An Evaluation of an Annual 2005 MM5 Simulation to Support Photochemical and Emissions Modeling Applications

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INTRODUCTION

The entire year of 2005 is simulated with the Fifth-Generation NCAR / Penn State Mesoscale Model (MM5) v3.7 to develop meteorological inputs to support emissions and photochemical modeling. MM5 consists of the Mesoscale model MM5 and a suite of pre-processors including PREGRID, REGRIDDER, RAWINS, LITTLE R, INTERPF, INTERPX, and TERRAIN (Dudhia, 1993 and Grell et al, 1994).

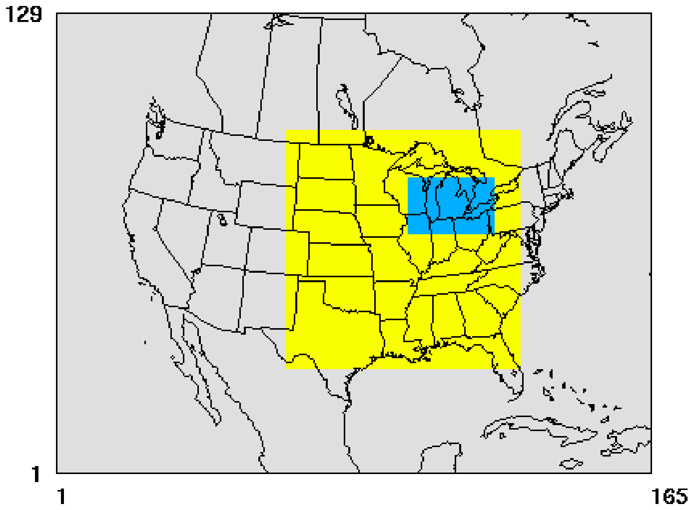
The model parameterizations and physics options outlined in this document were chosen based on the results of a series of sensitivity runs. The performance of the sensitivity tests provided a clear indication of an optimal configuration for the Upper Midwest based on temperature, mixing ratio, and wind field (Johnson, 2003).

The annual 36/12 km and summer season 4 km MM5 modeling was completed by Dennis McNally of Alpine Geophysics, L.L.C. under contract from a consortium of industrial stakeholder groups from the central United States. Wusheng Ji from Wisconsin DNR also completed 36/12 km MM5 runs for the summer season of 2005.

TERRAIN

The TERRAIN processor defines the horizontal grid of the MM5 application. The 24 category USGS 2 minute (~4 km) data is used for the 36/12/4 km domains. The National RPO grid is a Lambert conic projection centered at coordinates –97, 40 with first and second true latitudes at 33 and 45 degrees (See Figure 1).

Figure 1. Horizontal Domains



The 36 km grid contains 165 x 129 grid cells and the 12 km has 193 x 199 grid cells. The 12 km grid is two-way nested within the mother grid to allow fine grid feedback into the coarse grid. Additional options are set to allow generation of data to support the Pleim-Xiu land surface module. Variables LSMDATA and IEXTRA are both set equal to TRUE. The 4 km grid is one-way nested from the 12 km grid and has 241 cells in the X direction and 142 cells in Y direction.

Table 1. Modeling Domain Specifications

Domain ID	Grid	X Cells (East-West)	Y Cells (North-South)	Cell Size (km)	Mother Domain ID	Lower Left X,Y of Nest
1	National RPO	165	129	36	1	1, 1
2	Midwest	193	199	12	1	66, 30
3	Great Lakes	241	142	4	2	

PREGRID

The PREGRID processor converts meteorological analyses data such as NCEP or ETA to an intermediate data format that the REGRIDDER processor can utilize. For PREGRID, the following options were set:

- ETA/AWIP 3D and SF analyses data (ds609.2) is used to initialize the REGRID processor.
- Snow cover is estimated from water equivalent snow depth.
- The input analyses data is processed 3 hourly (10,800 seconds).
- The AWIP grib definition tables are used to map ETA data into MM5.
- The ETA skin temperature is used as the source of sea surface temperature.
- The ETA analysis files with the extension “.tm12” are not used since they are the "cold start" global analysis files.

REGRIDDER

The REGRIDDER processor takes the data extracted from analyses fields and interpolates the data to user specified pressure levels and to the user specified horizontal grid.

LITTLE R

The RAWINS and LITTLE R processors perform objective analysis on the output from REGRIDDER using surface and upper air observation data. Since these observations are incorporated into the ETA analysis fields this step is considered redundant.

Results of sensitivity tests where ETA 3-hourly analysis was utilized to initialize with and without RAWINS objective analysis demonstrated little or no difference in model performance (Baker, 2002).

Even though this step is redundant, LITTLE R is applied to enable surface nudging of soil moisture and temperature in the Pleim-Xiu land surface module. NCEP ADP surface (ds 464.0) and upper air (ds 353.1 and ds 353.4) data are the appropriate data to input into LITTLE R and/or RAWINS.

