

Supplementary data published online for the paper entitled:

Responses of Future Air Quality to Emission Controls over North Carolina, Part I: Model Evaluation for Current-Year Simulations

Xiao-Huan Liu^{1,2}, Yang Zhang^{1,*}, Kristen M. Olsen¹, Wen-Xing Wang², Bebhinn A. Do³, and George M. Bridgers³

¹ Department of Marine, Earth, and Atmospheric Sciences, North Carolina State University, Raleigh, NC 27695, USA

² Environment Research Institute, Shandong University, 27 Shanda Nanlu, Jinan, Shandong Province, P.R China 250100

³ Division of Air Quality, North Carolina Department of Environment and Natural Resources, Raleigh, NC 27699, USA

1. Description of “actual” and “typical” emissions used in model simulations

The 2002 actual emission inventories were developed base on the U.S. EPA’s 1999 National Emission Inventory (NEI), Version 2 Final (NEI99V2) and recent updates from VISTAS/ASIP states. The 2002 typical emission inventories were developed to avoid anomalies in emissions due to variability in economic, meteorology, and outage factors in 2002. The differences between 2002 actual and typical emission inventories are the fire and EGUs emissions. While actual emission scenarios used 2002 day-specific fire emissions and continuous emissions monitoring data for EGUs, the 2002 typical EGUs and fire emissions were based on the 2000-2004 average to avoid atypical EGU outages and fire activities in 2002 (Morris et al., 2007; Barnard and Sabo, 2008). Projected emissions were generated for each source category to account for control scenarios under the promulgated and proposed control programs at the national, state, and local levels. In 2009 and 2018, the projected emission reductions from their levels in 2002 in NC are 19.7% and 32.6% for carbon monoxide (CO), 35.4% and 56.2% for nitrogen oxide (NO_x), 46.3% and 68.0% for sulfur dioxide (SO₂), and 24.8% and 35.1% for volatile organic compounds (VOCs), respectively.

2. Locations and names of observational sites within the modeling domain

Figures S-1 to S-4 show the locations of sites for meteorological, O₃, PM_{2.5}, and wet deposition measurements within the modeling domain. Tables S-1 to S-4 provide the full names and coordinates of these sites. Figure S-5 shows the three physiographic regions in North Carolina.

* Corresponding author. Yang Zhang, Tel: +1 919 515 9688; fax: +1 919 515 7802.
Email address: yang_zhang@ncsu.edu

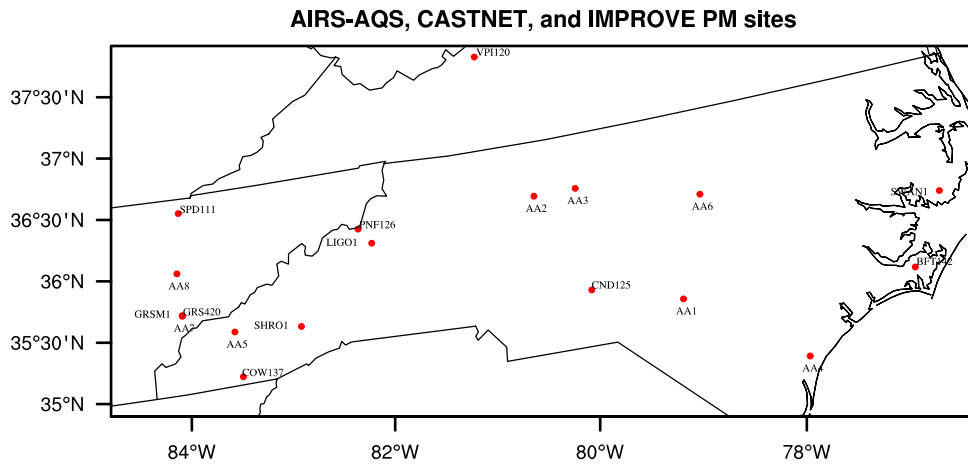


Figure S-3. The locations of sites for PM_{2.5} and its component measurements in the networks of AIRS-AQS, CASTNET, and IMPROVE. Note that the STN sites are included as part of the AIRS-AQS. Note that the four IMPROVE sites (GRSM1, LIGO1, SHRO1, SWAN1) are also the sites for visibility measurements. See the full names of all sites in Table S-3.

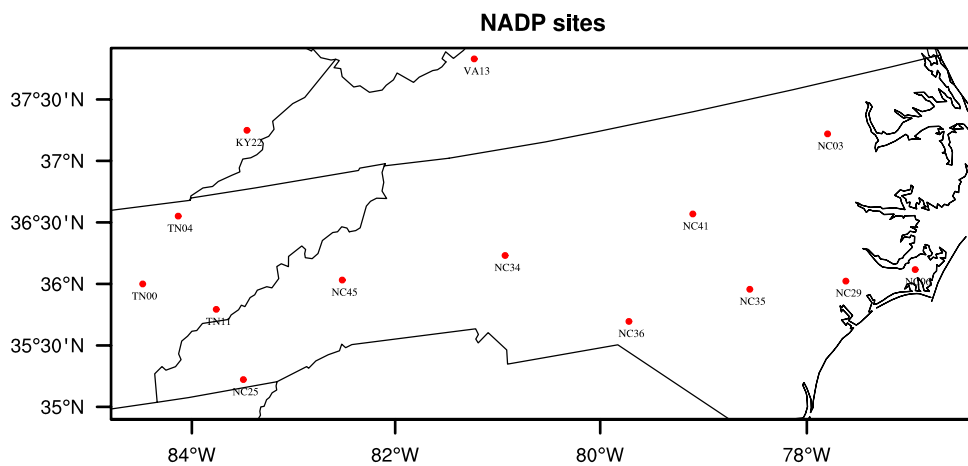


Figure S-4. The locations of wet deposition measurement sites in the NADP network. See the full names of all sites in Table S-4.

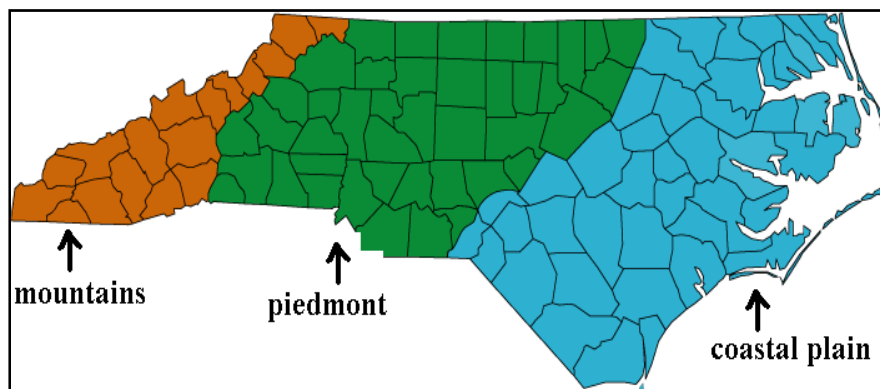


Figure S-5. The three physiographic regions in North Carolina.

Table S-1. The meteorological measurement sites from CASTNET and SCO.

