Assessing Meteorological Model Performance and Meteorological Processes in a Photochemical Model

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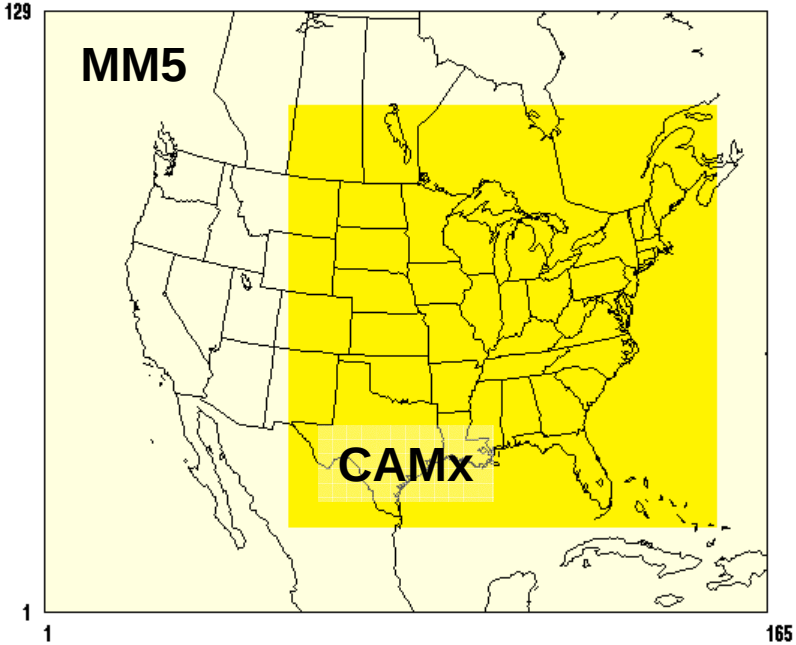
Background

- Wind field important to emission and chemical transport
- Temperature and relative humidity important for PM2.5 nitrate formation
- Wet and dry deposition are important removal processes for annual and regional scale modeling applications
- Meteorological inputs to the photochemical model are assessed by comparing to observation data collected near the ammonia network sites (U.S. Airways data)

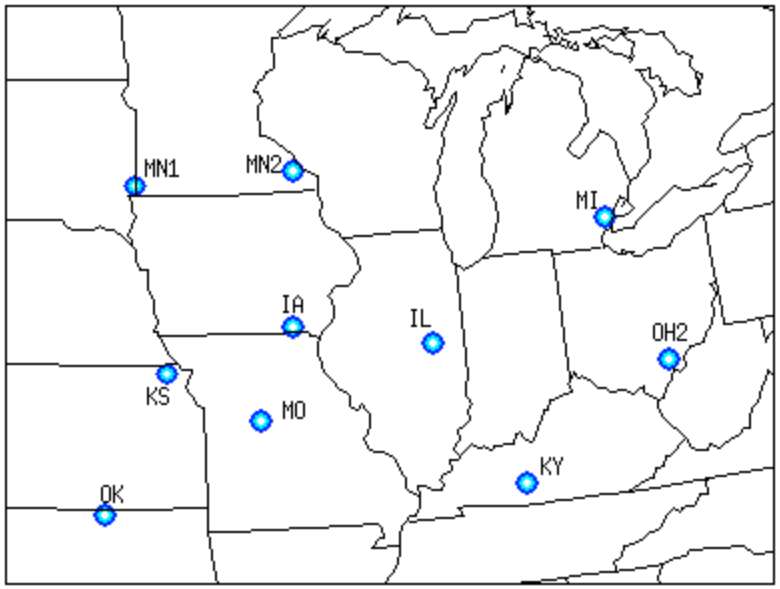


Configuration	36km Domain
Explicit Moisture	Mixed Phase (Reisner I)
Cumulus	Kain-Fritsch 2
PBL	Pleim-Chang (ACM)
Radiation	RRTM
Multi-Layer Soil Model	Pleim-Xu
Shallow convection	No
4-D Data Assimilation	Analysis nudging on above PBL
Moist Physics Table	No

k(MM5)	sigma	press.(mb)	height(m)	depth(m)
34	0.000	10000	14662	1841
33	0.050	14500	12822	1466
32	0.100	19000	11356	1228
31	0.150	23500	10127	1062
30	0.200	28000	9066	939
29	0.250	32500	8127	843
28	0.300	37000	7284	767
27	0.350	41500	6517	704
26	0.400	46000	5812	652
25	0.450	50500	5160	607
24	0.500	55000	4553	569
23	0.550	59500	3984	536
22	0.600	64000	3448	506
21	0.650	68500	2942	480
20	0.700	73000	2462	367
19	0.740	76600	2095	266
18	0.770	79300	1828	259
17	0.800	82000	1569	169
16	0.820	83800	1400	166
15	0.840	85600	1235	163
14	0.860	87400	1071	160
13	0.880	89200	911	158
12	0.900	91000	753	78
11	0.910	91900	675	77
10	0.920	92800	598	77
9	0.930	93700	521	76
8	0.940	94600	445	76
7	0.950	95500	369	75
6	0.960	96400	294	74
5	0.970	97300	220	74
4	0.980	98200	146	37
3	0.985	98650	109	37
2	0.990	99100	73	36
1	0.995	99550	36	36
0	1.000	100000	0	--SURF--

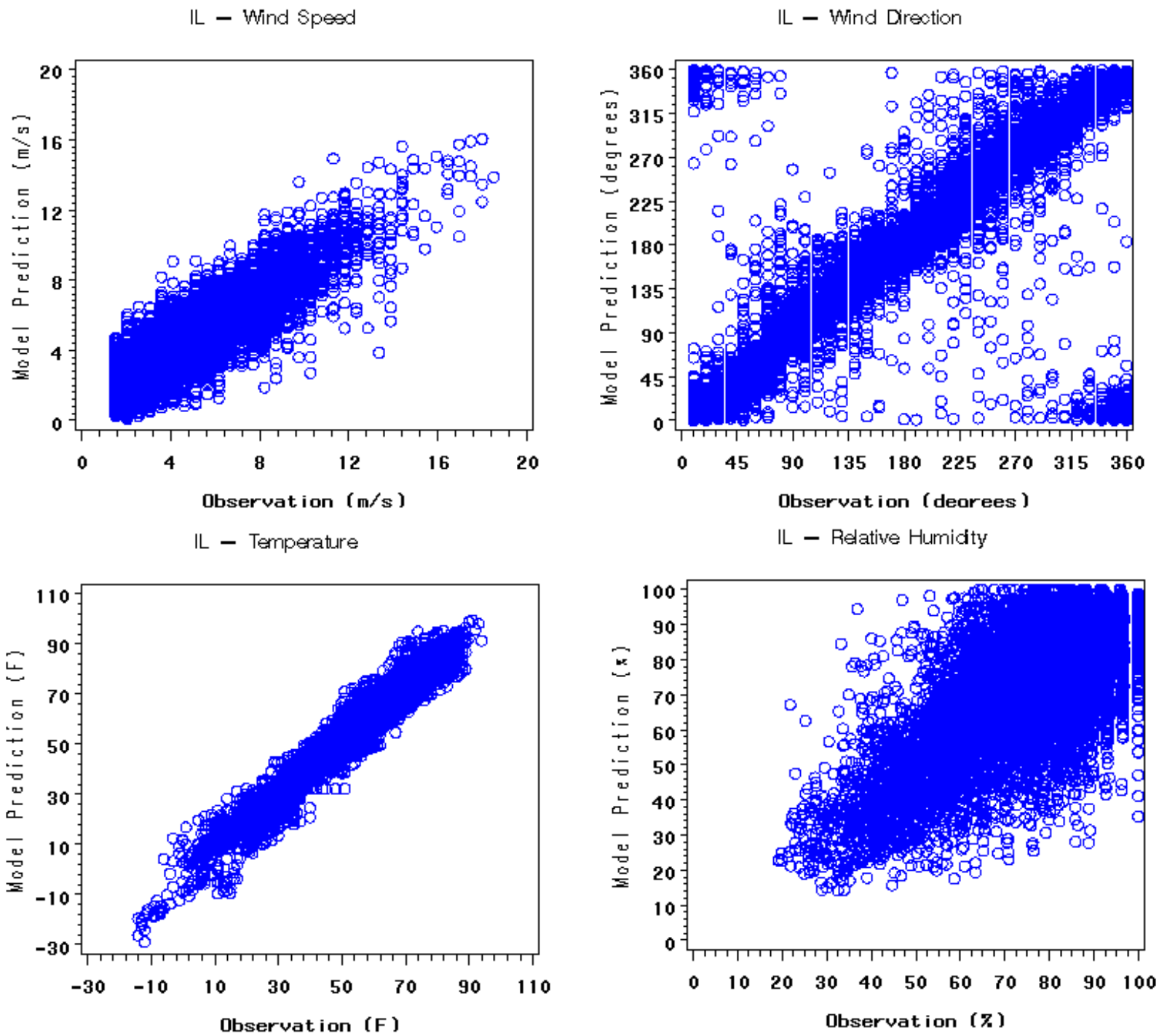
Ammonia Monitor Network

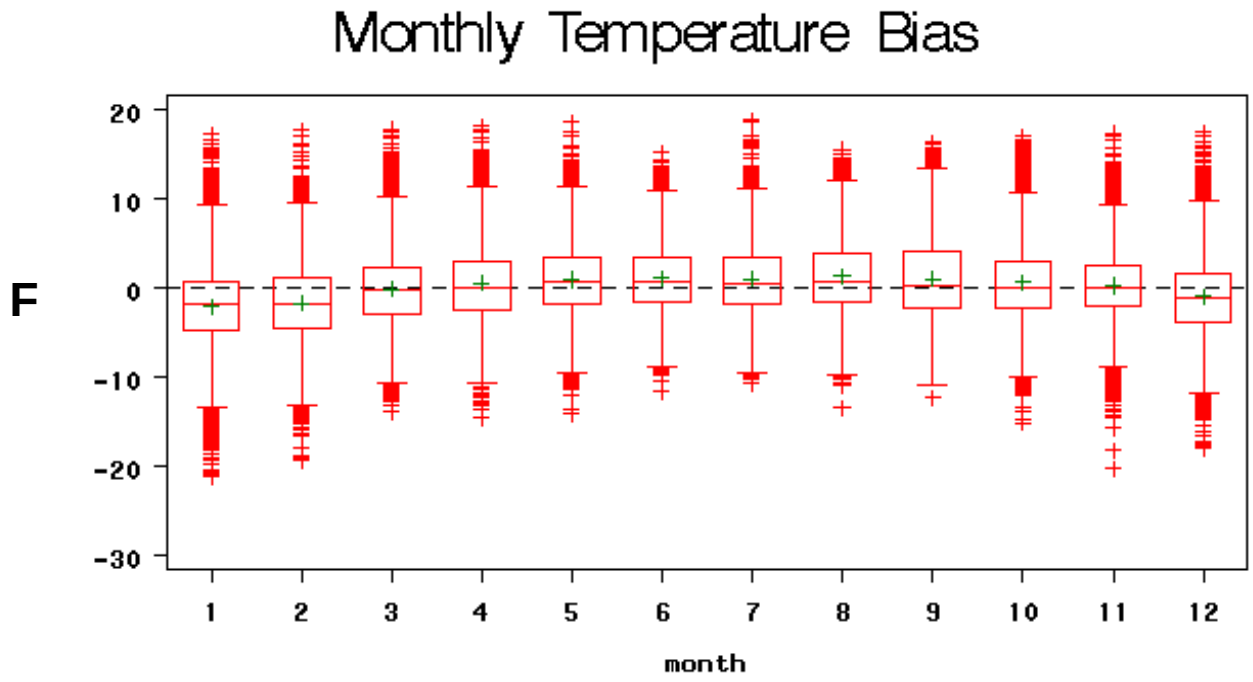
- 9 rural and 1 urban (MI)
- Measure SO4, SO2, NH4, NH3, NO3, HNO3
- 24-hr average sample every 6 days
- Analyzing data for entire year of 2004
- Samples at most sites use URG manual denuder
- IA, MO, and IL use R&P denuder