INTERPF

The INTERPF processor takes the REGRIDDER/LITTLE R output that is at standard pressure levels and interpolates that data to the vertical grid defined by the user (Table 2). The vertical grid is defined in terms of sigmas, where 1 is the surface and 0 is the top of the model atmosphere. The top of the MM5 simulation is 100 millibars, which is approximately 15 kilometers above ground level.

Table 2. Vertical Grid Structure

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--

The vertical atmosphere was resolved to 34 layers, with thinner layers in the planetary boundary layer. The layer configuration was selected to capture the important diurnal variations in the boundary layer while also having layers in the upper troposphere to try and resolve convective activity. Output from the INTERPF processor is ready for input into MM5.

INTERPX

The INTERPX processor is used to extract the soil temperature and soil moisture data from MM5 output files and overwrite the soil temperature and moisture fields on the MMINPUT file for the next 5 day simulation block. This allows soil moisture and temperature to be carried over to subsequent modeling simulations.

For example, to simulate 20 days in 4 blocks of 5 days, the first block of 5 days would use the standard MMINPUT to run MM5, and the subsequent 3 blocks of 5 days would take the MM5 output and extract soil temperature and moisture data for the next 5 day block. This option has been shown to introduce a cold bias for the temperature field, particularly in the winter months (Olerud, 2003). INTERPX was not used for any of the MM5 simulations.

MM5

The output from INTERPF, LITTLE R, and TERRAIN processors were used to run MM5. These files must be in the "./MM5/Run" directory and have the generic filenames given directly out of these processors. Three dimensional analysis nudging for temperatures, and moisture is applied above the boundary layer only. Analysis nudging for the wind field is applied above and below the boundary layer. Analysis nudging is not performed on the rotational wind field. In addition, the observation nudging flag is turned off. This type of nudging is appropriate when there is a very dense set of observation data from a field study, which this application lacked. The default nudging weighting factors are used for all simulations: 2.5×10^{-4} for wind fields and temperatures and 1.0×10^{-5} for moisture fields.

Table 3. Physics and configuration options

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

Table 3 outlines the model configuration used for MM5 modeling up to the date of this document. All simulations use the mixed phase moisture scheme so that all four phases of water will be explicitly output by MM5. This is important since the photochemical model is applied for an annual basis and correctly characterizing the phase of water is important for several physiochemical processes.

Atmospheric radiation is calculated every 15 minutes in the model. Vertical moisture and temperature advection are set to use linear interpolation. Other important variables switched to ON include: moist vertical diffusion in clouds, temperature advection using potential temperature, diffusion using perturbation temperature, 3D coriolis force, and upper radiative boundary condition. Sea surface temperature and snow cover are set to vary with time.

The Pleim-Xiu land surface module requires that 3 additional variables be set in the MM5 deck: ISMRD, NUDGE, and IFGROW. ISMRD is set to use soil moisture fields from the ETA analyses. NUDGE is set to nudge soil moisture data to the analyses fields. IFGROW is set to option 2, which takes vegetative growth into account based on vegetative fraction data from the TERRAIN file.

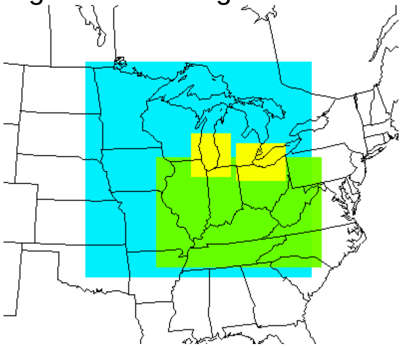
MODEL EXECUTION

MM5 was executed in 5 day blocks (7200 minute simulation) initiated at 12Z with a 90 second time step. Model results are output every 60 minutes and the model output files are written out (i.e. split) every 24 hours to accommodate post-processing utilities. The 36 and 12 km domains were run for the entire year of 2005. The 4 km summer season simulation was initiated on May 29 and was run through September 20.

MODEL PERFORMANCE EVALUATION

Model performance was assessed quantitatively with the METSTAT tool from Environ (Emery et al, 2001). Model predictions are compared to Techniques Data Laboratory U.S. and Canada surface hourly observations (NCAR dataset ds472.0). The MM5 model outputs predictions approximately 15 meters above the surface while observations are at 10 meters. METSTAT applies micro-meteorological adjustments to the MM5 estimates to approximate 10 m values. MM5 outputs near-instantaneous values (90 second time step) as opposed to the values with longer averaging times taken at monitor stations. This should be considered when interpreting model performance metrics.