CASTNET Meteorological Sites

No.	Site Code	Full Name	Site Coordinate
1	PNF126	Cranberry	(36.1058, -82.0454)
2	BFT142	Beaufort	(34.8848, -76.6203)
3	COW137	Coweeta	(35.0608, -83.4305)
4	SPD111	Speedwell	(36.47, -83.8268)
5	VPI120	Horton Station	(37.3297, -80.5578)
6	GRS420	Great Smoky NP – Look Rock	(35.631, -83.942)
7	CND125	Candor	(35.2632, -79.8365)

SCO Meteorological Sites

No.	Site Code	Full Name	Site Coordinate
1	KAKH	Gastonia Municipal Airport	(35.2, -81.15)
2	KAVL	Asheville Regional Airport	(35.4333, -82.55)
3	KBCB	Blacksburg	(37.22, -80.42)
4	KCLT	Douglas International Airport	(35.2133, -80.9486)
5	KDPL	Duplin County	(35, -77.98)
6	KEQY	Monroe	(35.0199, -80.6203)
7	KEWN	Mount Mitchell State Park	(35.0833, -77.05)
8	KEXX	Davidson County	(35.78, -80.3)
9	KFAY	Fayetteville	(35, -78.8833)
10	KFBG	Simmons Army Airfield	(35, -78.8833)
11	KFQD	Rutherford County	(35.43, -81.94)
12	KGSB	Seymour Johnson	(42.8833, -85.5167)
13	KGSO	Greensboro	(36.0833, -79.95)
14	KGWW	Goldsboro-Wayne Municipal	(33.5, -90.0833)
15	KHBI	Asheboro Municipal	(35.66, -79.9)
16	KHFF	Mackall U.S. Army Airfield	(41.7333, -72.65)
17	KHKY	Hickory	(35.75, -81.3833)
18	KHRJ	Harnett County	(35.38, -78.74)
19	KIGX	Chapel Hill-Williams	(35.935, -79.0658)
20	KINT	Smith Reynolds	(36.1333, -80.2333)
21	KIPJ	Lincoln County	(35.48, -81.16)
22	KISO	Stallings AFB	(35.3167, -77.6333)
23	KJNX	Johnston County	(35.54, -78.38)
24	KJQF	Sampson County	(35.38, -80.71)
25	KLBT	Lumberton Municipal	(34.6, -79.07)
26	KMEB	Laurinburg-Maxton	(34.7914, -79.3681)
27	KMRH	Beaufort Smith Field	(34.7325, -76.6569)
28	KMRN	Morganton / Lenoir	(35.82, -81.61)
29	KMWK	Surry County	(36.46, -80.55)
30	KNKT	Cherry Point MCAS	(34.85, -76.8833)
31	KOAJ	Albert Ellis	(34.8167, -77.6167)
32	KOQT	Memphis International Ap	(36.02, -84.23)
33	KPGV	Pitt / Greenville	(35.63, -77.4)
34	KPOB	Pope AFB	(40.92, -88.63)
35	KPSK	Dublin/New River Valley	(37.13, -80.68)
36	KRDU	Raleigh-Durham	(35.8667, -78.7833)
37	KRHP	Andrews-Murphy	(35.1944, -83.8647)
38	KSOP	Moore County	(35.23, -79.4)
39	KSVH	Statesville Municipal	(35.76, -80.96)
40	KTNB	Boone-Watauga Hospital	(36.2, -81.65)
41	KTYS	Hatteras Weather Service Office	(35.8167, -83.9833)
42	KUZA	Rock Hill-York County	(34.98, -81.06)
43	KVUJ	Stanly County Airport	(35.42, -80.15)

Table S-2. The O₃ measurement sites from CASTNET and AIRS-AQS.

CASTNET O₃ Sites

No.	Site Code	Full Name	Site Coordinate
1	PNF126	Cranberry	(36.1058, -82.0454)
2	BFT142	Beaufort	(34.8848, -76.6203)
3	COW137	Coweeta	(35.0608, -83.4305)
4	SPD111	Speedwell	(36.47, -83.8268)
5	VPI120	Horton Station	(37.3297, -80.5578)
6	GRS420	Great Smoky NP – Look Rock	(35.631, -83.942)
7	CND125	Candor	(35.2632, -79.8365)

AIRS-AQS O₃ Sites

No.	Short Site Code*	Full Site Code*	Site Coordinate
1	A1	132130003	(34.785,-84.6269)
2	A2	210130002	(36.6081,-83.7369)
3	A3	211130001	(37.8933,-84.5892)
4	A4	211930003	(37.2831,-83.2203)
5	A5	211950002	(37.4828,-82.5353)
6	A6	370030003	(35.9036,-81.1842)
7	A7	211990003	(37.0975,-84.6117)
8	A8	370210030	(35.5,-82.6)
9	A9	370110002	(35.9717,-81.9342)
10	A10	370270003	(35.9358,-81.5303)
11	A11	370330001	(36.307,-79.4674)
12	A12	370510008	(35.1587,-78.728)
13	A13	370370004	(35.7572,-79.1597)
14	A14	370511003	(34.9689,-78.9625)
15	A15	370590002	(35.8093,-80.5591)
16	A16	370610002	(34.9548,-77.9608)
17	A17	370630013	(36.0356,-78.9042)
18	A18	370650099	(35.9883,-77.5828)
19	A19	370670022	(36.1106,-80.2267)
20	A20	370670028	(36.2031,-80.2158)
21	A21	370670027	(36.2364,-80.4106)
22	A22	370671008	(36.0508,-80.1439)
23	A23	370690001	(36.0962,-78.4637)
24	A24	370810011	(36.1133,-79.7039)
25	A25	370770001	(36.1411,-78.7681)
26	A26	370870035	(35.3792,-82.7925)
27	A27	370870004	(35.5053,-82.9647)
28	A28	370990005	(35.5244,-83.2361)
29	A29	370870036	(35.59,-83.0775)
30	A30	371070004	(35.2315,-77.5688)
31	A31	371010002	(35.5908,-78.4619)
32	A32	371090004	(35.4386,-81.2767)
33	A33	371170001	(35.8107,-76.8978)
34	A34	371191005	(35.1131,-80.9197)
35	A35	371190041	(35.2403,-80.7856)
36	A36	371191009	(35.3486,-80.6936)
37	A37	371450003	(36.307,-79.092)
38	A38	371310002	(36.4844,-77.62)
39	A39	371470099	(35.5833,-77.5989)
40	A40	371510004	(35.8306,-79.8653)

AIRS-AQS O₃ Sites (continued)