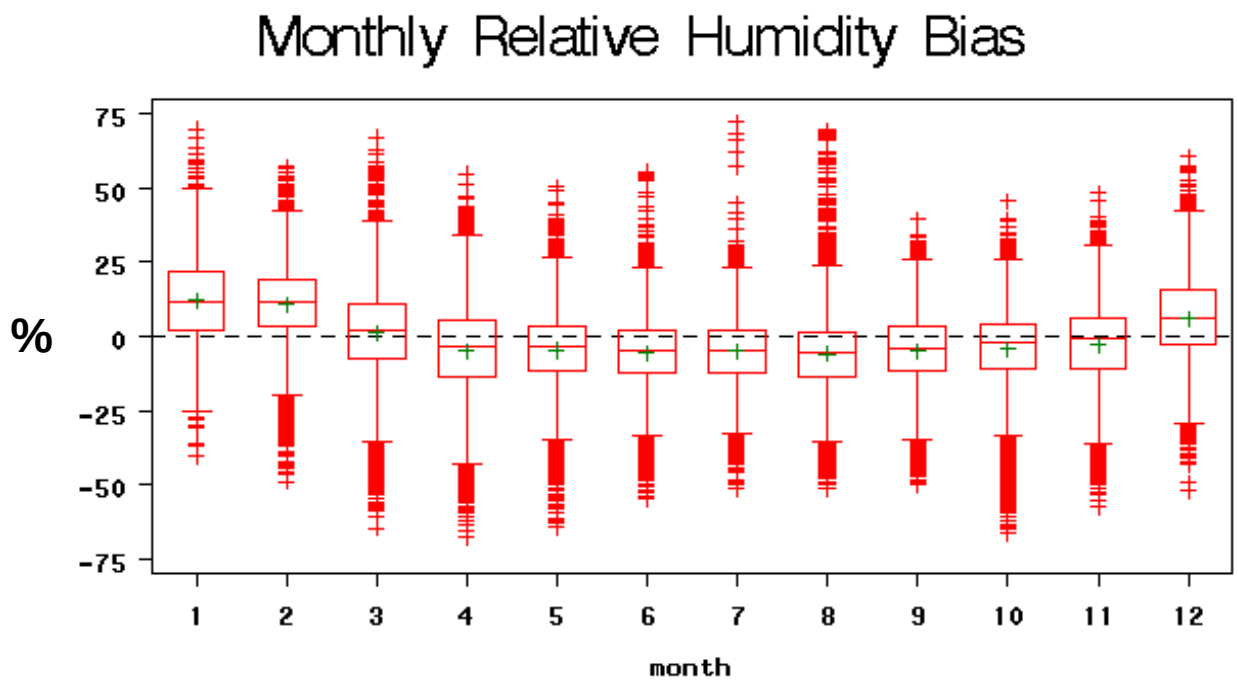


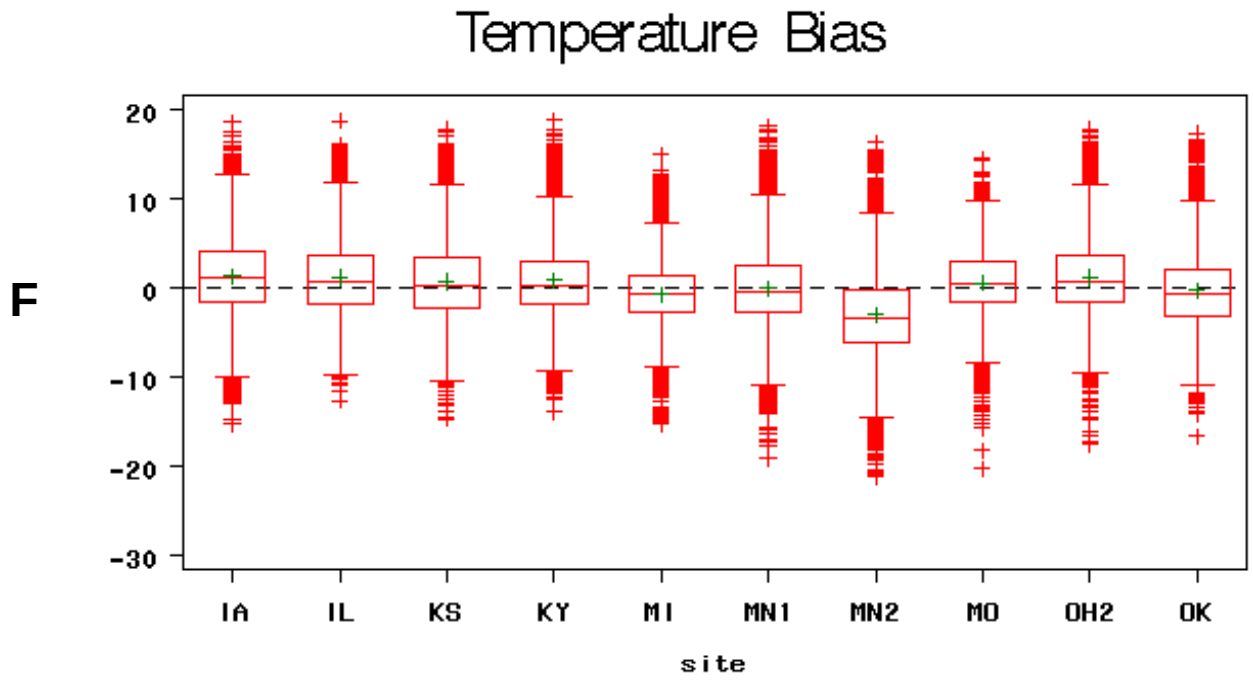
Mean model performance metrics

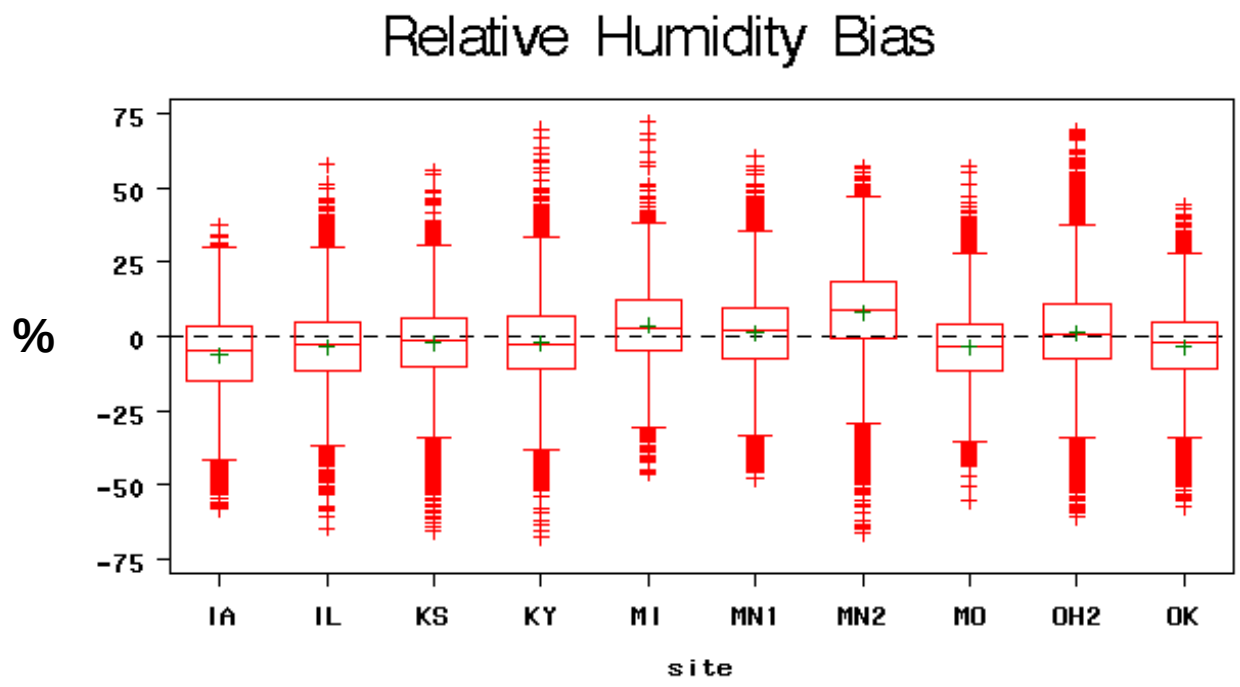
Metric	Variable	N	MEAN	STD
Bias	Temperature (F)	86,474	-0.49	5.16
Bias	Relative Humidity (%)	86,373	-0.71	15.06
Bias	Wind Speed (m/s)	76,480	0.34	1.40
Error	Temperature (F)	86,474	3.82	3.51
Error	Relative Humidity (%)	86,373	11.50	9.76
Error	Wind Speed (m/s)	76,480	1.12	0.91
Fractional Bias	Temperature (F)	86,474	-0.11	1.03
Fractional Bias	Relative Humidity (%)	86,373	-2.12	23.74
Fractional Bias	Wind Speed (m/s)	76,480	9.09	36.62
Fractional Error	Temperature (F)	86,474	0.75	0.72
Fractional Error	Relative Humidity (%)	86,373	17.41	16.27
Fractional Error	Wind Speed (m/s)	76,480	28.69	24.50
Wind Displacement (km)		74,612	18.01	15.19
Wind Displacement (grid cells)		74,612	0.50	0.42

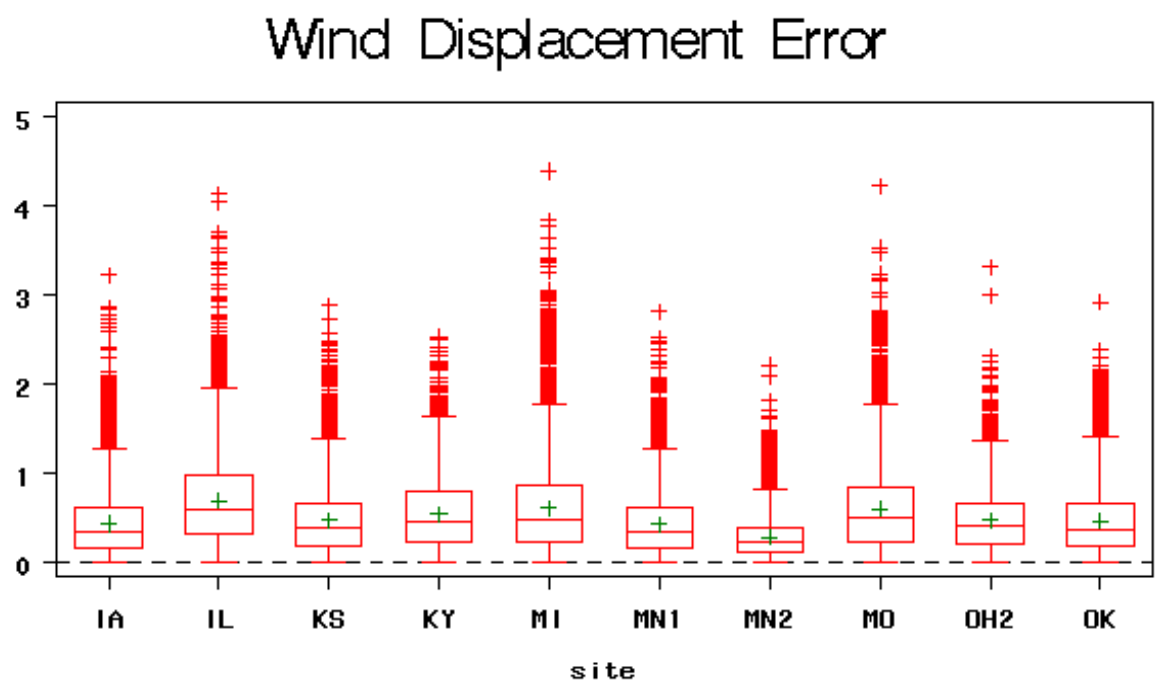

IL — Wind Speed
Model Prediction (m/s)
Observation (m/s)
0
4
8
12
16
20
IL — Wind Direction
Model Prediction (degrees)
Observation (degrees)
0
45
90
135
180
225
270
315
360
IL — Temperature
Model Prediction (F)
Observation (F)
-30
-10
10
30
50
70
90
110
IL — Relative Humidity
Model Prediction (%)
Observation (%)
0
10
20
30
40
50
60
70
80
90
100

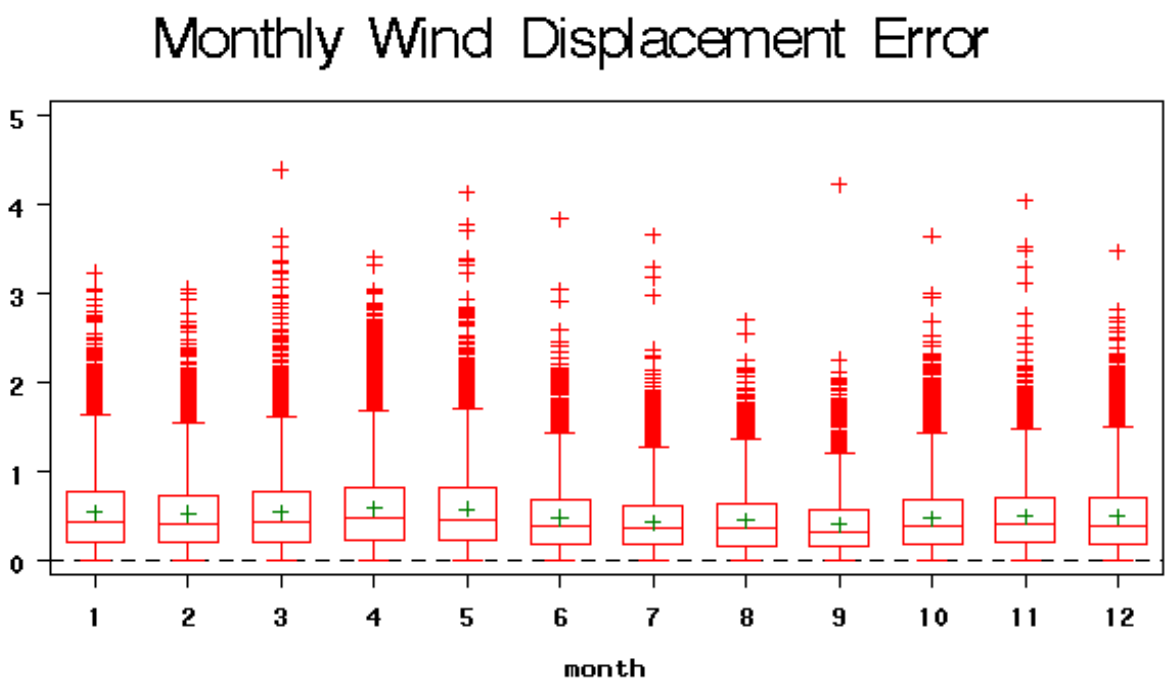

Monthly Temperature Bias
F
20
10
0
-10
-20
-30
1
2
3
4
5
6
7
8
9
10
11
12
month


Monthly Relative Humidity Bias
%
75
50
25
0
-25
-50
-75
1
2
3
4
5
6
7
8
9
10
11
12
month

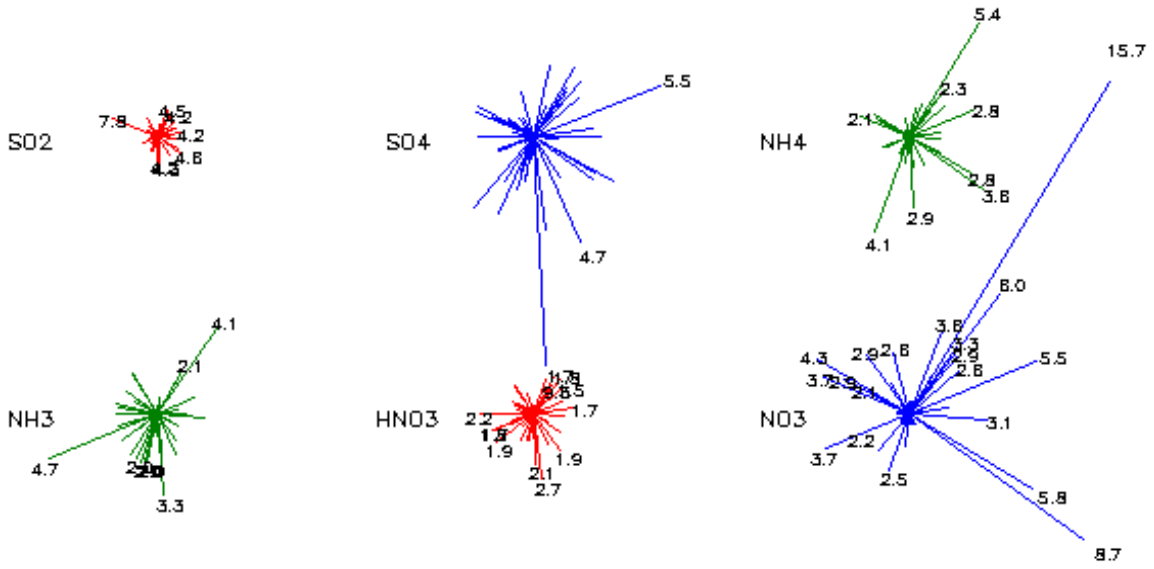

Temperature Bias
F
20
10
0
-10
-20
-30
IA
IL
KS
KY
MI
MN1
MN2
MO
OH2
OK
site


Relative Humidity Bias
%
75
50
25
0
-25
-50
-75
IA
IL
KS
KY
MI
MN1
MN2
MO
OH2
OK
site

