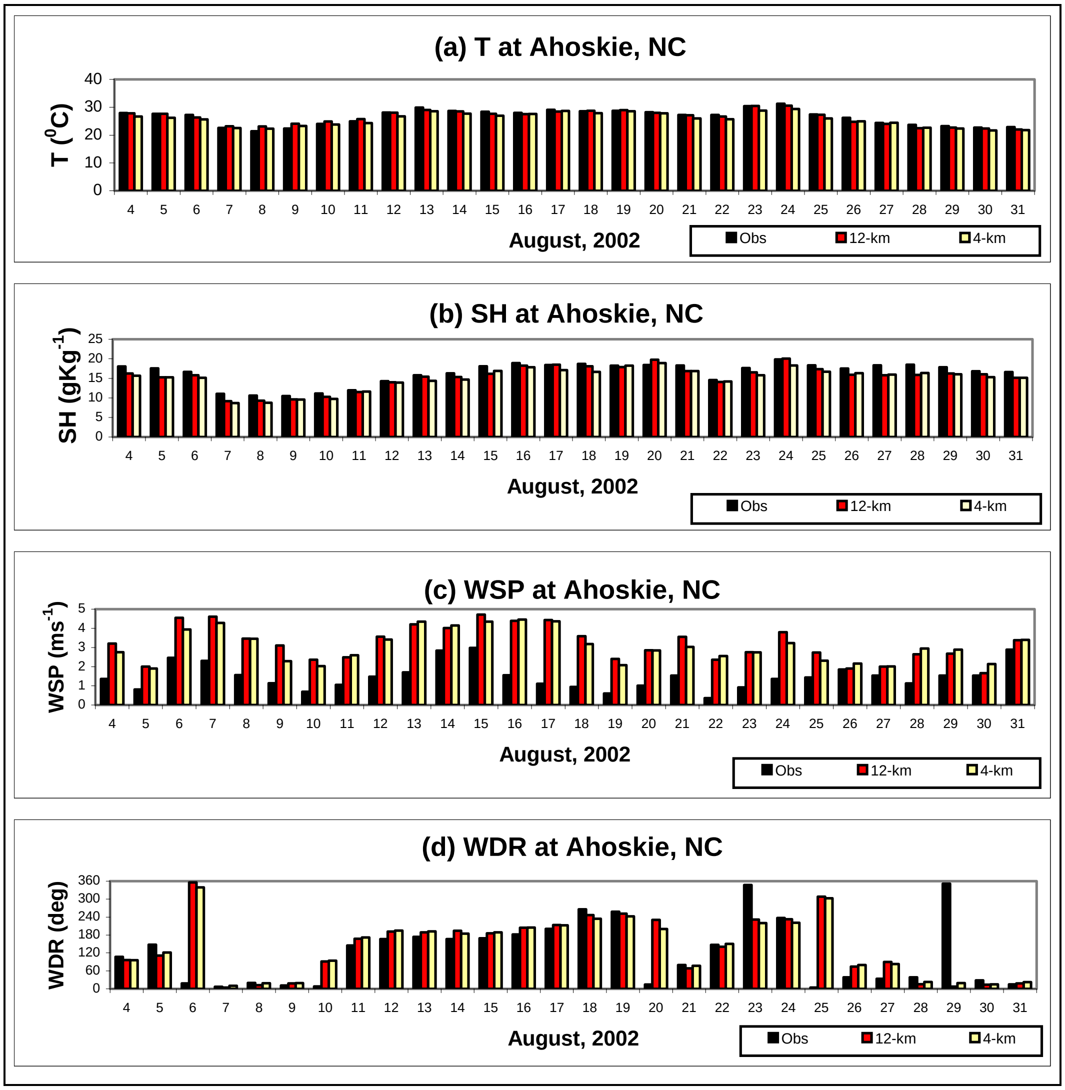

Figure 3. The observed and simulated daily-average (a) T, (b) SH, (c) WSP, and (d) WDR with 4- and 12-km horizontal grid spacings at Tri-County, Ahoskie, NC, in August 2002. The data on August 1-3 are excluded because of errors in initialization in the 12-km simulation.

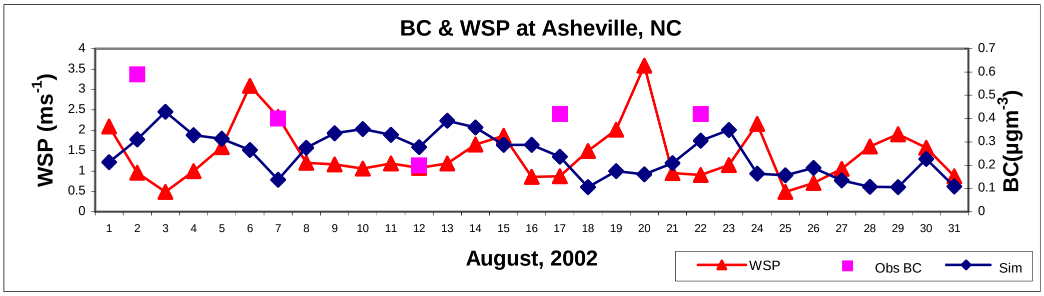

Figure 4. The observed and simulated daily-average BC concentrations and the simulated WSP at a 4-km grid spacing at Asheville Airport, NC, during August 2002.