No.	Short Site Code*	Full Site Code*	Site Coordinate
41	A41	371590021	(35.5519,-80.395)
42	A42	371570099	(36.3089,-79.8592)
43	A43	371730002	(35.4355,-83.4437)
44	A44	371590022	(35.5345,-80.6676)
45	A45	371790003	(34.9739,-80.5408)
46	A46	371830014	(35.8561,-78.5742)
47	A47	371830016	(35.5969,-78.7925)
48	A48	371830015	(35.79,-78.6197)
49	A49	371830017	(35.6764,-78.5353)
50	A50	371990003	(35.7377,-82.2852)
51	A51	450070003	(34.775,-82.4903)
52	A52	450230002	(34.7925,-81.2036)
53	A53	450210002	(35.1303,-81.8164)
54	A54	450770002	(34.6861,-82.8387)
55	A55	450730001	(34.805,-83.2375)
56	A56	450830009	(34.9886,-82.0756)
57	A57	450910006	(34.9356,-81.2283)
58	A58	470090101	(35.6314,-83.9436)
59	A59	470010101	(35.965,-84.2233)
60	A60	470090102	(35.6031,-83.7836)
61	A61	470630003	(36.3078,-83.1345)
62	A62	470650028	(35.0764,-85.1517)
63	A63	470651011	(35.1403,-85.17)
64	A64	470930021	(36.0847,-83.7647)
65	A65	470890002	(36.1144,-83.6011)
66	A66	471210104	(35.2889,-84.9461)
67	A67	470931020	(36.0194,-83.8736)
68	A68	471550101	(35.6967,-83.6097)
69	A69	471550102	(35.5628,-83.4981)
70	A70	471632002	(36.5411,-82.4261)
71	A71	471632003	(36.5822,-82.4858)
72	A72	511611004	(37.2856,-79.8842)
73	A73	518000005	(36.6675,-76.7314)

* The O₃ sites in the AIRS-AQS network are given as 9-digit site codes such as 132130003. No full site names are provided. The short site codes such as A1 are used in the map, as the full site codes are too long to be included in the site map.

Table S-3. The sites for PM_{2.5} and its component measurements from AIRS-AQS, CASTNET, and IMPROVE.AIRS-AQS PM_{2.5} Sites

No.	Short Site Code*	Full Site Code*	Site Coordinate
1	AA2	370510009	(35.041, -78.953)
2	AA3	370670022	(36.111, -80.227)
3	AA4	370810013	(36.109, -79.801)
4	AA5	371290002	(34.364, -77.839)
5	AA6	371730002	(35.436, -83.444)
6	AA7	371830014	(35.856, -78.574)
7	AA8	470931013	(35.981, -83.933)
8	AA9	470090101	(35.631, -83.944)

* The PM_{2.5} sites in the AIRS-AQS network are given as 9-digit site codes such as 130890002. No full site names are provided. The short site codes such as AA1 are used in the map to be consistent with the AIRS-AQS site map for O₃.

CASTNET Speciated PM_{2.5} Sites*

No.	Site Code	Full Name	Site Coordinate
1	PNF126	Cranberry	(36.1058, -82.0454)
2	BFT142	Beaufort	(34.8848, -76.6203)
3	COW137	Coweeta	(35.0608, -83.4305)
4	SPD111	Speedwell	(36.47, -83.8268)
5	VPI120	Horton Station	(37.3297, -80.5578)
6	GRS420	Great Smoky NP – Look Rock	(35.631, -83.942)
7	CND125	Candor	(35.2632, -79.8365)

* CASTNET speciated PM_{2.5} include sulfate, nitrate, and ammonium.

IMPROVE PM_{2.5} and Visibility Sites

No.	Site Code	Full Name	Site Coordinate
1	GRSM1	Great Smoky Mountains	(35.6334, -83.9416)
2	LIGO1	Linville Gorge	(35.9721, -81.9331)
3	SHRO1	Shining Rock WA	(35.3936, -82.7743)
4	SWAN1	Swanquarter	(35.4509, -76.2074)

Table S-4. The locations of wet deposition measurement sites in the NADP network.

No.	Site Code	Full Name	Site Coordinate
1	KY22	Lilley Cornett Woods	(37.0778, -82.9936)
2	NC03	Lewiston	(36.1325, -77.1714)
3	NC06	Beaufort	(34.8845, -76.6214)
4	NC25	Coweeta	(35.0605, -83.4305)
5	NC29	Hofmann Forest	(34.9206, -77.3227)
6	NC34	Piedmont Research Station	(35.697, -80.6225)
7	NC35	Clinton Crops Research Station	(35.0258, -78.2783)
8	NC36	Jordan Creek	(34.9708, -79.5283)
9	NC41	Finley Farm	(35.7283, -78.6803)
10	NC45	Mt. Mitchell	(35.7353, -82.2861)
11	TN00	Walker Branch Watershed	(35.9614, -84.2872)
12	TN04	Speedwell	(36.4692, -83.8272)
13	TN11	Great Smoky Mountains National Park-ElkmonT	(35.6645, -83.5903)
14	VA13	Horton's Station	(37.3314, -80.5575)

3. Evaluation of meteorological predictions

Figures S-6 and S-7 in the supplementary data show spatial distributions of simulated monthly-mean T1.5, RH1.5, WSP10, and WDR10, and hourly precipitation with observations overlaid in January and July, respectively, 2002. The analysis of these figures is provided in the main text of the paper.

Figure S-8 shows temporal variations of simulated T1.5, RH1.5, WSP10, and WDR10 from 4-km and 12-km simulations and the observations at one SCO site (i.e., the Raleigh-Durham

Airport site) and four CASTNET sites (i.e., Cranberry, Beaufort, Speedwell, and Candor). Beaufort is a coastal site, Cranberry is a mountain site with an elevation of 1219 m, Speedwell is a rural site located at the west side of Appalachian Mountains, and Candor and Raleigh-Durham Airport are located in the Piedmont area, representing urban and rural areas, respectively. MM5 at 12-km captures the temporal variations and magnitudes of T1.5 on most days in both months, although cold biases mostly occur during daytime. The heavy snow that occurred in NC during 2-4 January started to melt on 5 January and completely disappeared after 9 January. While the simulated temporal variations of T1.5 at 4-km are consistent with those at 12-km at all sites except for Candor and Raleigh, it gives a snow cover persistently presented during 8-12 January over the central NC, resulting in significantly lower T1.5 values than those observed and from the 12-km simulations at Candor and Raleigh. This may indicate some limitations of the snow melting treatment in the MM5/PX-LSM that gives a slower snow melt, resulting in higher snow cover and lower temperature and precipitation over this particular region at 4-km. As indicated in Gilliam et al. (2007), due to limited snow and surface energy balance representation, PX-LSM does not perform as well as other LSMs over snow surfaces such as the NOAH LSM, with the latter still having some limitations such as a faster snow melt, as compared with other LSMs with more sophisticated snow physics. Such a limitation at 4-km also indicates a need for more sophisticated snow representations with a more realistic snow pack evolution, sub-grid scale variability, vegetation interactions, and blowing snow to improve current model capability in simulating snow. At the two mountain sites (i.e., Cranberry and Speedwell), the 4-km simulation gives better agreement with observed T1.5 than the 12-km simulation during 8-12 January, indicating less accurate the snow melt/pack treatments over the mountain regions at 12-km. MM5 generally captures RH1.5 variations with similar temporal variation trends at 4- and 12-km (except for 8-12 January at Candor and Raleigh due to abnormal T1.5 predictions). Some underpredictions occur at both grid

resolutions at most sites during some days in January and most days in July. WSP10 is overpredicted on most days at most sites in both months, especially in the coastal plain and mountain areas. The 12-km simulation gives slightly better results than 4-km at Cranberry in both months. The time variations of WDR10 are captured during most time periods at most sites. Large discrepancies exist at Speedwell where WDR10 may be affected by the orographic weather in the Appalachian Mountains, which is difficult to simulate. The “seemingly” large discrepancies between simulated and observed WDR10 at Cranberry on some days (e.g., 4, 6-10, 11, 13, 15, 17, 21, 25 January) indicate the limitation of time series plots in representing a vector WDR10, as they are indeed much smaller in magnitude in the wind rose plots. Simulated WDR10 values at 4- and 12-km at the five sites are fairly consistent in January. Slightly large differences exist in July, especially at Cranberry during 1-6 July.