Figure 2. Sub-regions for metric estimation



Model performance metrics were applied to sub-regions (Figure 2) of the modeling domain, meaning the metrics are hourly spatial averages of multiple monitor locations. This is done to gain a better understanding of MM5 performance for sub-regions of interest: Lake Michigan, Detroit-Cleveland, the Ohio Valley, and Upper Midwest. All metrics are calculated within the specified model performance region for an hourly and daily time period. Mean wind direction is estimated by averaging the U and V wind vector components and converting those averages to compass degrees.

Additional analysis of rainfall is done on a monthly basis. Rainfall observation analysis data is available from the National Weather Service Climate Prediction Center (CPC) on an hourly basis for the Continental United States (National Weather Service, 2006). The rainfall analysis resolution is 0.25 degree longitude by 0.25 degree latitude (approximately 40 km by 40 km) and extends from 140W to 60W and 20N to 60N. The CPC rainfall analysis data does not include any portion of Canada, Mexico, or anywhere off-shore of the United States.

METRICS

Model performance is described using quantitative metrics: mean bias and mean (gross) error (EPA, 2001; Boylan et al., 2006). These metrics are useful because they describe model performance in the units the meteorological term is measured in. Performance is best when these metrics approach 0. Rainfall performance is examined qualitatively with side-by-side monthly total rainfall plots.

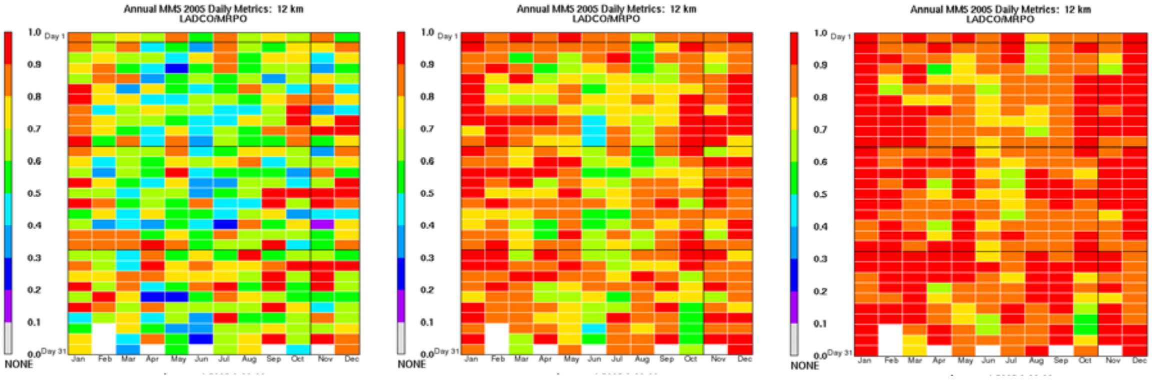
Table 4. Model Performance Metrics

Mean Bias	$= \frac{1}{N \times M} \sum_{i=1}^{N} \sum_{j=1}^{M} \left(A_i^j - B_i^j \right)$
Mean (Gross) Error	$= \frac{1}{N \times M} \sum_{i=1}^{N} \sum_{j=1}^{M} \left\| A_i^j - B_i^j \right\|$

A = model prediction and B = observation

The index of agreement metric is commonly used to describe meteorological model performance. This metric is not used in this document because the index of agreement is largely a function of the number of observation-prediction pairs being used to estimate the metric. This is illustrated using the mixing ratio index of agreement in Figure 3 for the Detroit-Cleveland region, the Ohio Valley region, and the upper Midwest region.

Figure 3. Humidity Index of Agreement at 12 km for the Detroit-Cleveland region (left), Ohio Valley region (center), and Upper Midwest region (right)