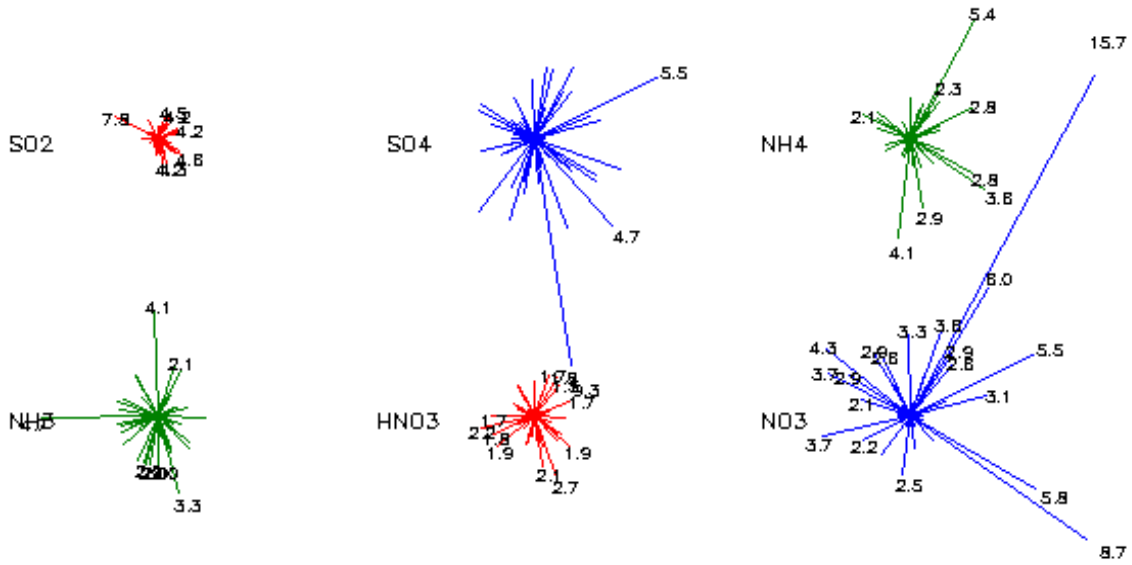

Wind Displacement Error
5
4
3
2
1
0
IA
IL
KS
KY
MI
MN1
MN2
MO
OH2
OK
site


Monthly Wind Displacement Error
5
4
3
2
1
0
1
2
3
4
5
6
7
8
9
10
11
12
month

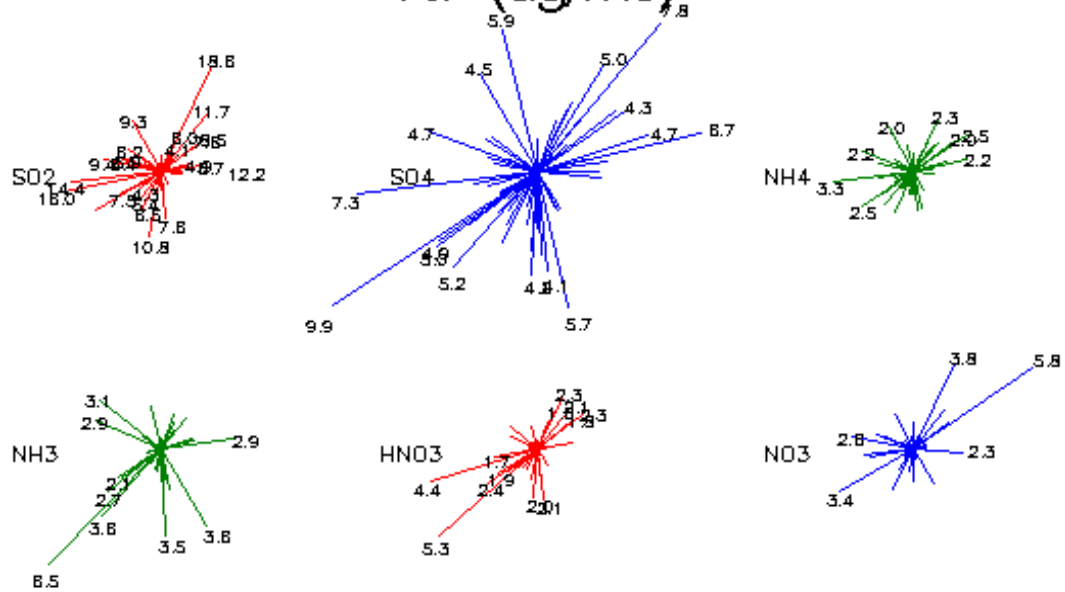
IA (ug/m3)



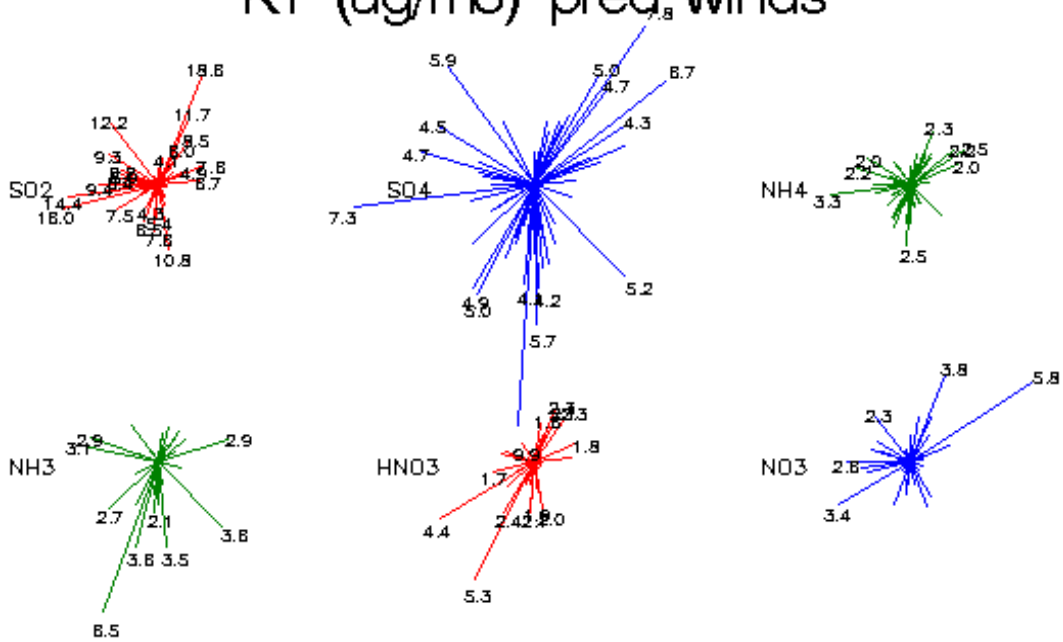
IA (ug/m3) pred winds



KY (ug/m3)



KY (ug/m3) pred. winds

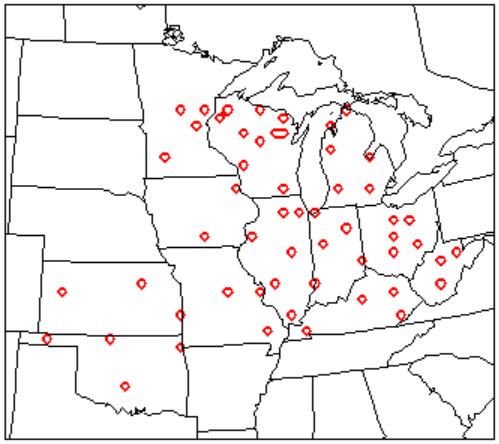


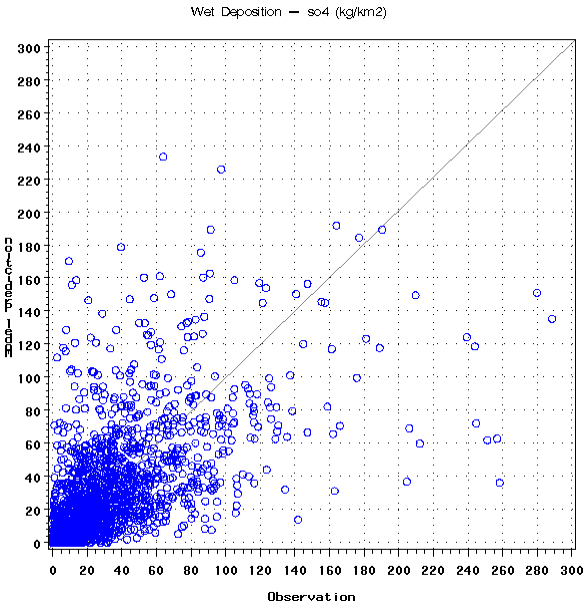
Meteorological Metrics Correlated to Photochemical Species Metrics

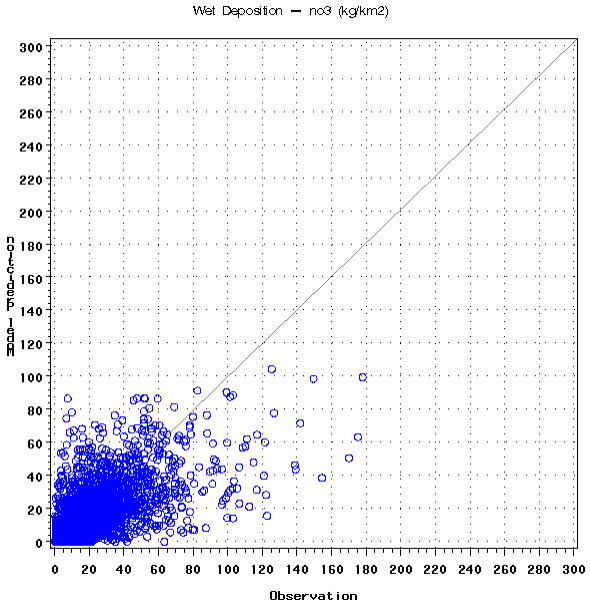
PCM	Met	N	RSQ	Month
Error NH4	Error RH	37	0.36	1
Error NH4	Error T	30	0.30	11
Error NH3	Error T	35	0.30	1
Error SO2	Error RH	45	0.27	3
Bias NH4	Bias T	30	0.27	11
Bias NO3	Bias T	43	0.25	12
Error HNO3	Error T	30	0.25	12
Bias HNO3	Bias RH	26	0.24	11
Error NO3	Error WS	26	0.23	9
Bias SO2	Bias RH	35	0.23	11
Bias HNO3	Bias T	35	0.23	1
Bias NH4	Bias RH	45	0.21	2
Error SO4	Error T	36	0.21	11
Error HNO3	Error WS	26	0.20	11

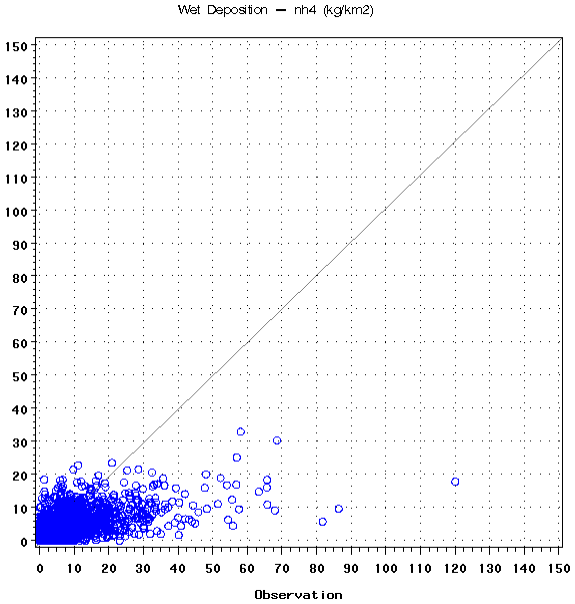
Wet Deposition (kg/km^2) – NADP sites

Season	N	Fractional Bias NO_3^-	Fractional Bias $SO_4^=$	Fractional Bias NH_4^+	Fractional Error NO_3^-	Fractional Error $SO_4^=$	Fractional Error NH_4^+
Winter	496	-73	-91	-113	92	108	122
Spring	535	-27	-9	-50	64	64	81
Summer	493	-14	14	-19	70	74	78
Fall	458	-28	-48	-64	68	81	87