4. Evaluation of chemical predictions

Figures S-9 and S-10 show the simulated monthly-mean 24-h average concentrations of $PM_{2.5}$ composition in January and July 2002. The detailed analysis is provided in the main text.

Figure S-11 compares dry deposition amounts of SO_2 , HNO_3 , NH_4^+ , SO_4^{2-} , and NO_3^- simulated by CMAQ with those estimated by MLM in July 2002 at two sites: Beaufort (BFT) and Coweeta (COW), NC. While both models give comparable dry deposition amounts of HNO_3 and SO_2 at the coastal site BFT where the terrain is flat and agriculture is the primary land use, large differences exist at COW where the terrain is complex and forest is the dominant land use, indicating the challenges and uncertainties in simulated dry deposition over complex terrain. Such large differences are mainly due to differences in V_d used in both models, e.g., the V_d values used in MLM are 2-3 orders of magnitude lower for SO_2 and 2-4 orders of magnitude lower for HNO_3 than those used in CMAQ (figures not shown), consistent with the differences in the dry deposition amounts. MLM gives higher dry deposition amounts than CMAQ at both sites, with the largest

differences (by up to 7 orders of magnitudes) in that of NO_3^- , indicating a large variability in the V_d of NO_3^- used by both models. Some differences exist between simulated dry deposition amounts by CMAQ at the 12- and 4-km, due to their sensitivity to model inputs (e.g., land cover/use) and meteorological and chemical predictions that are different at different horizontal grid resolutions.

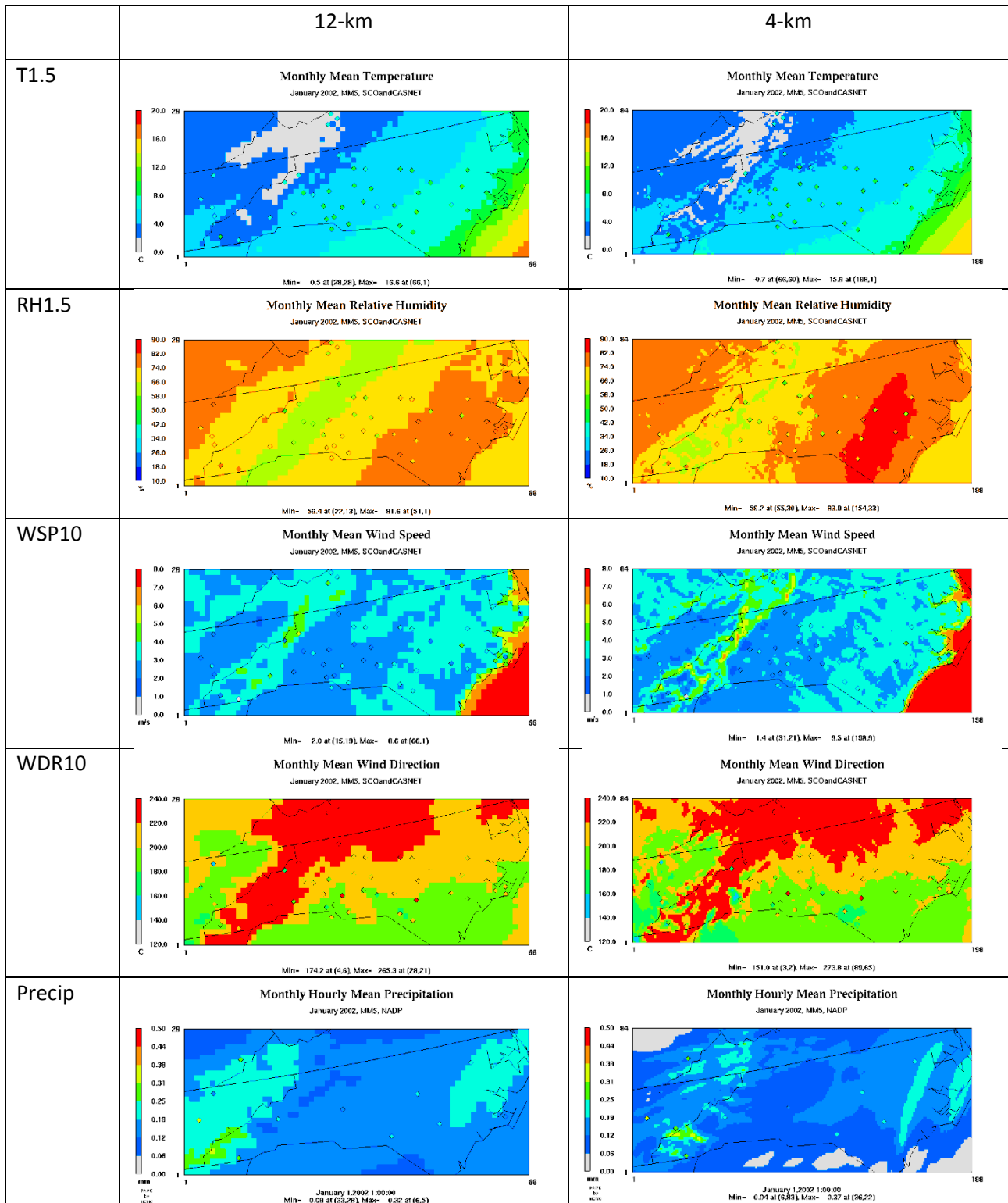


Figure S-6. Simulated vs. observed (diamond symbols) monthly-mean temperature at 1.5 m (T1.5), relative humidity at 1.5 m (RH1.5), wind speed at 10 m (WSP10), wind direction at 10 m (WDR10), and hourly precipitation (Precip) in January, 2002.