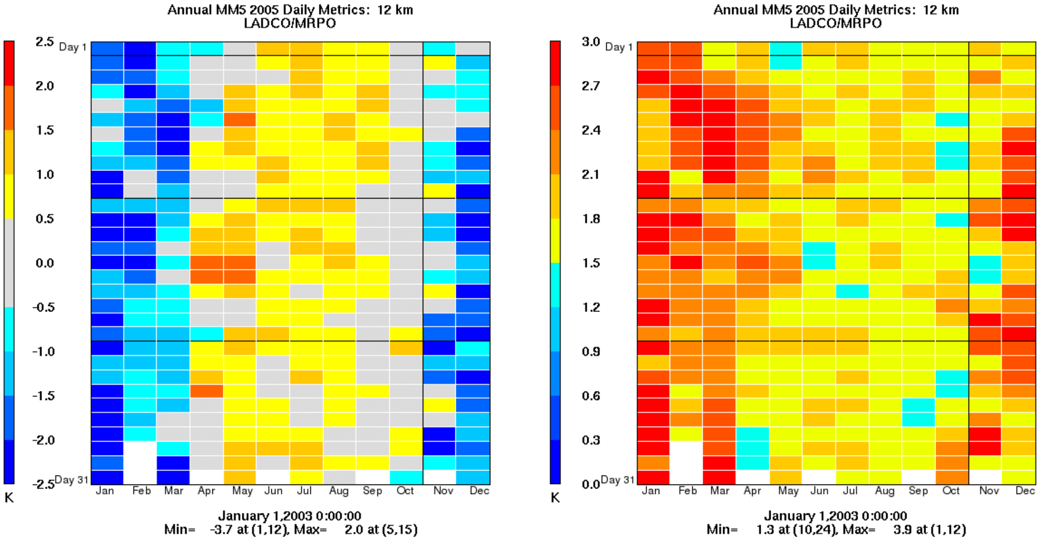


This figure clearly shows that as more stations are included in the calculation, the metric estimates get closer to 1.0, which is considered excellent model performance. This metric is clearly a function of prediction-observation pairs and is not a good indicator of model performance. The example shown is using mixing ratio, but a similar trend is seen for temperature and wind speed.

TEMPERATURE

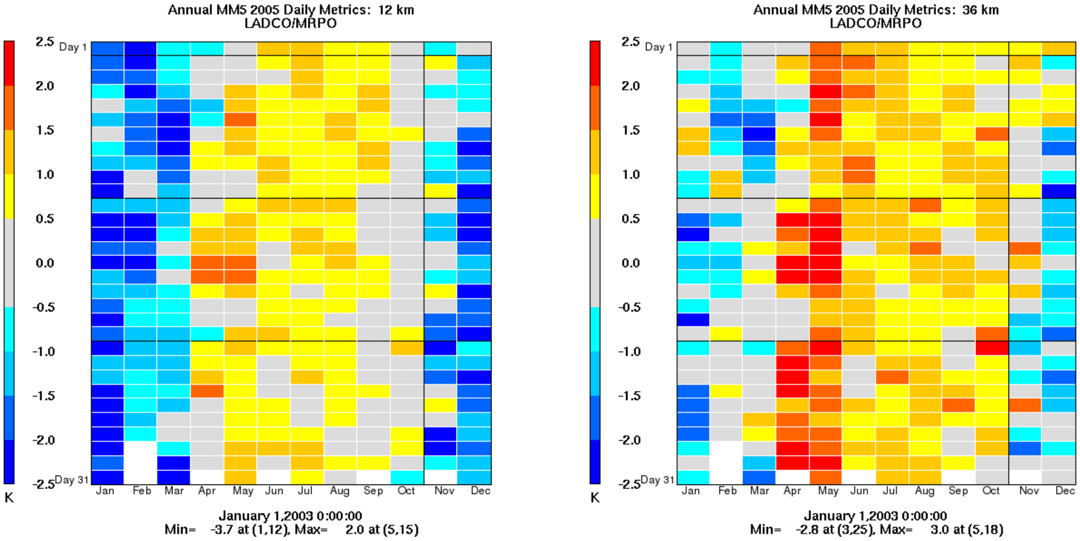
Daily average temperature bias and error metrics are shown in Figure 4 for the 12 km MM5 output covering the upper Midwest domain. The MM5 modeling system tends to under-predict temperature in the coldest months, November to March, and over-predict daily average temperatures in the warmest months. The daily average error is highest during the coldest months. The over-predictions in the summer months are driven by over-estimates during the night-time hours.

Figure 4. Temperature bias (left) and error (right) for 12 km Upper Midwest region



The 36 km MM5 output covering the upper Midwest domain show a systematically higher day-to-day bias and error (Figure 5).

Figure 5. Temperature (K) for the Upper Midwest region at 12 km (left) and 36 km (right)