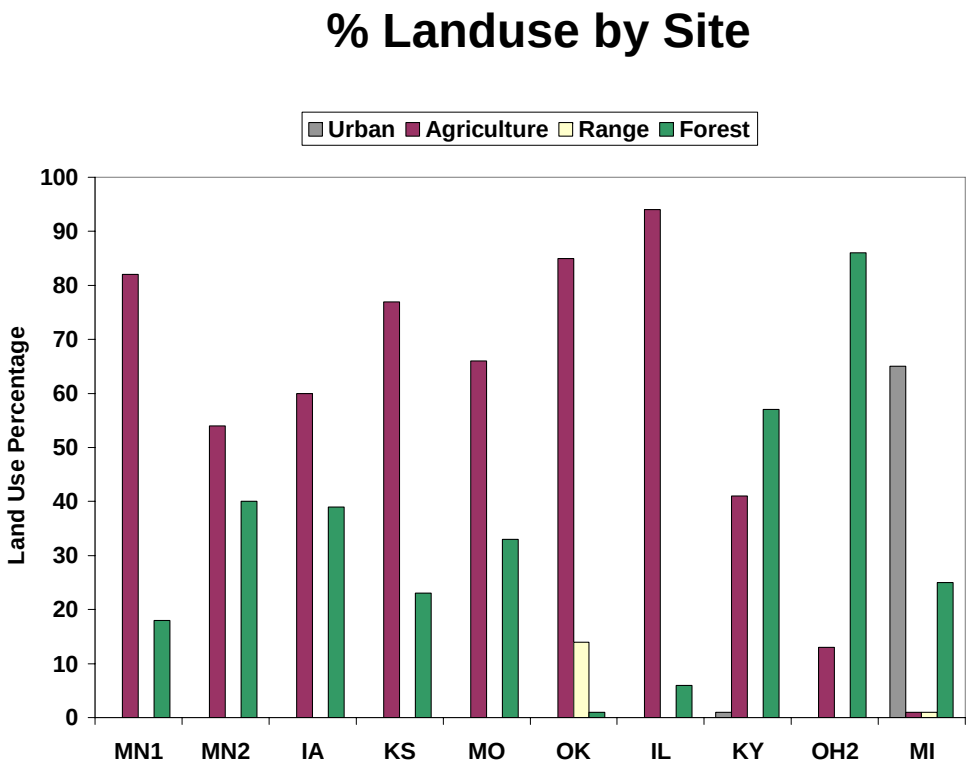




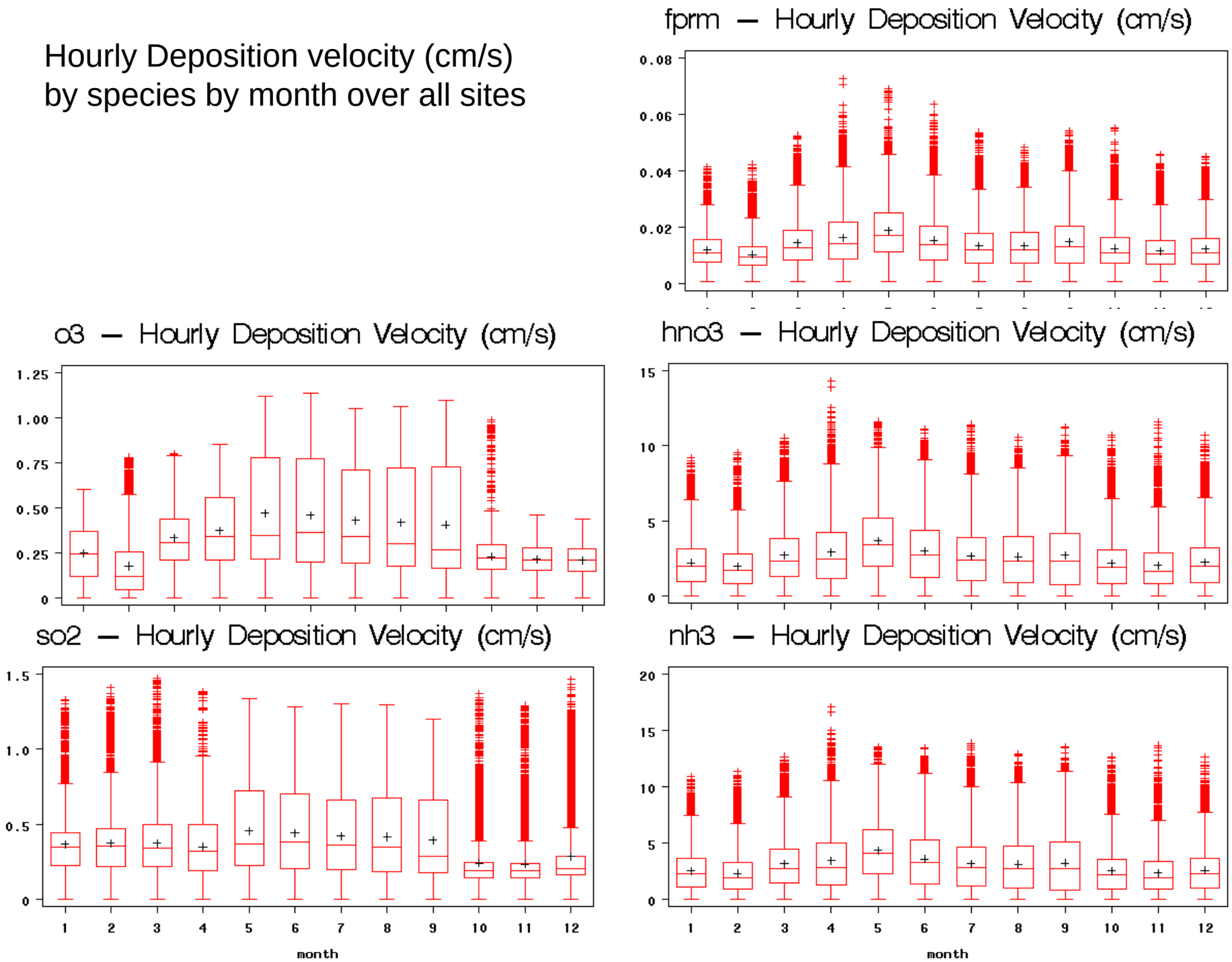


Dry Deposition

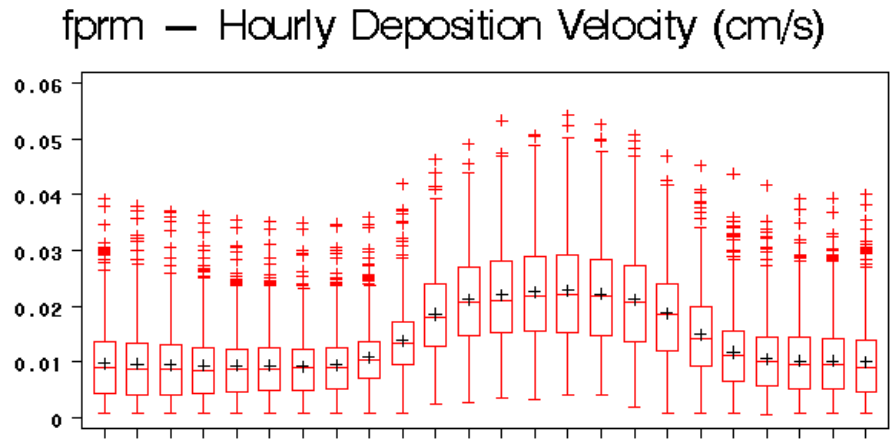
- Compare dry deposition velocities to published studies over forest and agricultural landuse
- SO2
- HNO3
- NH3
- Other: O3, H2O2

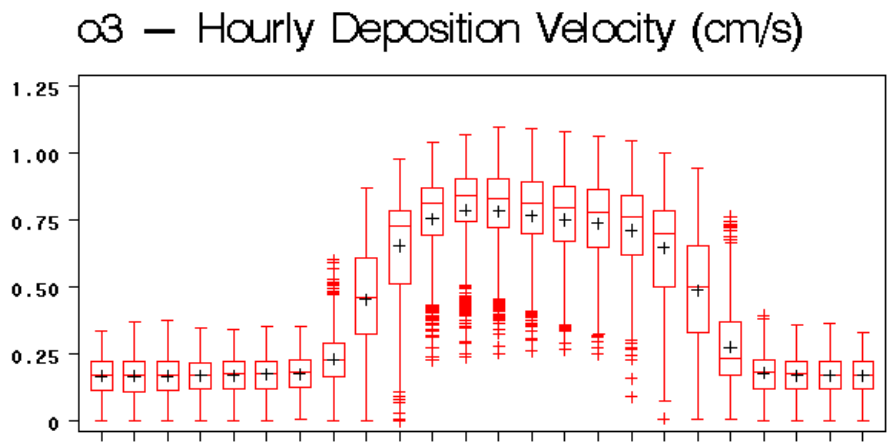


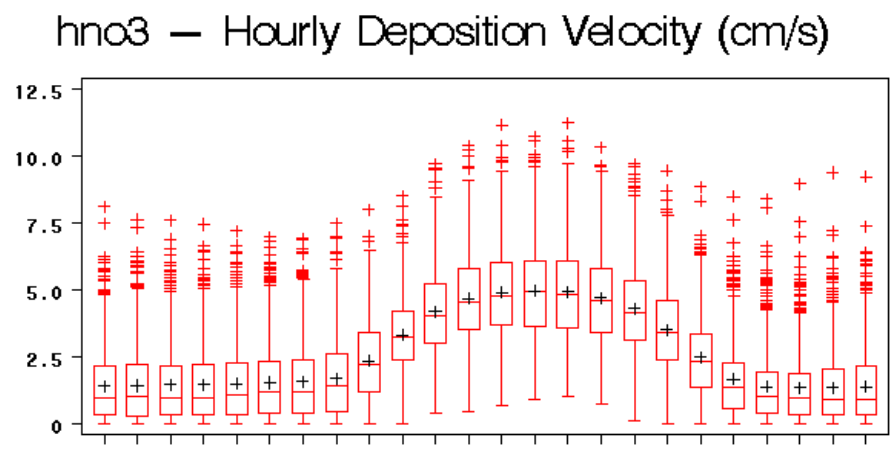
Hourly Deposition velocity (cm/s)
by species by month over all sites

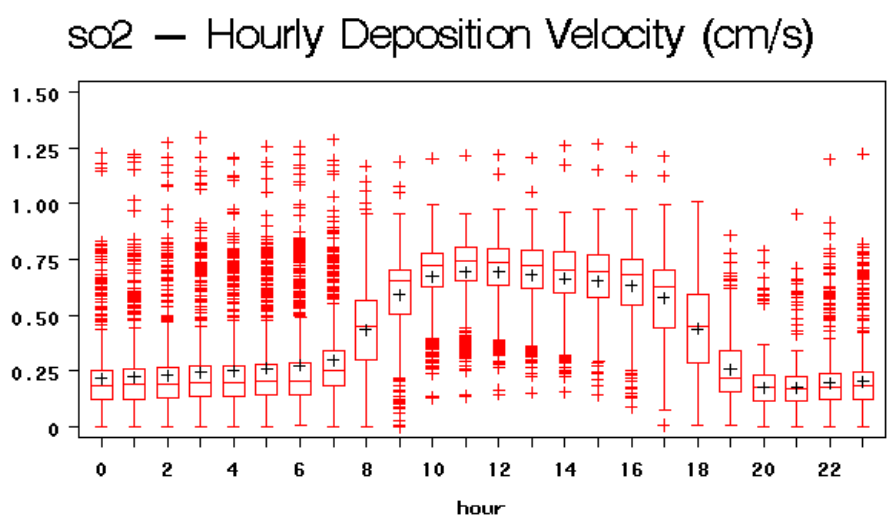


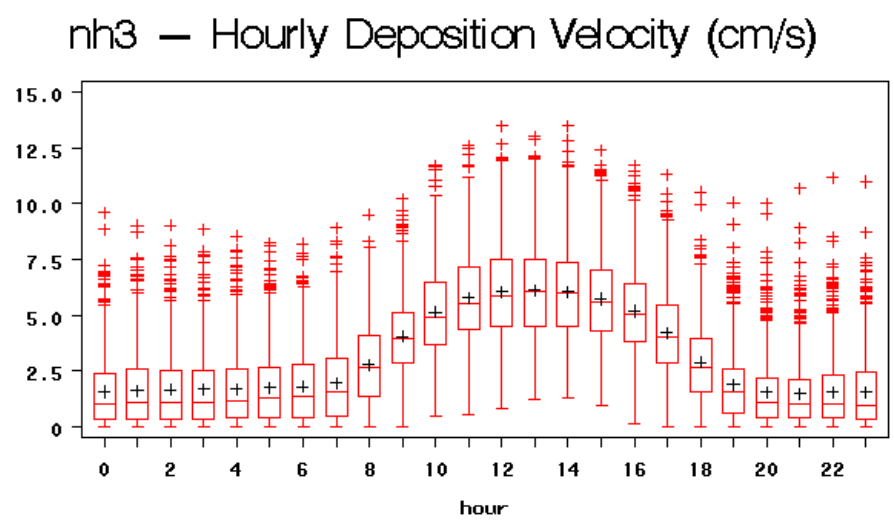
Hourly Deposition velocity (cm/s)
by species by hour over all sites



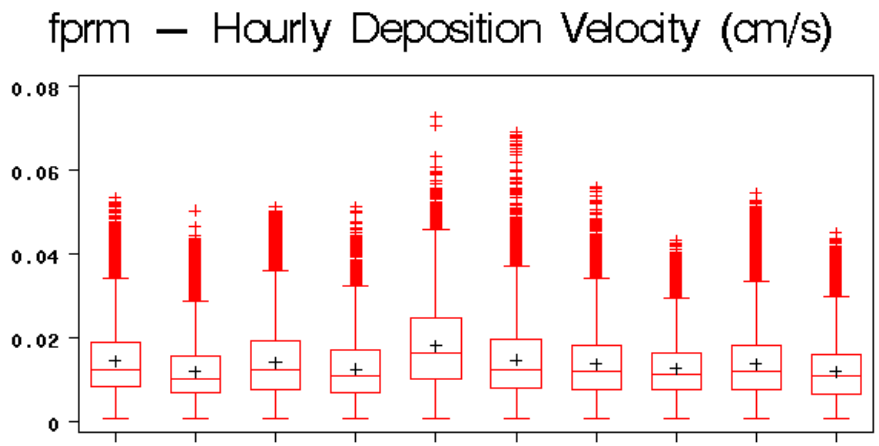


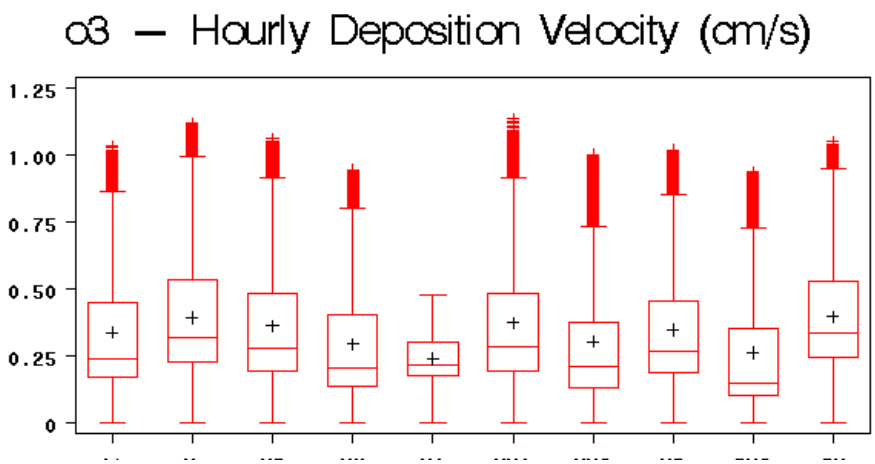


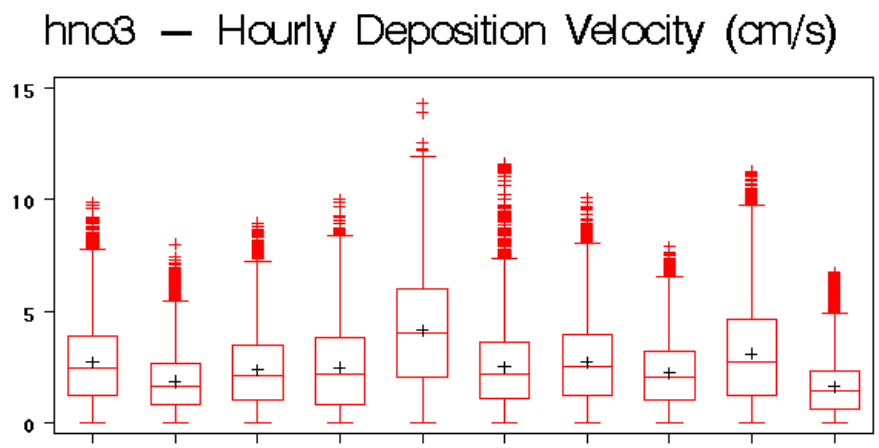


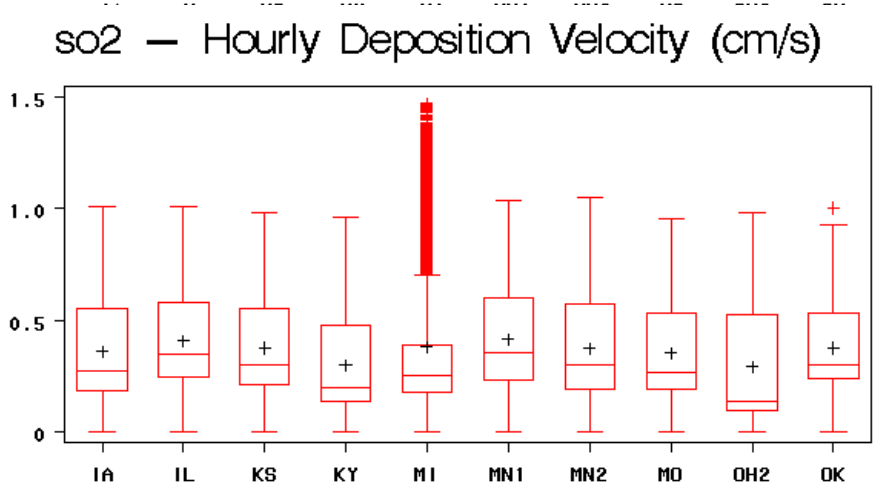


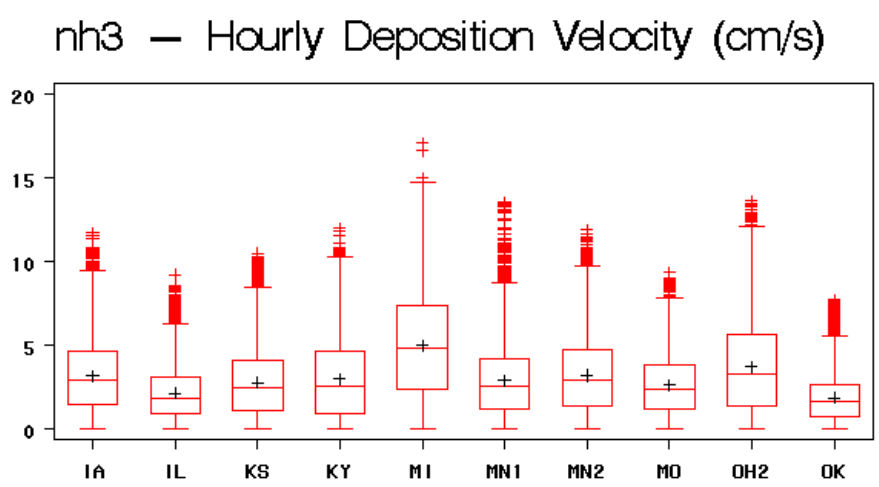
Hourly Deposition velocity (cm/s)
by species by site