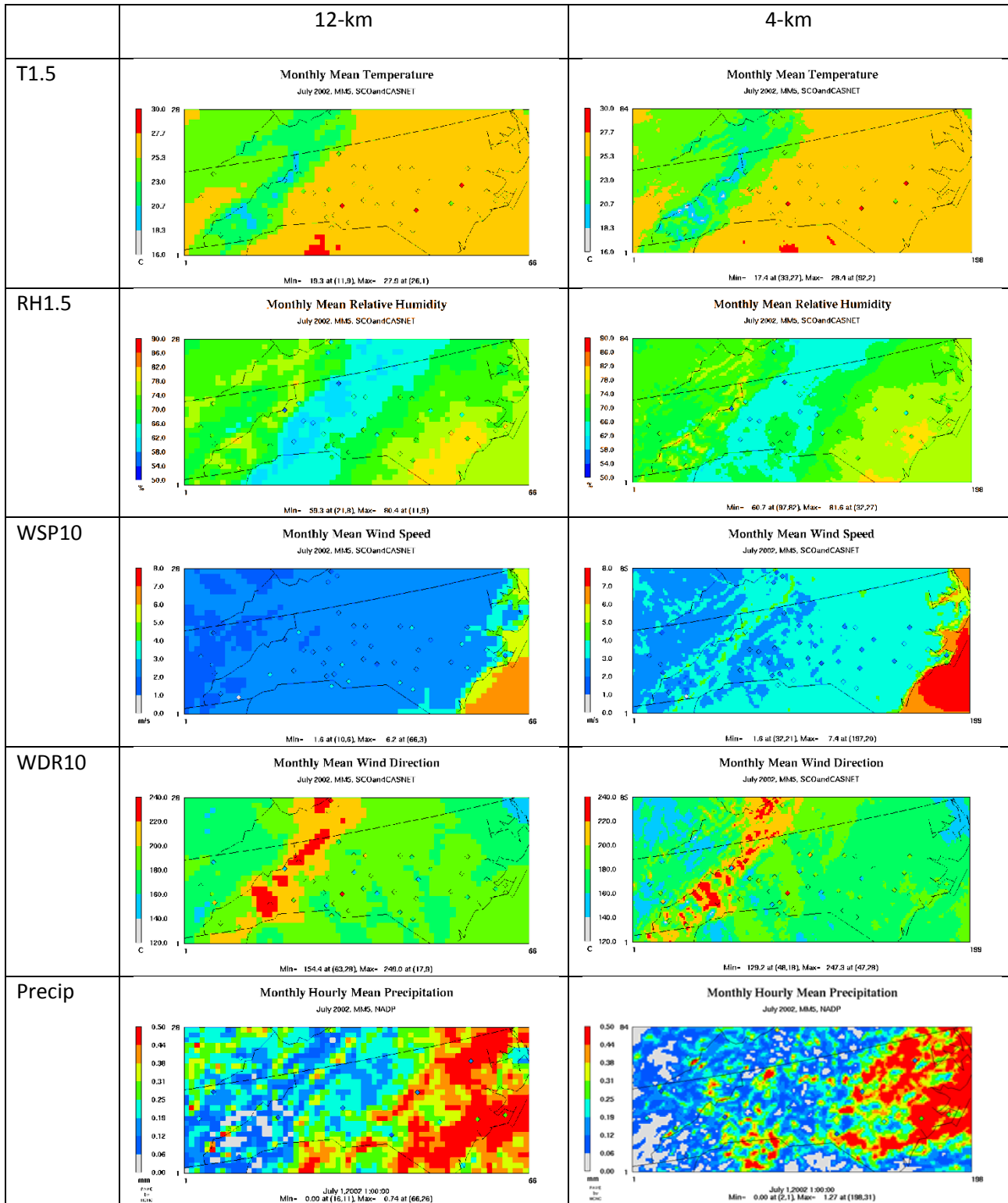
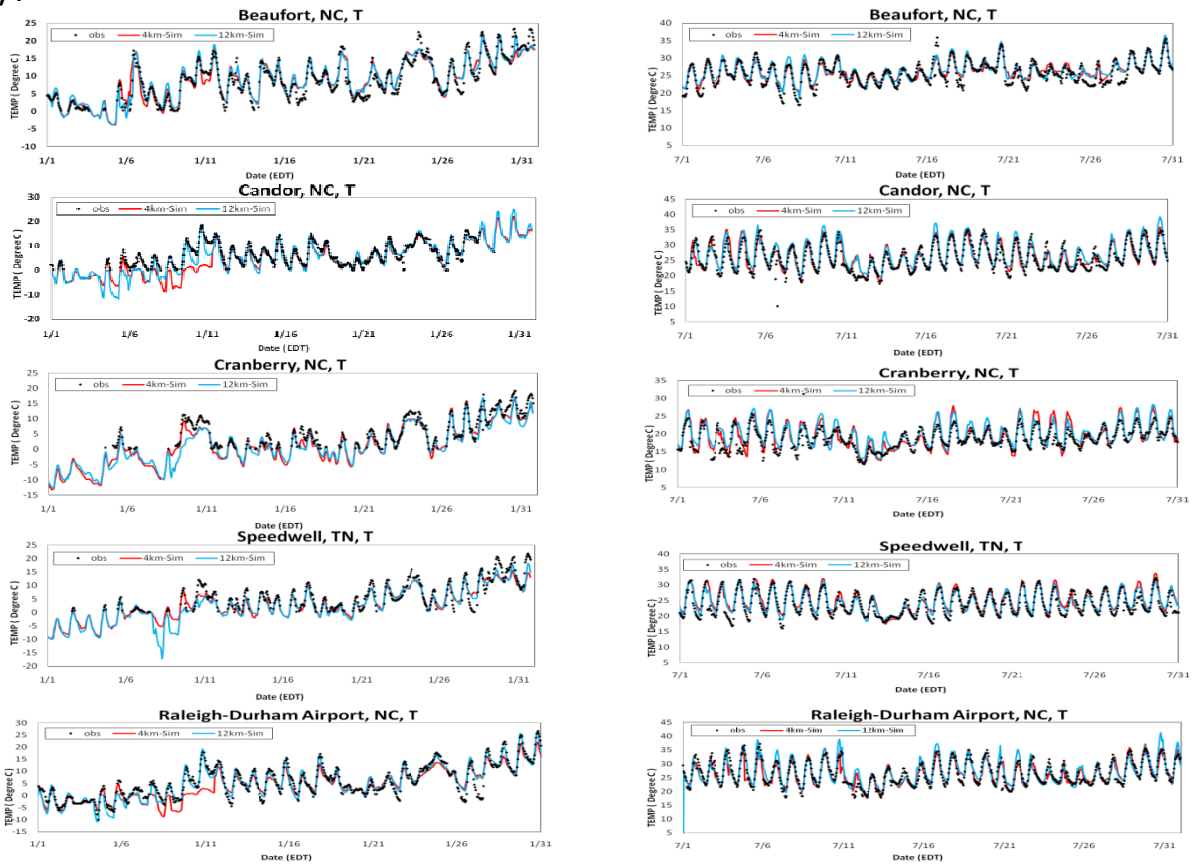


Figure S-7. Simulated vs. observed (diamond symbols) monthly-mean temperature at 1.5 m (T1.5), relative humidity at 1.5 m (RH1.5), wind speed at 10 m (WSP10), wind direction at 10 m (WDR10), and hourly precipitation (Precip) in July, 2002.