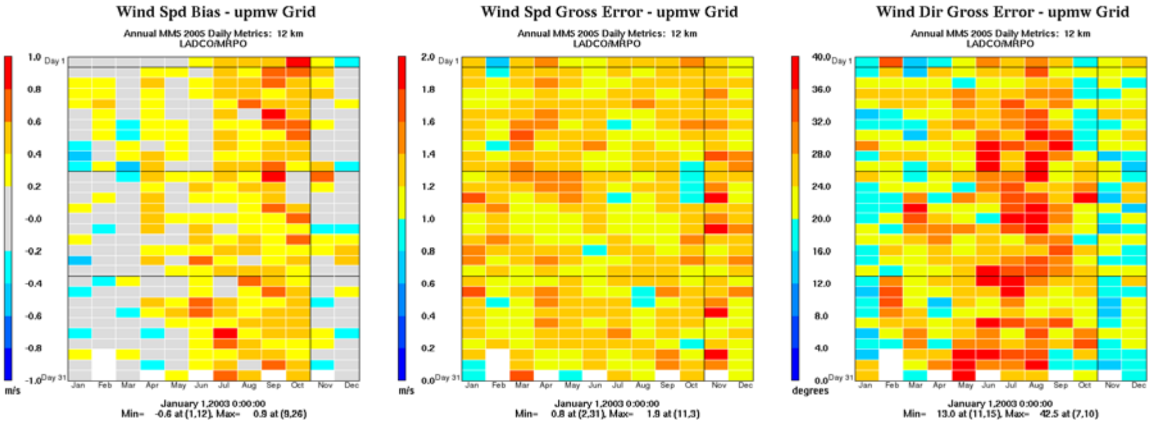


The cold bias in winter and night-time over-predictions in the summer are model performance features common to other annual MM5 simulations for the central United States. The photochemical model performed reasonably well for ozone and particulate matter using annual MM5 output from 2001, 2002, 2003, and 2004 with similar temperature performance features (Baker, 2005a; Baker, 2005b). The typical 1 degree Kelvin under-prediction of temperature during cold months is not enough to result in systematic performance degradation for PM2.5 ammonium nitrate (Baker & Scheff, 2007).

WIND FIELD

Daily average wind speed bias, wind speed error, and wind direction error are shown for MM5 12 km output covering the upper Midwest domain in Figure 6. Wind speed bias is minimal in the cold months and slightly over-predicted in the summer months. The largest over-predictions are seen in the early fall months of September and October. Wind speed bias is consistently between 1.0 and 1.5 m/s for most days of the annual simulation. The daily wind direction error is typically between 15 to 30 compass degrees. The highest wind direction error is in the summer when generally between 25 to 40 compass degrees.

Figure 6. Wind Speed (left) bias, Wind Speed error (center), and Wind Direction error (right) for 12 km Upper Midwest region

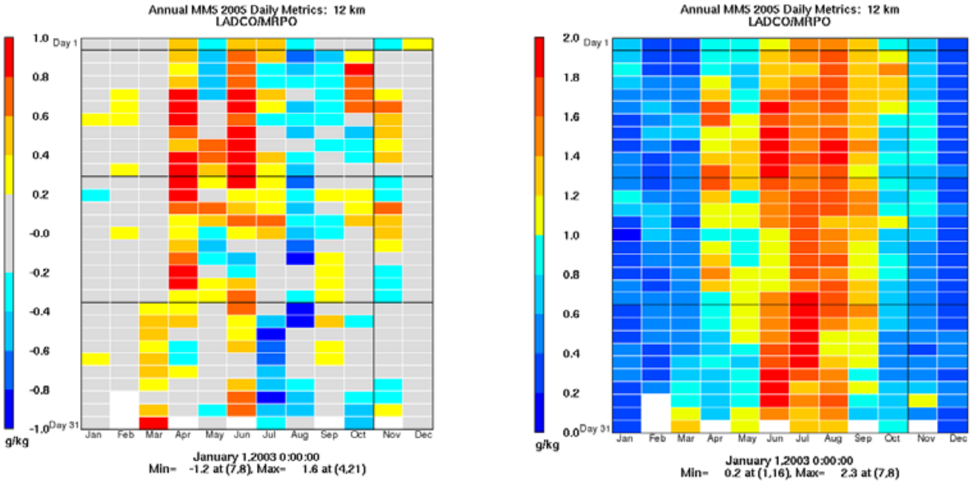


Wind speed and wind direction error is very similar at 12 and 36 km over the upper Midwest region. The wind speed bias tends to be slightly higher at 36 km compared to 12 km.

MIXING RATIO

Daily average mixing ratio bias and error are shown for the MM5 12 km output over the upper Midwest domain in Figure 7.

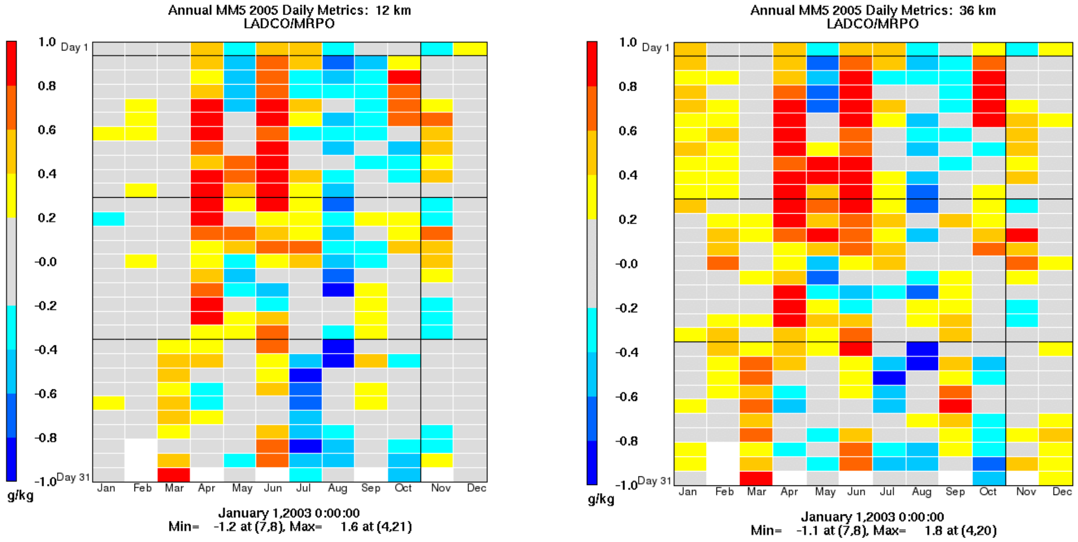
Figure 7. Mixing ratio bias (left) and error (right) for 12 km Upper Midwest region