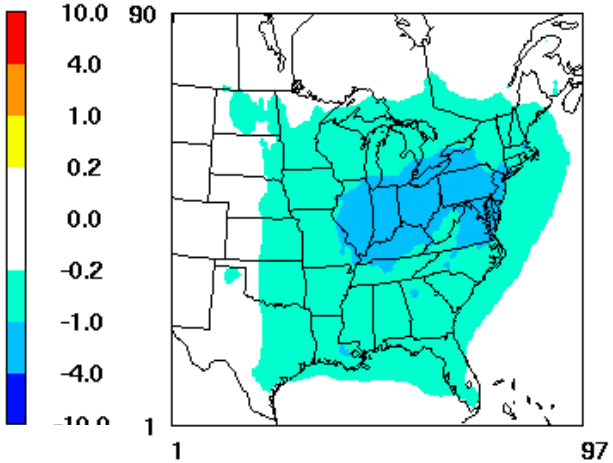




Meteorological Sensitivity Runs

- SO2 dry deposition velocity*2
- NH3 surface resistance reduced (deposition velocities decreased)
- Temperature sent to the inorganic chemistry module ISORROPIA increased by 1 K to compensate for the systematic temperature under-prediction in winter

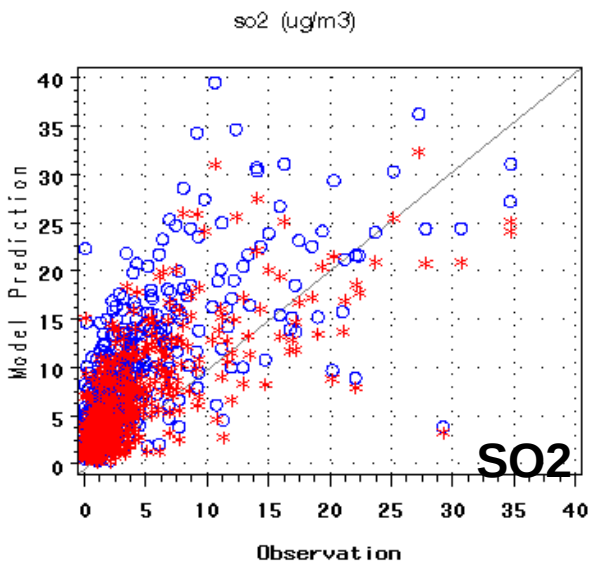
Quarter 4 Seasonal Average Difference Plot: SO2MOD-BASE

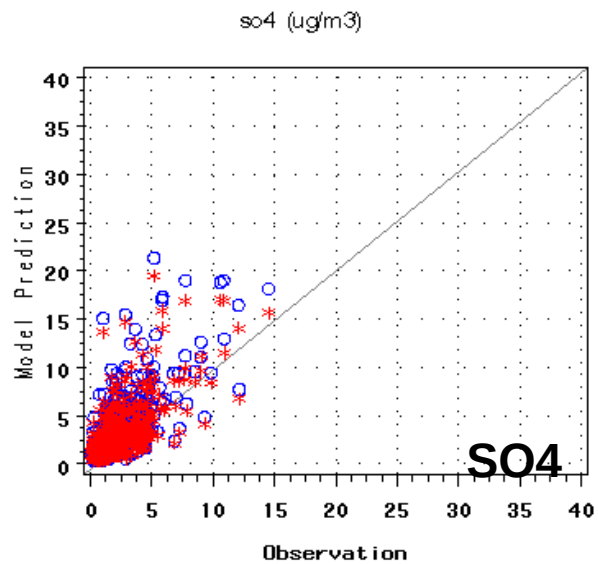


SO2 & SO4 performance metrics

Metric	Species	N	BASE	SO2 SENS	Units
Bias	SO_2	559	4.0	2.2	ug/m^3
Bias	$SO_4^=$	537	1.0	0.7	ug/m^3
Error	SO_2	559	4.5	3.1	ug/m^3
Error	$SO_4^=$	537	1.5	1.3	ug/m^3
Frac Bias	SO_2	559	90.1	68.1	%
Frac Bias	$SO_4^=$	537	31.3	23.5	%
Frac Error	SO_2	559	96.6	80.8	%
Frac Error	$SO_4^=$	537	52.1	49.0	%

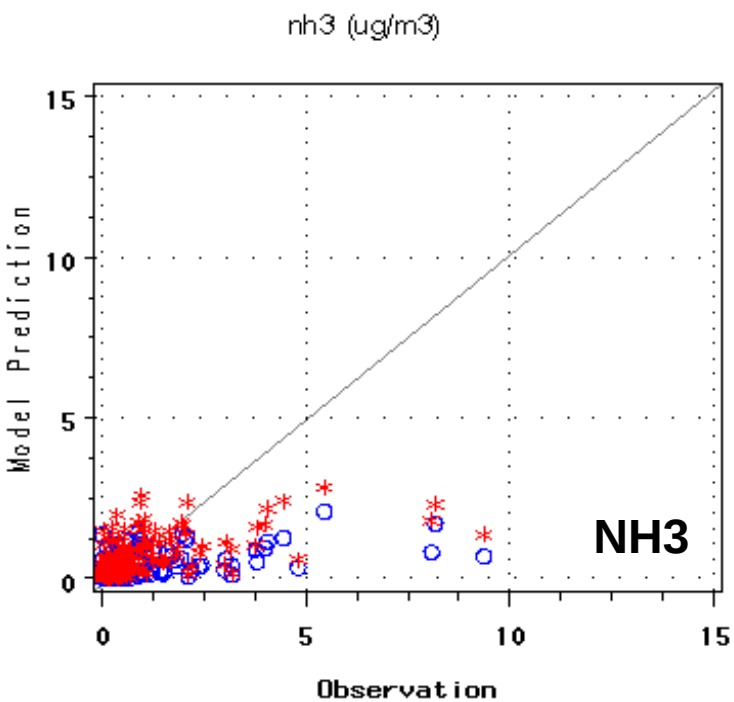
Model predictions with SO2 deposition velocity*2 (red) and without (blue)

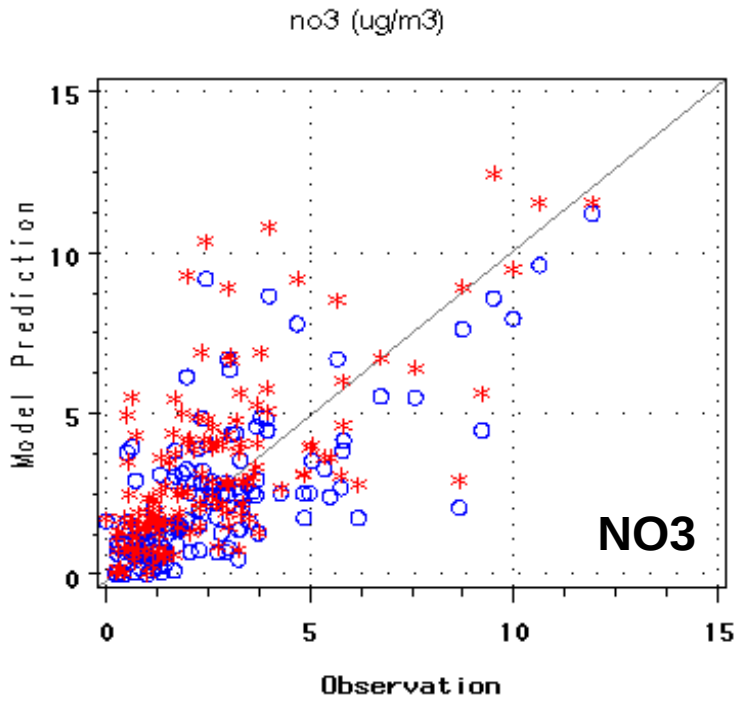




NH3 Deposition Adjustment

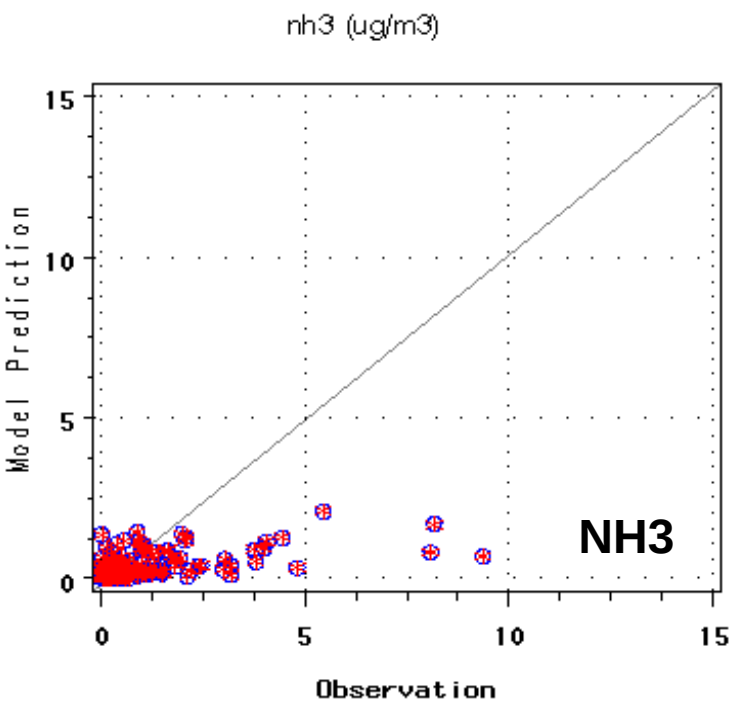
Species	N	BASE	SENS1	SENS2
NH_3	133	0.81	0.75	0.81
NO_3^-	135	1.24	1.50	1.26
HNO_3	128	0.54	0.49	0.55
SO_2	135	4.01	3.98	4.01
$SO_4^=$	136	1.01	1.06	1.01
NH_4^+	135	0.50	0.60	0.50

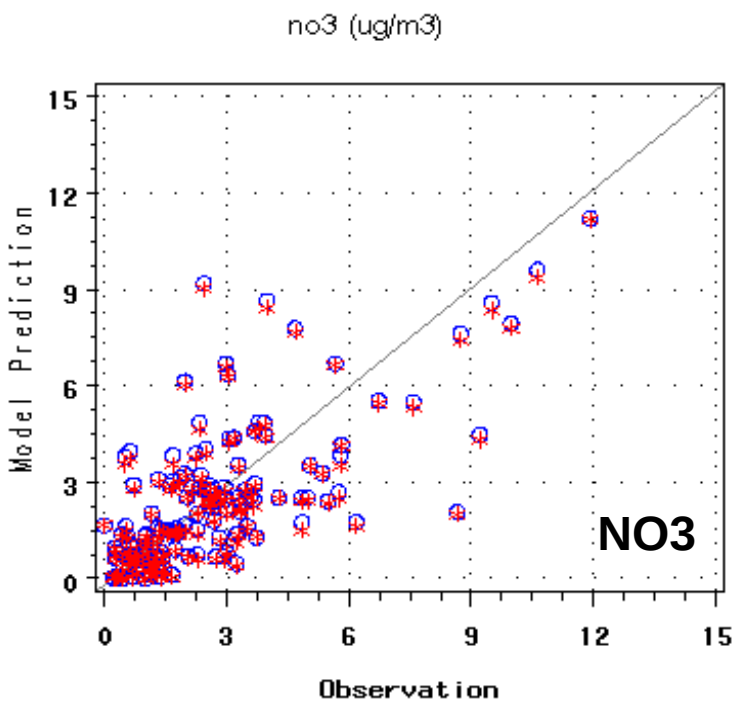




ISORROPIA Temperature Adjustment

Species	N	BASE	SENS1	SENS2
NH_3	133	0.81	0.75	0.81
NO_3^-	135	1.24	1.50	1.26
HNO_3	128	0.54	0.49	0.55
SO_2	135	4.01	3.98	4.01
$SO_4^=$	136	1.01	1.06	1.01
NH_4^+	135	0.50	0.60	0.50





Remarks

- Wind field, T, RH not systematically biasing model performance
- Wet deposition may be under-estimated in the winter
- Dry deposition for SO2 may be under-estimated by the photochemical landuse model
- Ammonia surface resistance not systematically introducing model error
- Meteorological variable bias/error not well correlated with photochemical model estimate bias/error