(1) T



(2) RH

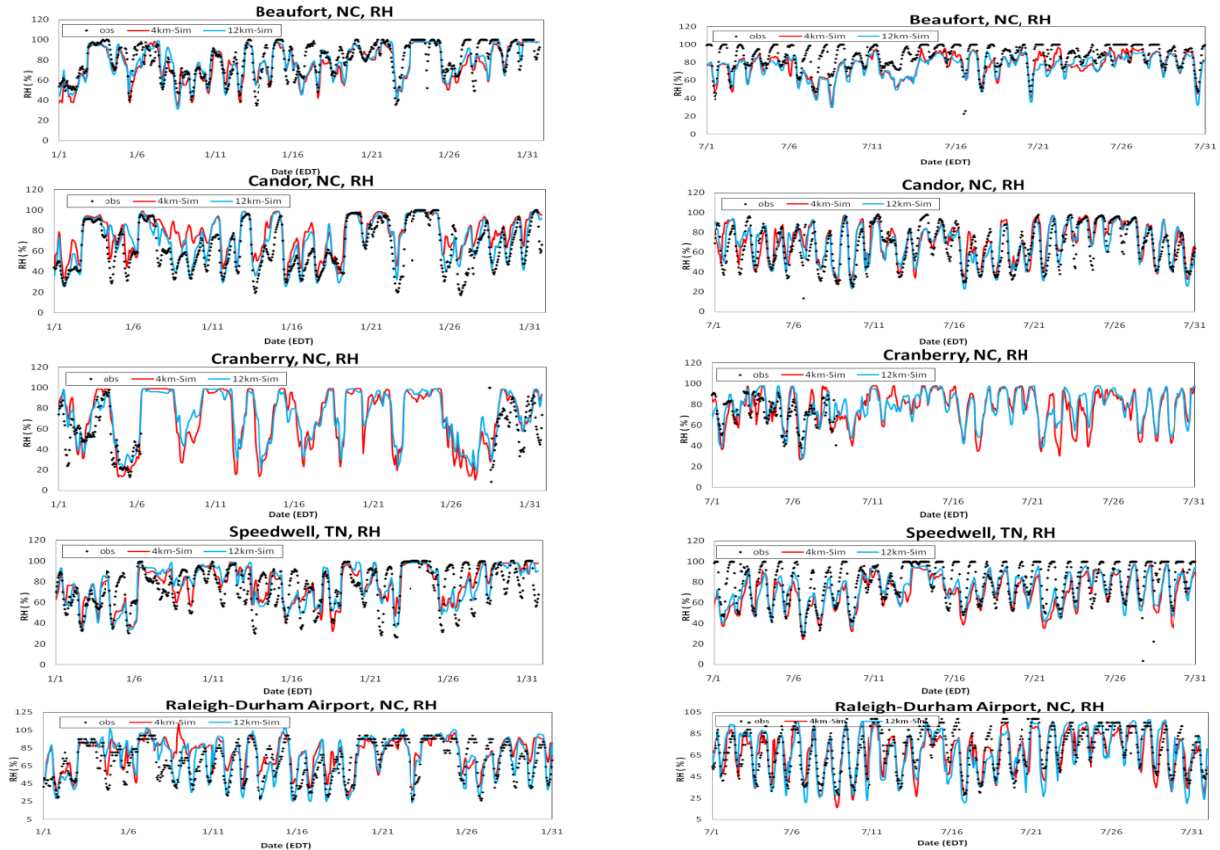
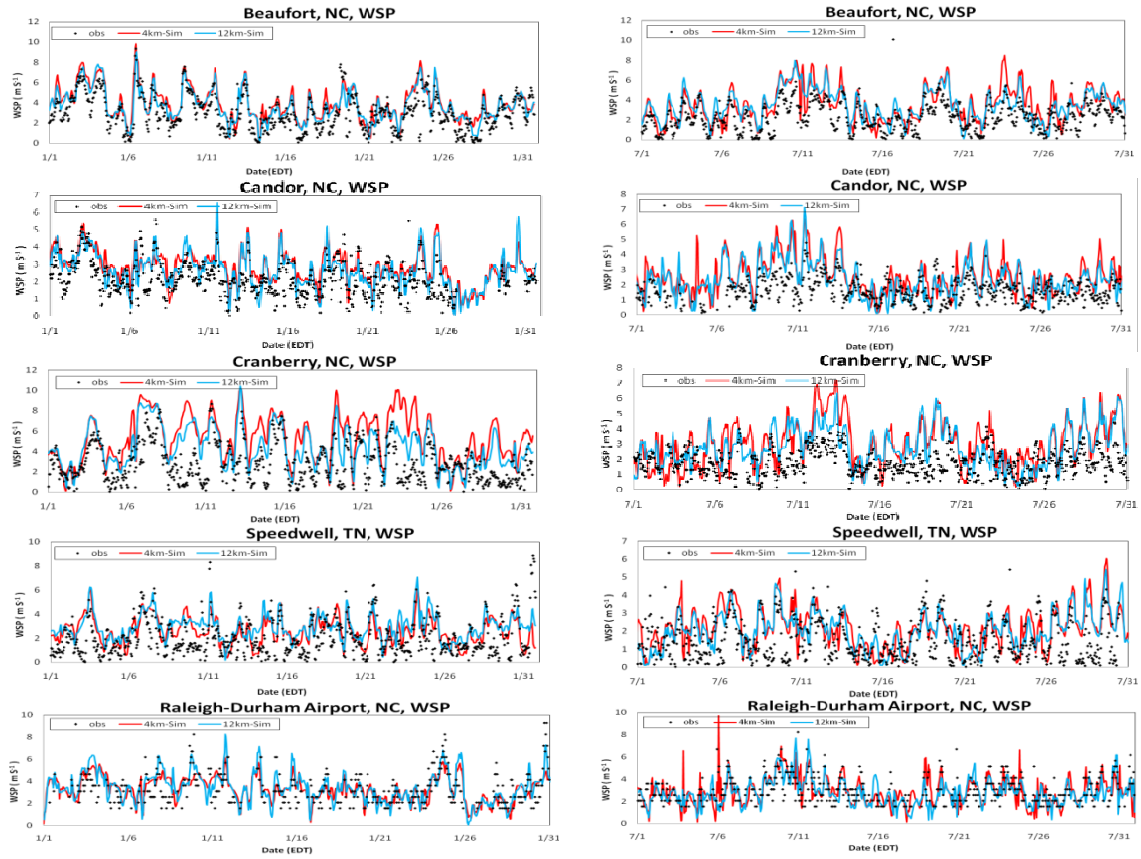


Figure S-8. Simulated vs. observed temporal variations of temperature at 1.5 m (T), relative humidity at 1.5 m (RH), wind speed at 10 m (WSP10), and wind direction at 10 m (WDR10) in January and Jul., 2002.