Mixing ratio is over-predicted in the model from late March to mid-April and again during June. Mixing ratio is under-predicted from late July to late August. The error is highest during the warmer months, starting in April and ending in mid-September. Little bias and error are seen in the winter since there is little moisture in the air during these months.

There is little difference in error when comparing the 36 km and 12 km performance over the upper Midwest domain. However, mixing ratio predictions are systematically higher at 36 km compared to 12 km as shown in the daily bias in Figure 8, most notably during the colder months.

Figure 8. Mixing ratio bias for the Upper Midwest region at 12 km (left) and 36 km (right)



RAINFALL

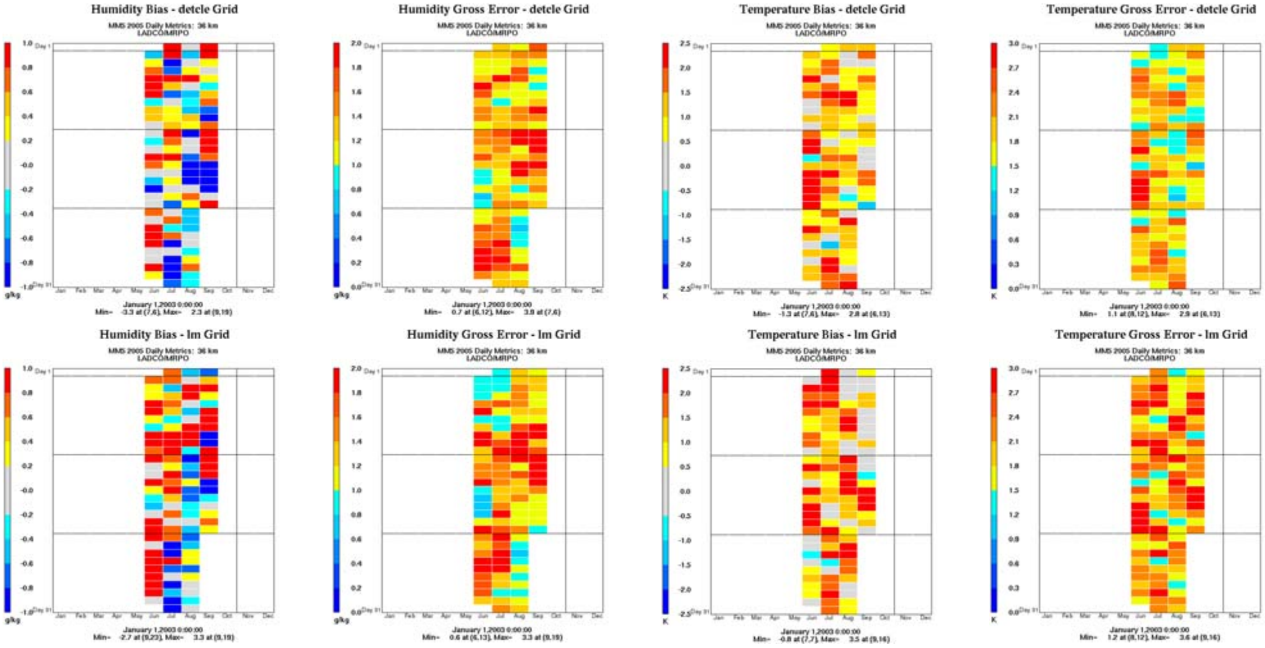
Monthly rainfall estimates from MM5 36 km output are compared qualitatively to rainfall analysis fields developed by NCEP for the central and eastern United States (Appendix A). Rainfall predictions match up well in magnitude and spatially during the coldest months. During the summer, rainfall is over-predicted by MM5 over most of the domain. This is consistent with other annual applications of MM5 using the same configuration and physics options. This over-prediction of rainfall in MM5 does not necessarily translate into over-prediction of wet deposition in the photochemical model (Baker and Scheff, 2006). CAMx does not explicitly use the convective and non-convective rainfall output by MM5, but estimates wet scavenging by hydrometers using cloud, ice, snow, and rain water mixing ratios output by MM5.

One interesting feature of rainfall performance is that the mixing ratio is under-predicted during August, but MM5 is clearly over-estimating rainfall in the Ohio Valley section of the upper Midwest domain. In June, the mixing ratio is over-predicted and rainfall is clearly over-predicted. In April, humidity is over-predicted but total rainfall predicted by MM5 shows fairly good agreement with observations.