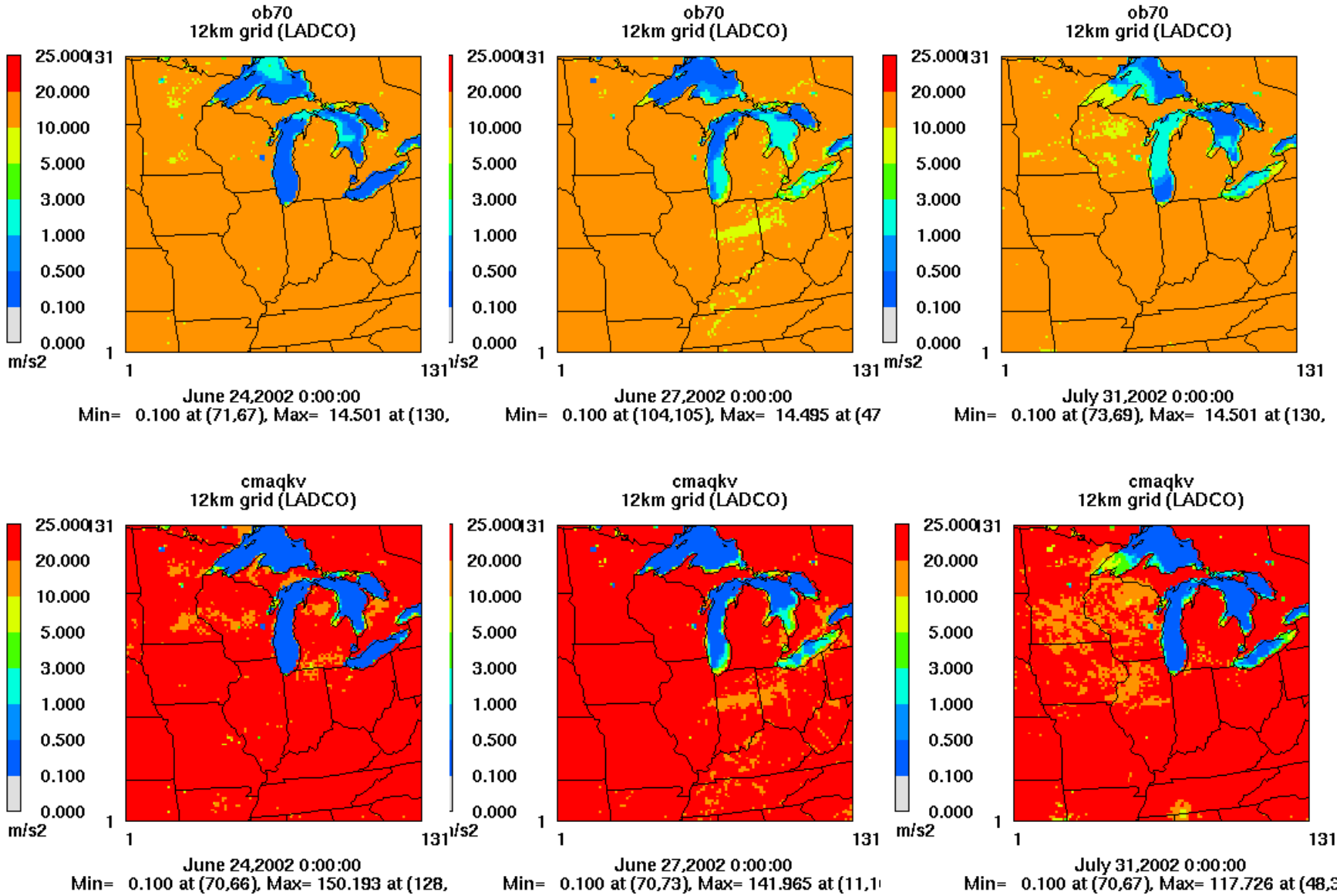
Average model deposition velocity (cm/s)

season	day	_TYPE_	_FREQ_	so2	nh3	hno3	o3	no	no2	h2o2	fprm	cprm
		0	87600	0.36	3.02	2.56	0.33	0.00	0.17	0.52	0.01	2.72
	0	1	32850	0.28	1.89	1.66	0.18	0.00	0.05	0.39	0.01	1.57
	1	1	54750	0.41	3.69	3.11	0.42	0.00	0.24	0.60	0.02	3.41
1		2	21600	0.37	2.66	2.30	0.25	0.00	0.08	0.59	0.01	2.39
2		2	21840	0.42	3.78	3.19	0.43	0.00	0.26	0.57	0.02	3.67
3		2	22080	0.41	3.16	2.64	0.42	0.00	0.28	0.54	0.01	2.70
4		2	22080	0.25	2.47	2.14	0.22	0.00	0.06	0.39	0.01	2.13
1	0	3	8100	0.36	1.94	1.70	0.19	0.00	0.04	0.55	0.01	1.64
1	1	3	13500	0.38	3.10	2.65	0.29	0.00	0.10	0.62	0.01	2.85
2	0	3	8190	0.25	2.20	1.92	0.20	0.00	0.05	0.33	0.01	1.87
2	1	3	13650	0.51	4.72	3.94	0.57	0.00	0.39	0.71	0.02	4.74
3	0	3	8280	0.24	1.64	1.44	0.17	0.00	0.05	0.29	0.01	1.27
3	1	3	13800	0.51	4.07	3.36	0.57	0.00	0.42	0.68	0.02	3.56
4	0	3	8280	0.27	1.79	1.58	0.17	0.00	0.05	0.38	0.01	1.49
4	1	3	13800	0.24	2.87	2.47	0.24	0.00	0.06	0.39	0.01	2.51

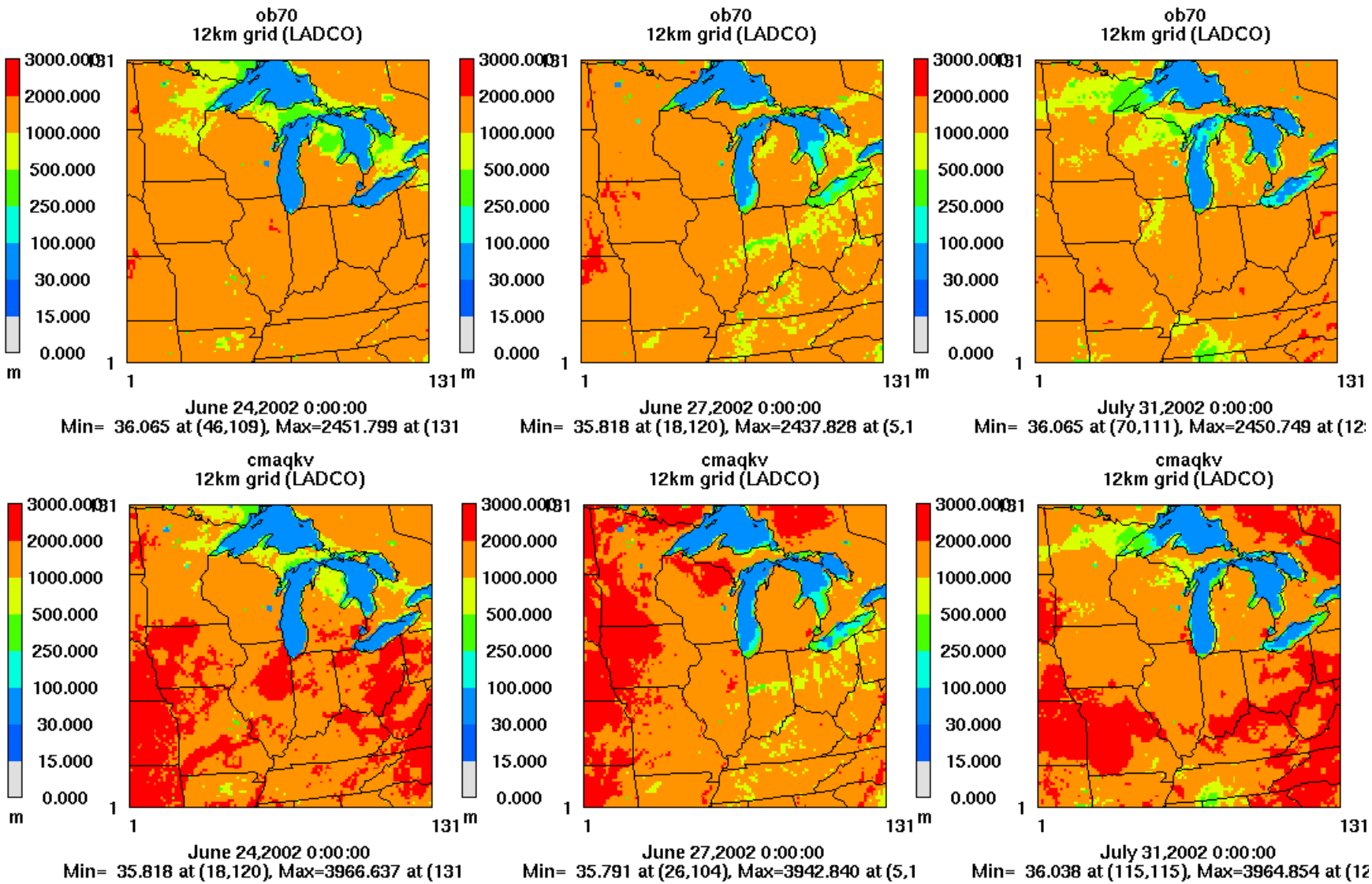
Kv diagnoses

- Plots for 3 different days (first day shown is a high ozone day in the Lake Michigan region)
- Plots show max Kv and max PBL (as diagnosed based on Kv values in metpave utility)
- Plot color bins designed to show detail over the Great Lakes
- There is a tiny bit of mixing over the Lakes on certain days; but both schemes have a gradient that can span several orders of magnitude between land and water—especially the cmaq Kv scheme
- Minimum Kv is .1; but can increase up to 1.5 in the lower 3 layers of the model if a grid cell is 100% urban (kvpatch)

Maximum Kv (Layer 1)



Maximum PBL Height

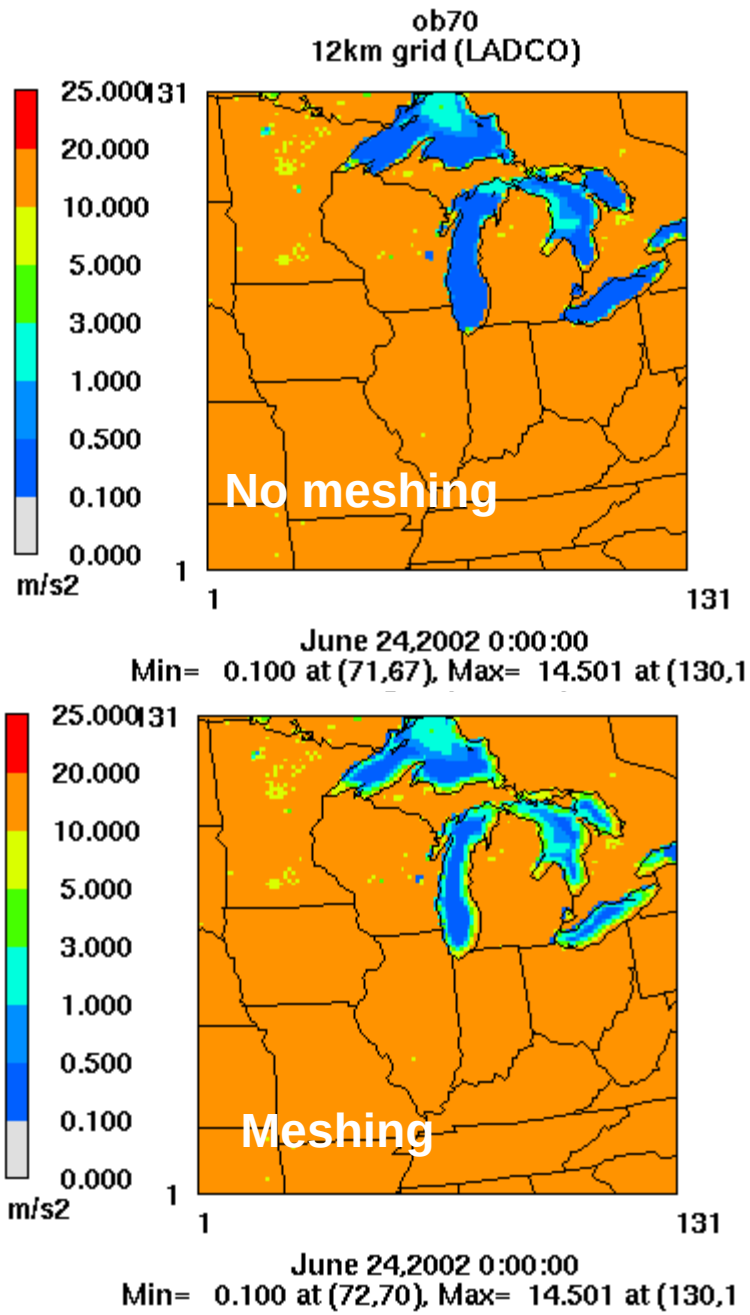


- Develop simple interpolation scheme to smooth Lake grid cells next to the shore and remove the sharp gradient

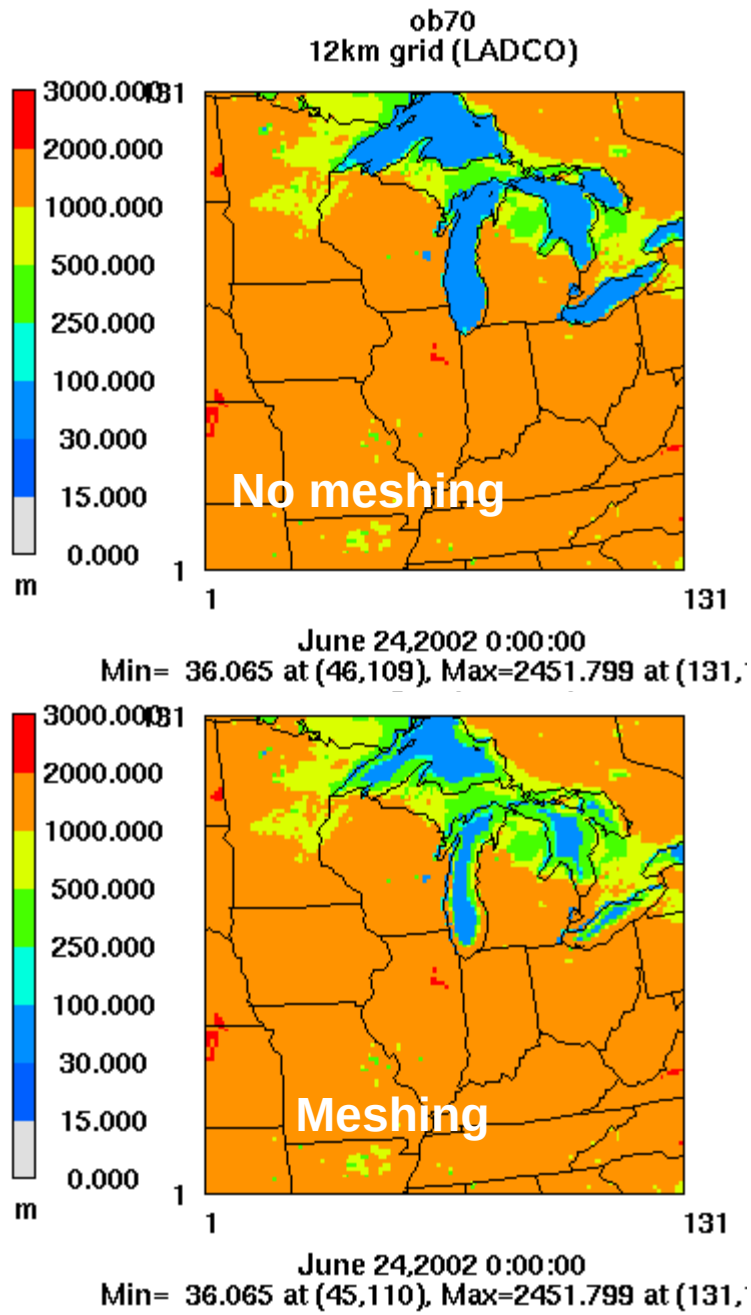
Kv adjustments

- Adjusting Kv values to better reflect transition of vertical mixing from land to Lakes – method called Kv “meshing”
- This technique increases the Kv values (which effectively increases the PBL height)
- Problems seen near Lake shore where complex high emissions are located at shore; Kv values are over 10 during the day on the shore grid cells and .1 on the Lake grid cells
- This seems to help perpetuate the model “NOX disbenefit” in some areas around Lake Michigan-most notably NW Indiana
- Plots on the next page show the Kv values and PBL values at noon for an episode day in the 12km domain: standard values on top and new KVMESH on bottom

