

**Supplementary Data to be published Online for the paper entitled:**

**Modeling Atmospheric Transport and Fate of Ammonia in North Carolina, Part I.  
Evaluation of Meteorological and Chemical Predictions**

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## Appendix I

Table A-1. Configurations of MM5 and CMAQ for the major processes.

MM5 Configurations		CMAQ Configurations	
Microphysics	Reisner 1 Mixed Ice	Sub-grid-scale Plumes	No Plume-in-Grid
Cumulus Scheme	Kain-Fritsch 2	Gas Phase Chemistry	CBM-IV
Planetary Boundary Layer	ACM PBL	Aerosol Chemistry	AE3/ISORROPIA
Radiation	RRTM	Secondary Organic Aerosols	SORGAM
Land Surface Model	P-X Land Surface Model (LSM)	Cloud Chemistry	RADM-type aqueous chemistry
Shallow Convection	None	Horizontal Diffusion	K-theory with Kh grid size dependence
Sea Surface Temperature	Eta Skin		
Snow Cover Effects	None	Vertical Diffusion	K-theory
Analysis Nudging (36-, 12-, and 4-km)	Winds (aloft) $2.5E-4^1$ , $1.0E-4^{1,2}$	Diffusivity Lower Limit	Kzmin = 1.0
	Winds (surface) $2.5E-4^1$ , $1.0E-4^{1,2}$	Planetary Boundary Layer	No Patch
	Temp (aloft) $2.5E-4^1$ , $1.0E-4^{1,2}$	Deposition Scheme	M3dry
	Temp(surface) not used	Gas Phase Chemistry Solver	EBI
	Moisture (aloft) $1.0E-5^1$ , $1.0E-5^{1,2}$	Horizontal Advection Scheme	Piecewise Parabolic Method (PPM)
	Moisture (surface) not used		

<sup>1</sup>The values are observation-nudging coefficients in  $s^{-1}$  for 36-, 12- and 4-km simulations.

<sup>2</sup>The same observation-nudging coefficients are used for 12- and 4-km simulations.

Table A-2. Summary of observational datasets used in the model evaluation.

Network	Variables		Sampling Period
TDL	Met	Wind speed/direction, temperature, humidity	Hourly
NADP	Met	Precipitation	Weekly
	PM	Wet deposition of $NH_4^+$ , $NO_3^-$ , and $SO_4^{2-}$	Weekly
NCDENR	GAS	$O_3$ , CO, $NO_2$ , $SO_2$	Hourly average
	PM	$PM_{2.5}$ , $NH_4^+$ , $NO_3^-$ , $SO_4^{2-}$ , EC, OC	$PM_{2.5}$ : 1 in 3 days; 24 hour average; other: weekly average
CASTNET	GAS	$O_3$ , $SO_2$	Hourly average
	PM	$NH_4^+$ , $NO_3^-$ , $SO_4^{2-}$	Weekly average
AQS	GAS	$O_3$	Hourly average
IMPROVE	PM	$PM_{2.5}$ , $NH_4^+$ , $NO_3^-$ , $SO_4^{2-}$ , EC, OC	1 in 3 days; 24 hour average
STN	PM	$PM_{2.5}$ , $NH_4^+$ , $NO_3^-$ , $SO_4^{2-}$ , EC, OC	1 in 3 days; 24 hour average

Table A-3. Domain-wide and Area-specific model performance statistics for hourly mean meteorological predictions for the August 2002 simulations with 4-km and 12-km grid spacings<sup>1</sup>.

		T		SH		WSP		WDR	
		4-km	12-km	4-km	12-km	4-km	12-km	4-km	12-km
<b>Overall</b>	<b>Obs</b>	24.8	24.8	14.3	14.3	3.1	3.1	155.2	155.2
	<b>Sim</b>	24.9	25.1	14.3	13.8	3.3	3.3	143.7	152.3
	<b>Data pair</b>	38678	38678	50500	50500	35370	35370	35369	35369
	<b>NMB,%</b>	0.4	1.3	-0.6	-4.0	8.8	7.0	-7.4	-1.8
	<b>NME,%</b>	7.9	6.5	10.2	11.9	35.8	35.5	34.6	35.0
<b>Coastal</b>	<b>Obs</b>	26.2	26.2	16.1	16.1	3.7	3.7	153.8	153.8
	<b>Sim</b>	25.8	25.9	15.5	15.3	4.2	4.3	148.8	151.7
	<b>Data pair</b>	4622	4622	4622	4622	3858	3858	3858	3858
	<b>NMB,%</b>	-2.0	-1.0	-4.0	-5.0	14.0	15.0	-3.0	-1.0
	<b>NME,%</b>	6.0	6.0	9.0	10.0	37.0	38.0	27.0	31.0
<b>Rural</b>	<b>Obs</b>	23.4	23.4	14	14	2.4	2.4	175.2	175.2
	<b>Sim</b>	23.5	23.6	13.5	13.1	3	3.2	161	176.6
	<b>Data pair</b>	2887	2887	2587	2587	1053	1053	1053	1053
	<b>NMB,%</b>	0.5	0.8	-4.0	-6.0	23.9	30.4	-8.1	0.8
	<b>NME,%</b>	7.6	7.1	10.9	12.0	45.1	50.0	36.9	40.3
<b>Urban</b>	<b>Obs</b>	26.6	26.6	14.3	14.3	3.1	3.1	149.2	149.2
	<b>Sim</b>	26.4	27.6	14.3	13.7	3.2	3.2	142	147.5
	<b>Data pair</b>	16603	16603	15912	15912	10719	10719	10719	10719
	<b>NMB,%</b>	0.0	0.1	0.0	-4.2	3.2	3.9	-4.8	-1.1
	<b>NME,%</b>	0.5	0.6	10.4	12.0	33.0	33.9	34.5	36.6
<b>Other</b>	<b>Obs</b>	24.7	24.7	14.1	14.1	3	3	157.6	157.6
	<b>Sim</b>	24.7	25.2	14.1	13.6	3.2	3.1	147.3	153.7
	<b>Data pair</b>	31170	31170	27383	27383	19740	19740	19740	19740
	<b>NMB,%</b>	-0.2	1.7	-0.3	-3.6	7.6	5.6	-6.5	-2.5
	<b>NME,%</b>	6.4	6.5	10.8	12.1	34.7	35.2	33.9	34.7

<sup>1</sup> The MM5 12-km model simulation results are taken from VISTAS and post-processed in this work.