4 KM PERFORMANCE

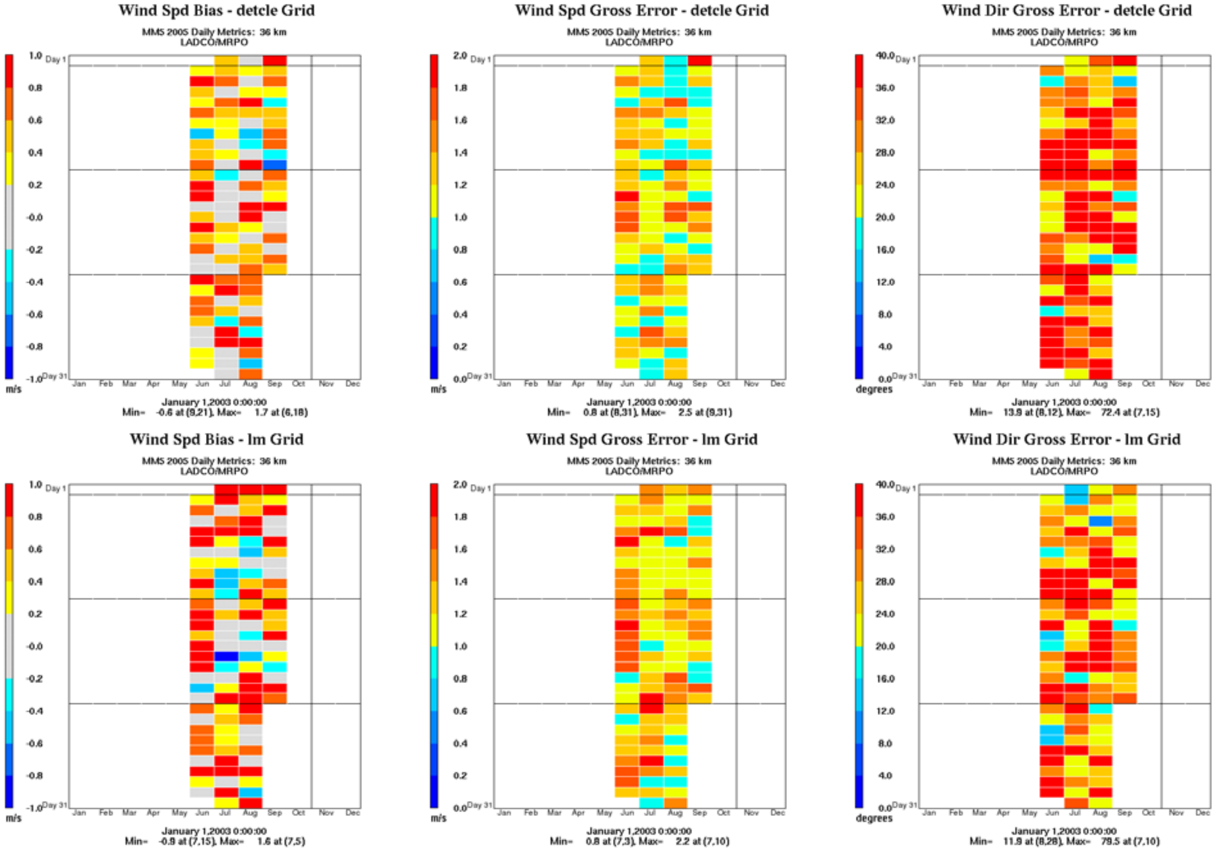
Daily metrics for the 4km MM5 output covering the Detroit-Cleveland and Lake Michigan domains are shown in Figure 9. The metrics shown in Figure 9 include mixing ratio bias, mixing ratio error, temperature bias, and temperature error. Both sub-regions of the 4 km MM5 output show very similar model performance for temperature and mixing ratio.

Figure 9. Detroit-Cleveland (top row) and Lake Michigan (bottom row) daily metrics from left to right: Mixing ratio bias, mixing ratio error, temperature bias, temperature error



Daily metrics for the wind field for both the Detroit-Cleveland and Lake Michigan domains are shown in Figure 10. Wind field performance is similar for both sub-regions of the 4 km MM5 output.