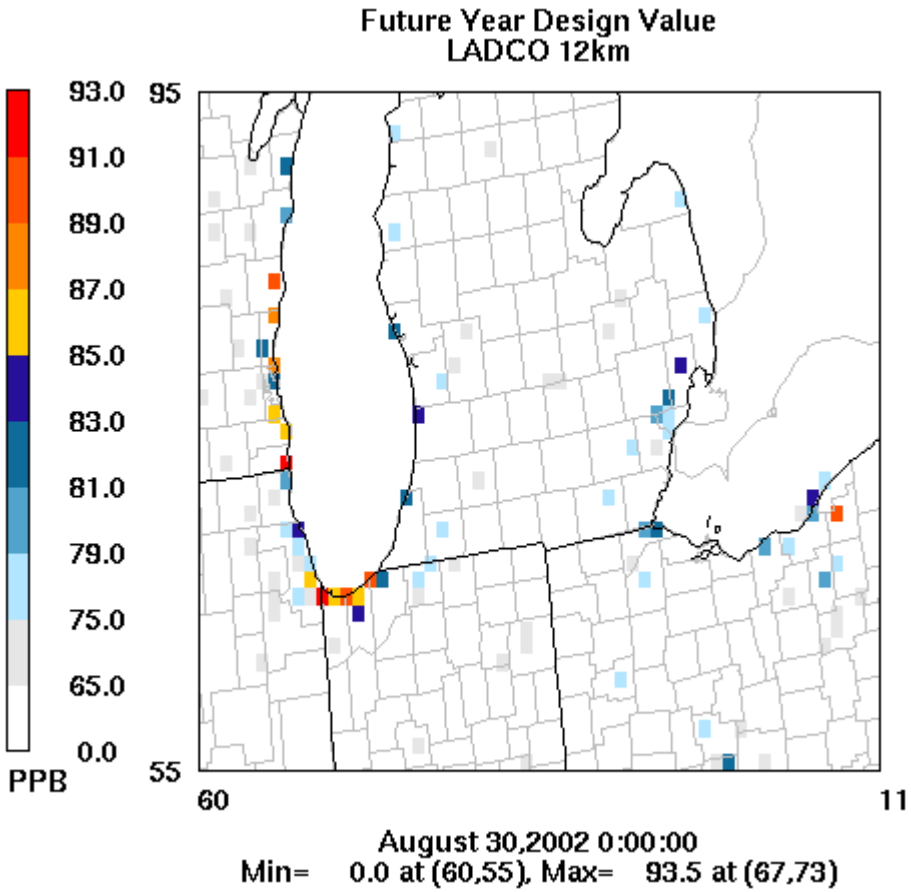
Vertical Diffusivity



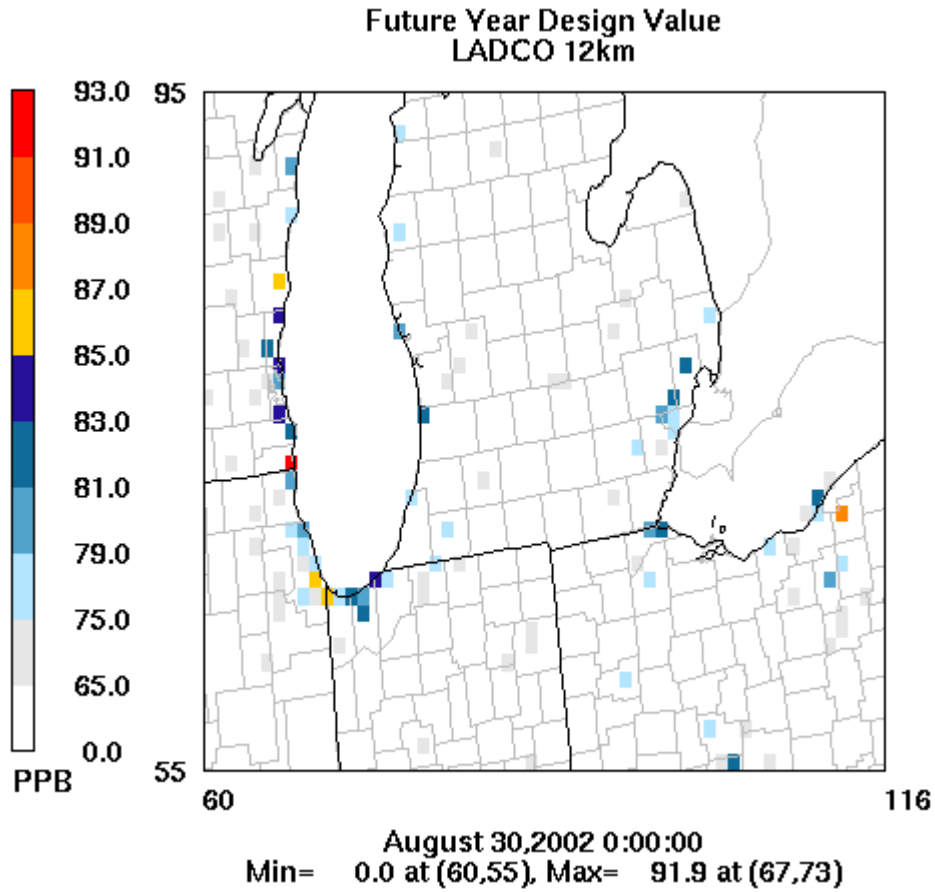
PBL Height



J2015R3S2 8hr O3



J2015R3S2 8hr O3 with the KVMESH Kv fields



Kvmesh Estimation

When grid cells have > 75% water, their Kv = the higher of the cell specific estimated value or the average of the 5x5 array of cells

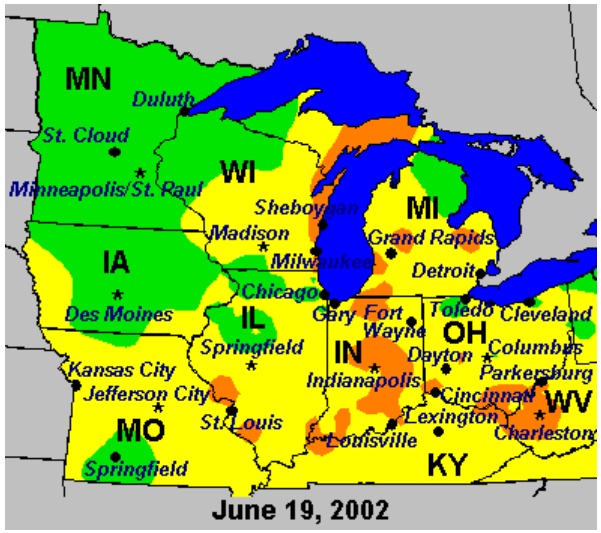
An additional adjustment is made to increase the Kv minimum to a landuse weighted value; this would mean a minimum Kv of 1.0 in an urban grid cell at at any hour of the day

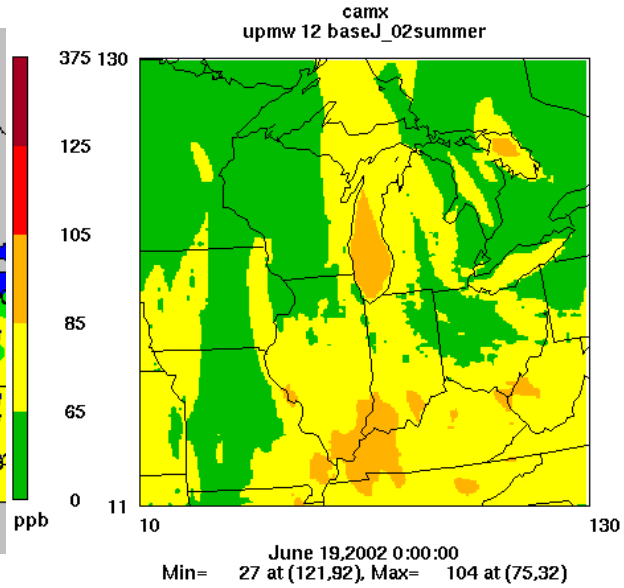
Spatial Plots – Model Performance

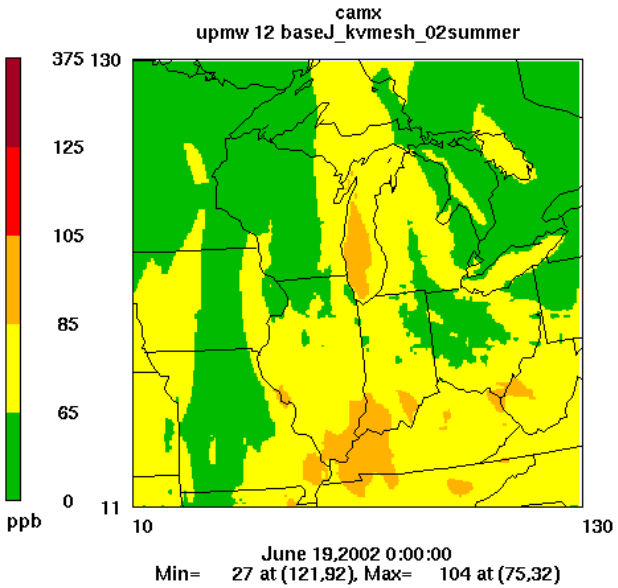
- 8 HR O3
- Daily Peak Plots
- 12 km Base J and base J with kvmesh
- AIRNOW spatial maps of observations
- No large differences in peak O3 model performance except over the Lakes