(3) WSP10



(4) WDR

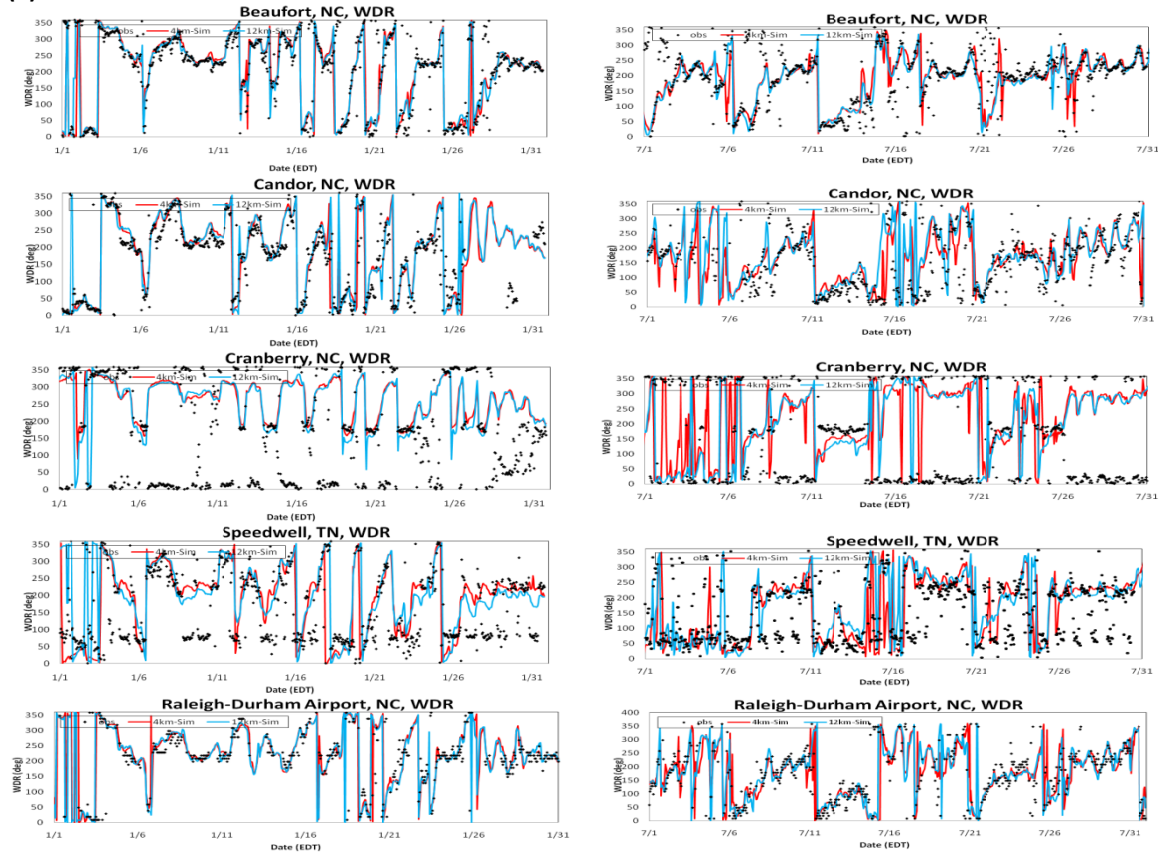


Figure S-8. Continued.

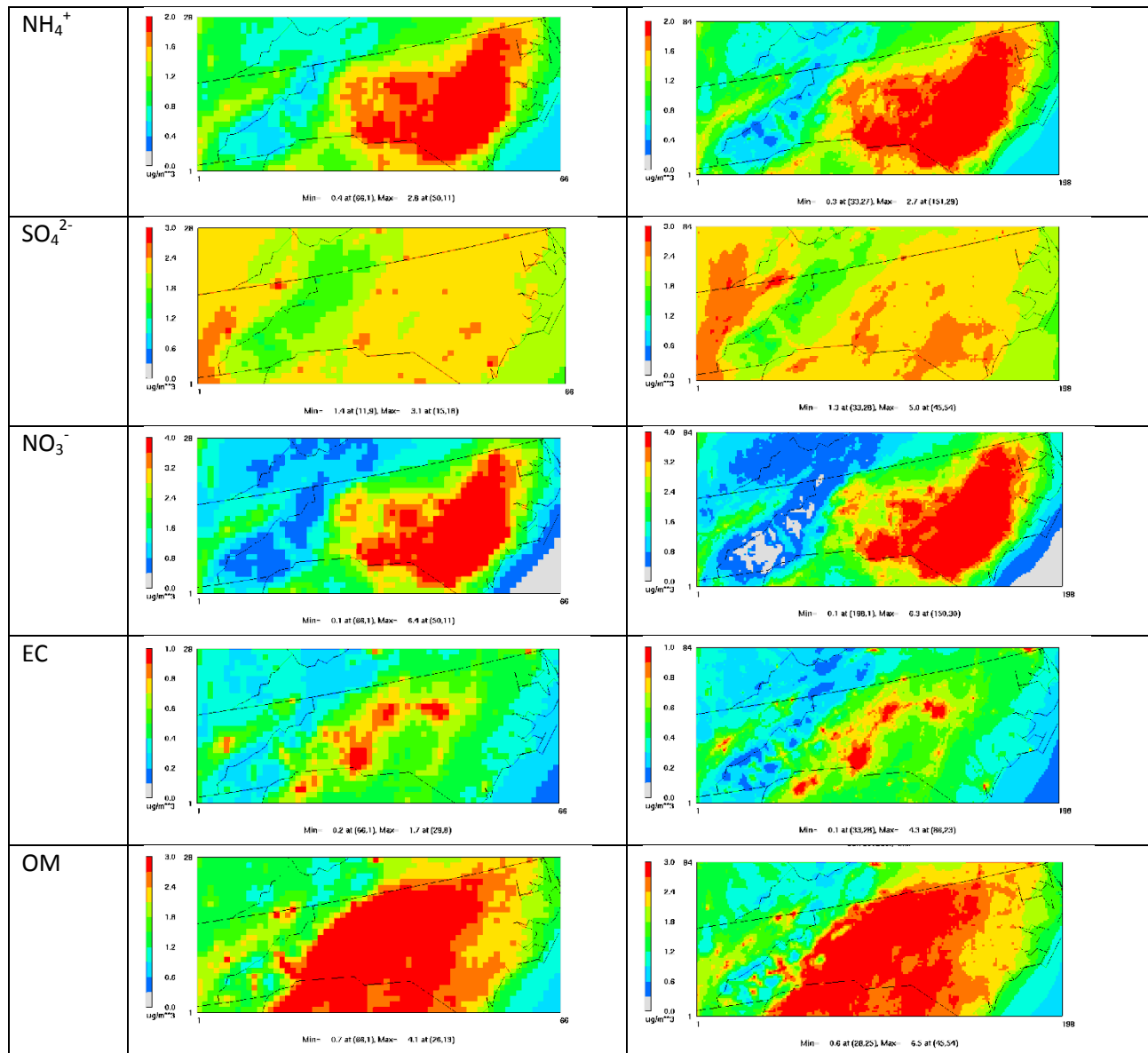


Figure S-9. Simulated monthly-mean 24-h average concentrations of $\text{PM}_{2.5}$ composition in January 2002.