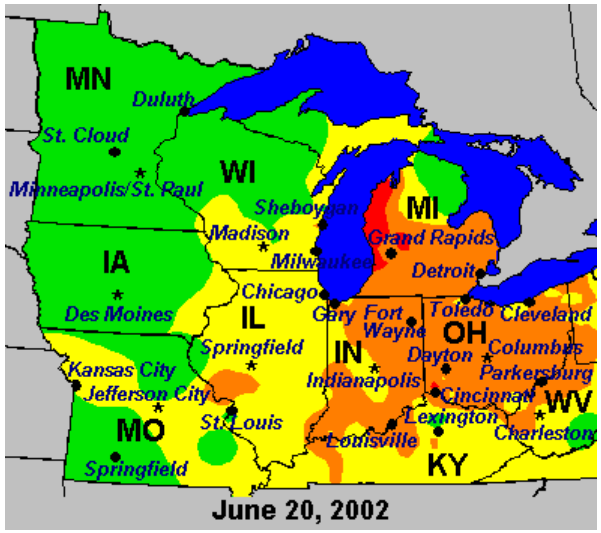
BASE J

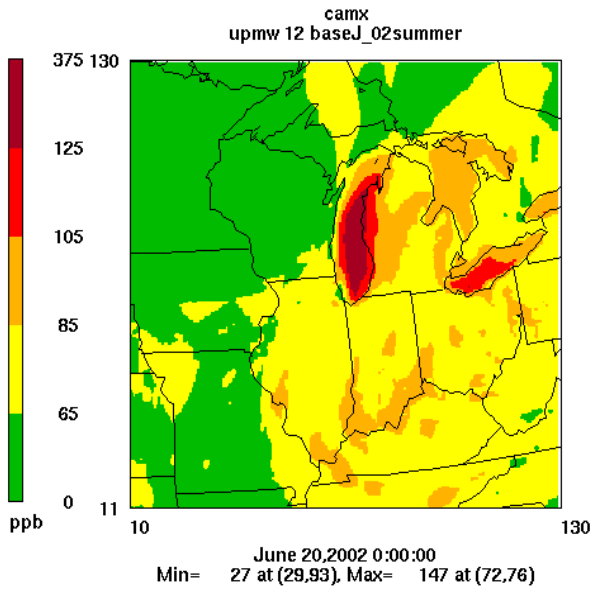
BASE J - KVMESH

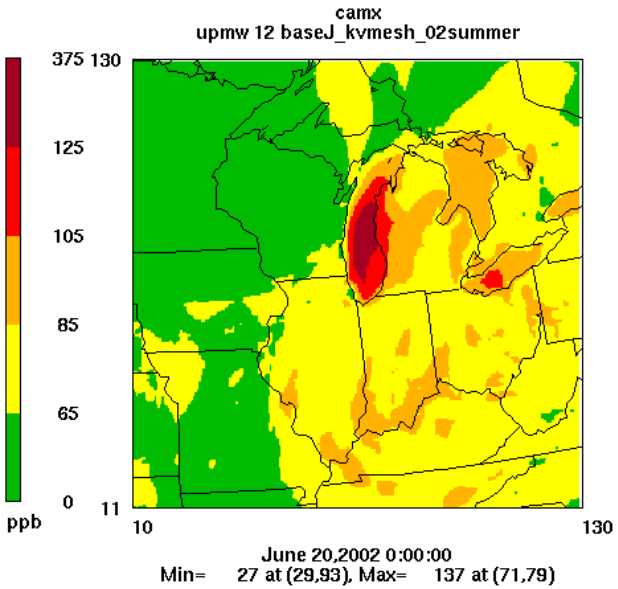






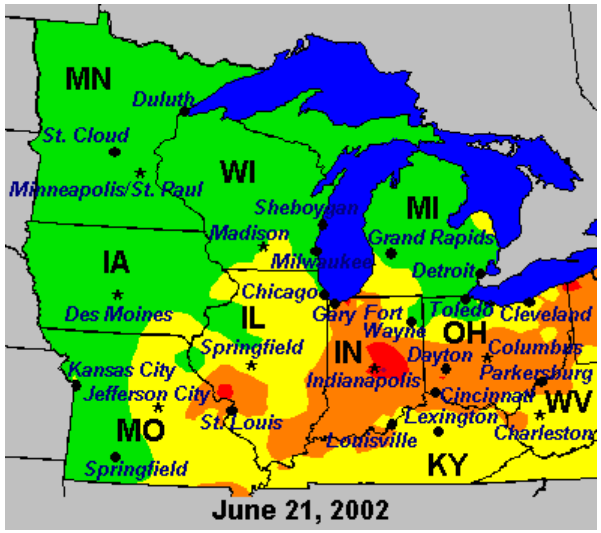


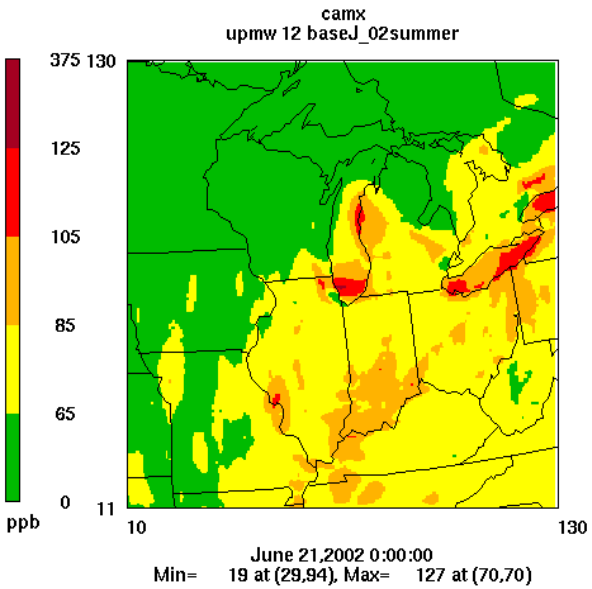


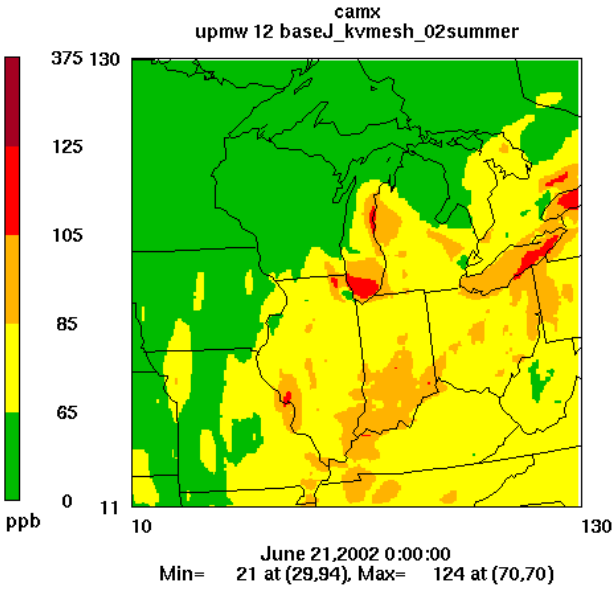


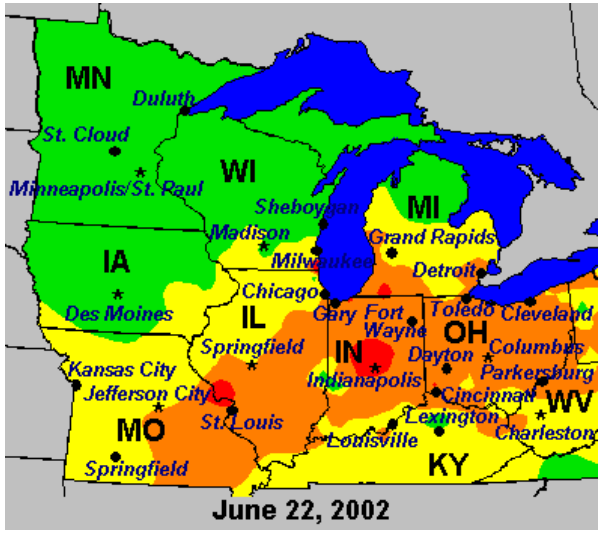
BASE J

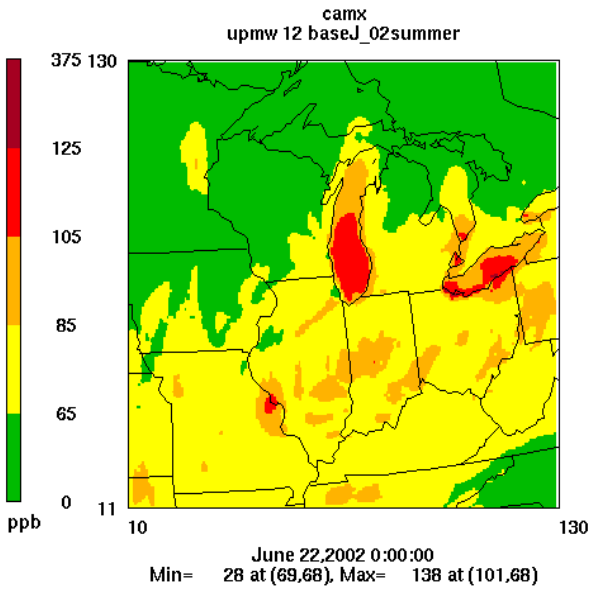
BASE J - KVMESH

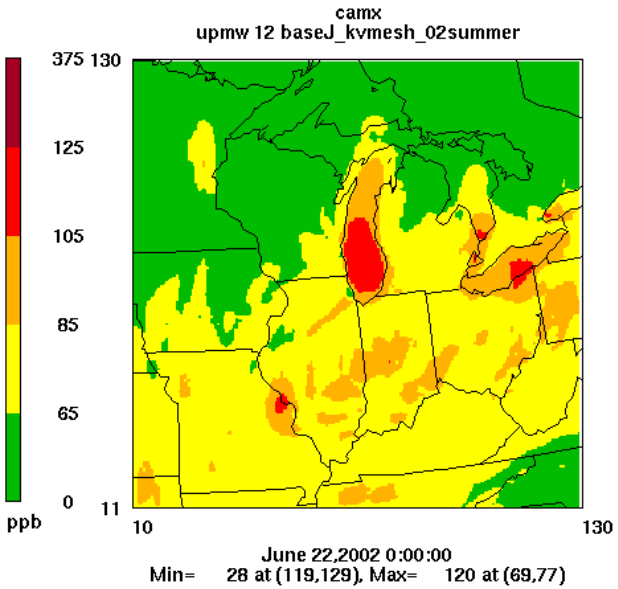






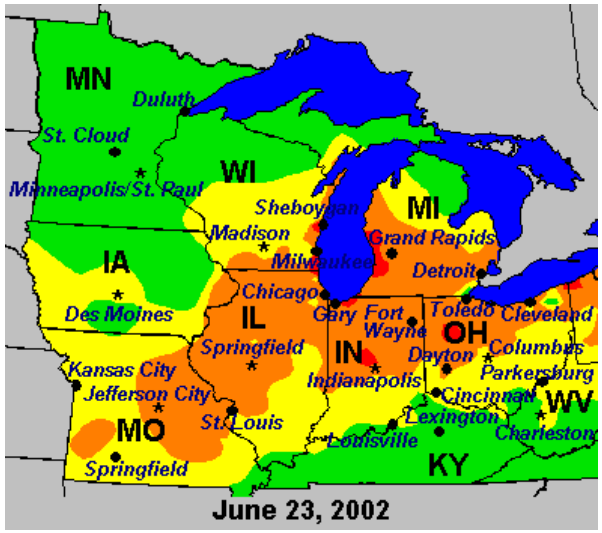


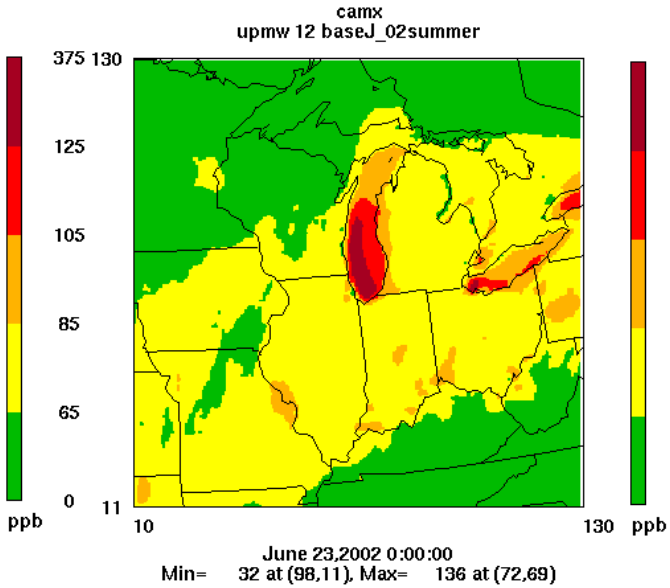


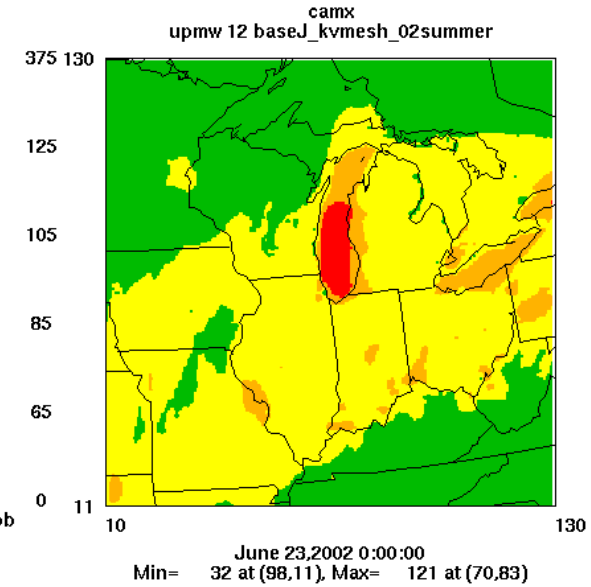


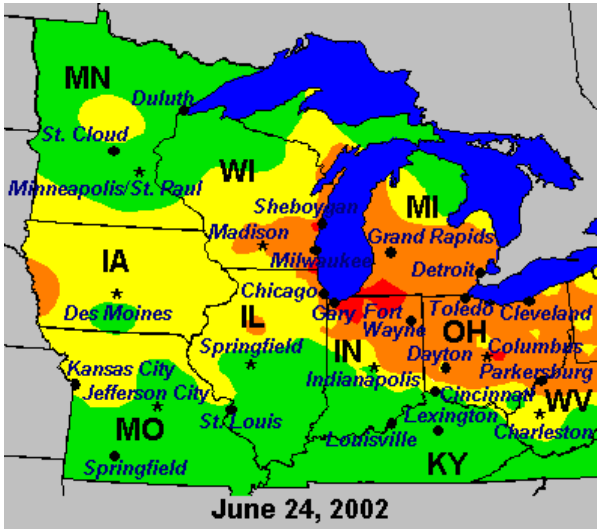
BASE J

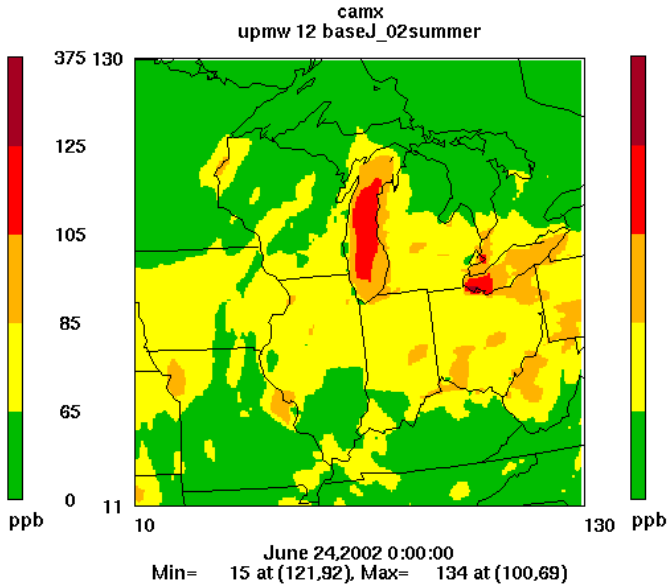
BASE J - KVMESH

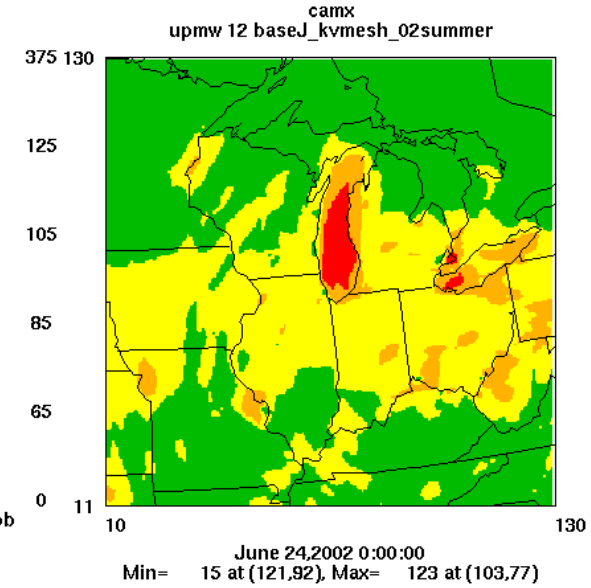


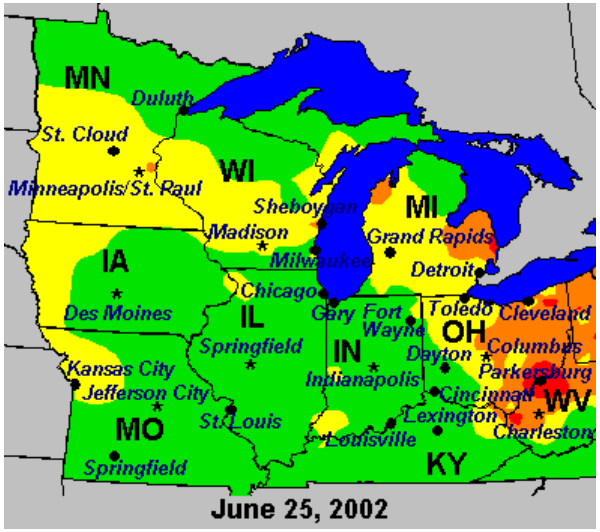
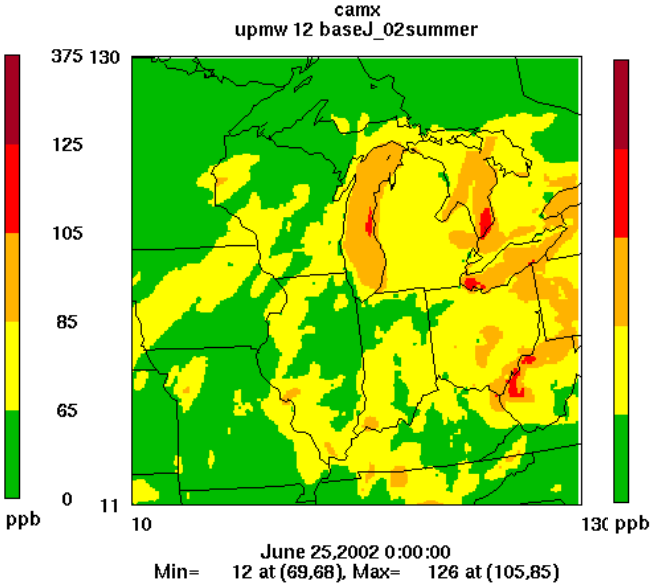
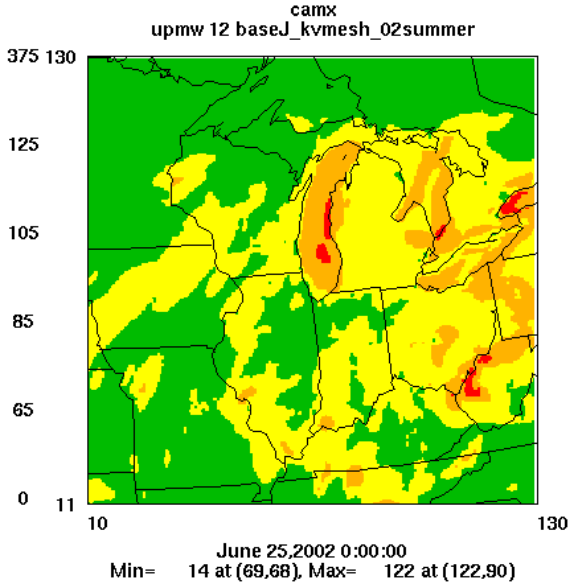










BASE J

BASE J - KVMESH