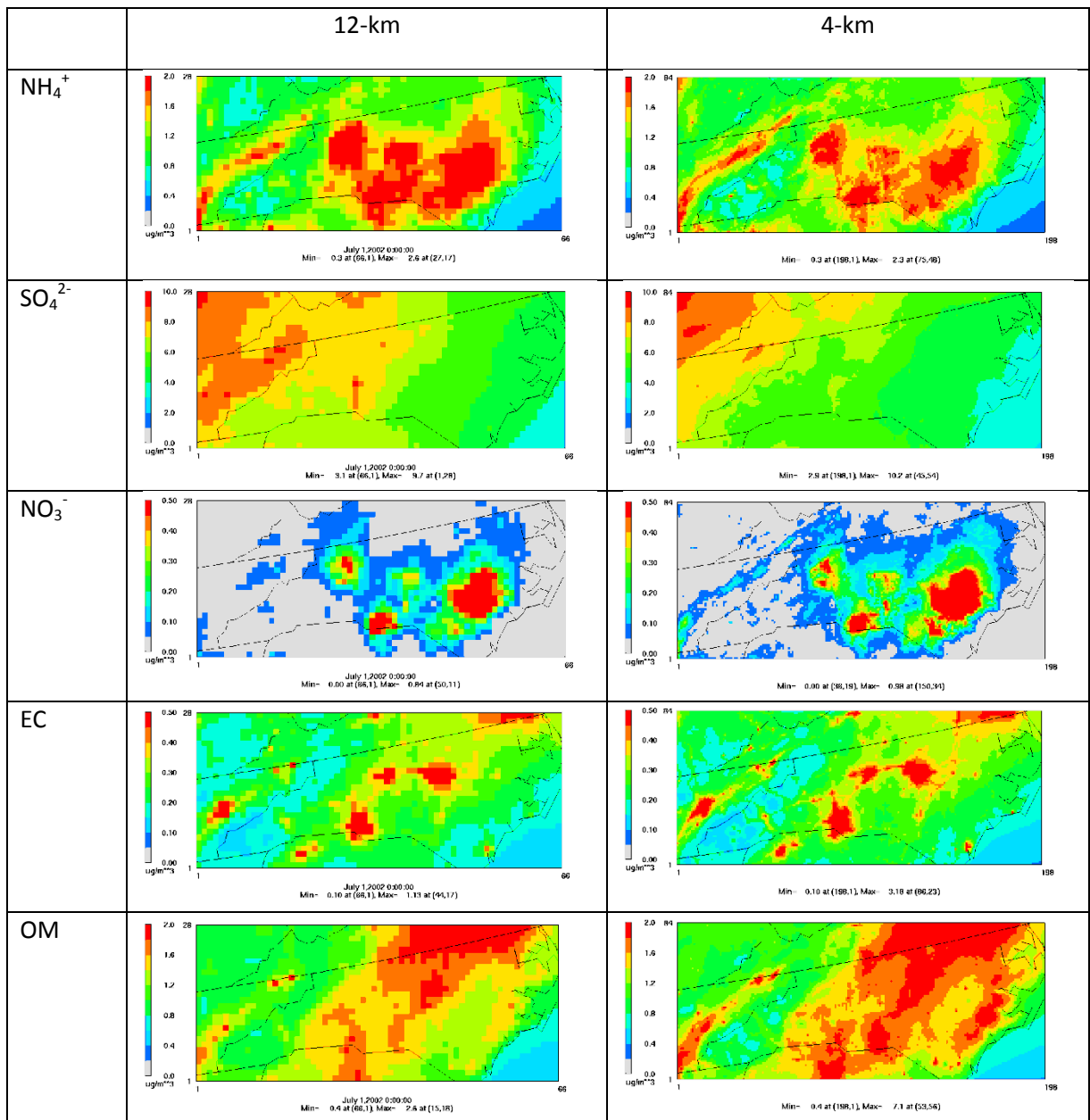


Figure S-10. Simulated monthly-mean 24-h average concentrations of $\text{PM}_{2.5}$ composition in July 2002.

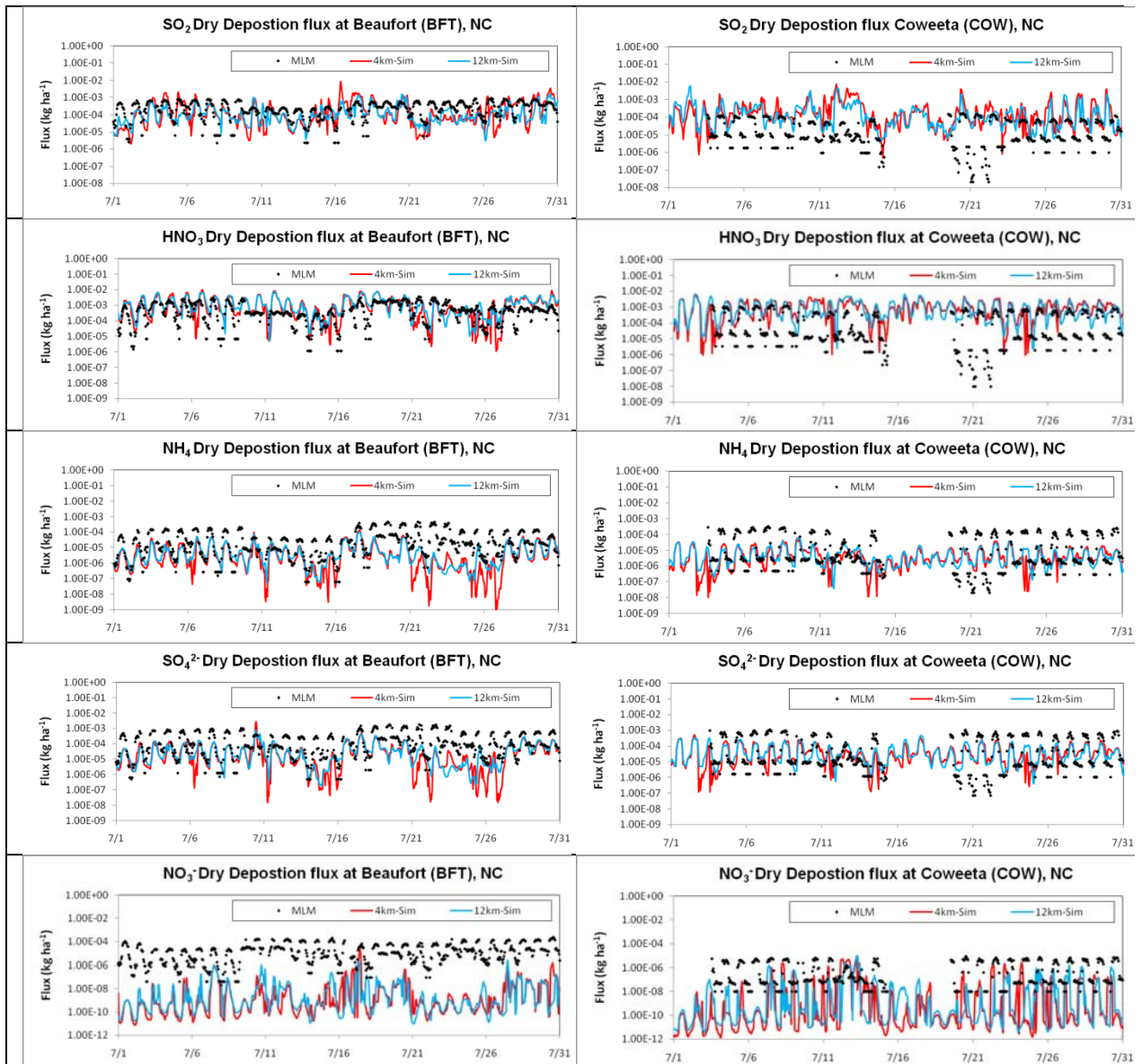


Figure S-11. The dry deposition fluxes of gaseous and PM species simulated by CMAQ 4- and 12-km simulations vs. estimated by the Multi-Layer Model (MLM) based on meteorological and chemical concentration measurements from CASTNET at 2 sites in NC in July 2002.