Figure 10. Detroit-Cleveland (top row) and Lake Michigan (bottom row) daily metrics from left to right: Wind speed bias, wind speed error, and wind direction error



Wind Spd Bias - detcle Grid

Wind Spd Gross Error - detcle Grid

Wind Dir Gross Error - detcle Grid

Wind Spd Bias - lm Grid

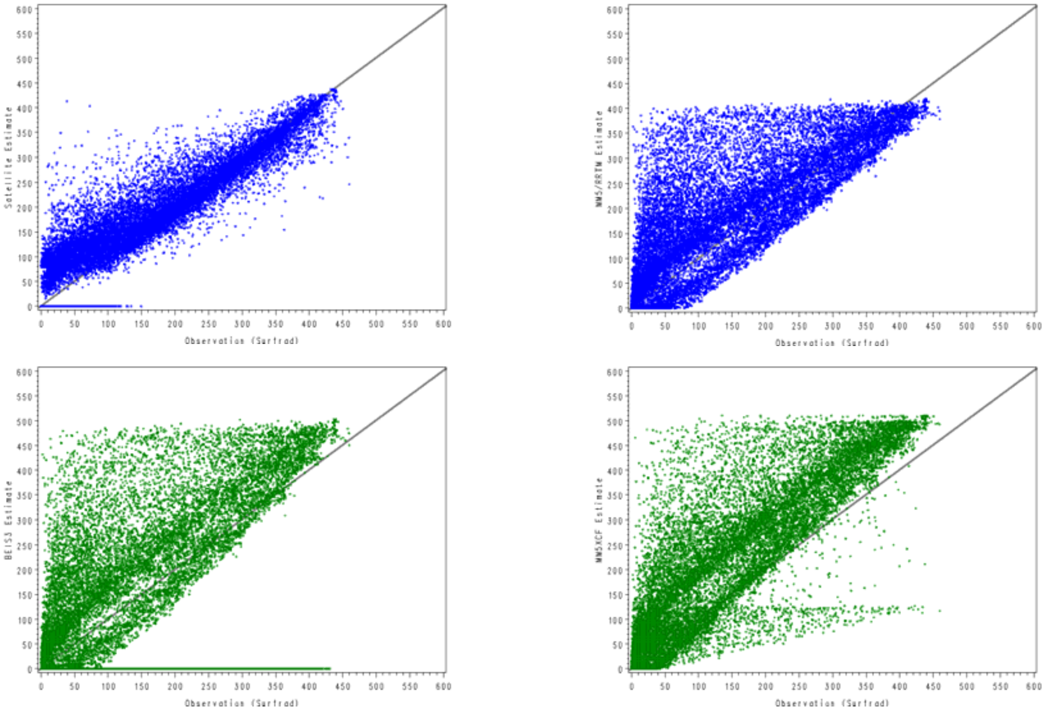
Wind Spd Gross Error - lm Grid

Wind Dir Gross Error - lm Grid

PAR

Biogenic emissions models uses photosynthetically activated radiation to estimate isoprene. The intermediate processor that converts MM5 output to emissions model (CONCEPT) has 3 different methods of estimating PAR: 1) MM5 output, 2) BEIS2 calculation, and 3) BEIS3 calculation. PAR data is also available from satellite estimates for the continental United States (Pinker and Laszlo, 1992). Each method is compared to 4 monitor locations in the central and eastern United States that measure PAR as part of the SURFRAD network: Bondville, IL; Goodwin Creek, MS; Penn State University, PA; and Sioux Falls, SD. Scatter-plots showing predictions against observations are shown in Figure 11. The satellite estimates of PAR match up very well with SURFRAD observations in the central and eastern United States. Alternative sources of PAR estimation were also compared to SURFRAD observations and are shown in Figure 11.

Figure 11. PAR observations compared to satellite (top left), MM5 (top right), BEIS2 (bottom left), and BEIS2 (bottom right) estimates



The satellite estimates show very good agreement with observation data. The BEIS2 estimates show several unusual features when compared to observations and are typically over-predicted. The BEIS estimation methods show odd features. The BEIS2 method estimates very low PAR when observations are high, but still tends to over-predict over all hours and days. The BEIS3 method also generally over-predicts over all hours and days, but often estimates a zero for fairly high observations.

MM5/RRTM also shows a tendency to over-predict low observed values. The satellite method to estimate PAR tends to slightly over-predict during the mid-day hours and misses early morning radiation between 7 and 9 am local time, but is clearly superior to the other methods.

SOIL MOISTURE

Soil moisture is an input to the MEGAN biogenics model for estimation of volatile organic compound emissions. Appendix B shows monthly averaged MM5 output soil moisture compared to NOAA Climate Prediction Center estimated monthly average soil moisture. The CPC soil moisture represents a depth of 1.6 meters and the MM5 soil moisture represents a soil depth of 1.0 meter. Both are representative of the root layer and are the appropriate depth to use as input to a biogenic emissions model. The CPC soil moisture is calculated using a one-layer hydrological model that uses precipitation and temperature as input (NOAA CPC, 2006; Huang et al., 1996; van den Dool et al., 2003).

The MM5 soil moisture data in general captures continental scale features, such as more moisture in the eastern United States compared to the central United States. The MM5 spatial pattern does not always match up well with CPC estimates.

CONCLUSION

The annual 2005 simulation at 36 and 12 km compares well for model performance of temperature, wind field, and humidity to other annual MM5 simulations used to support regulatory photochemical and emissions modeling applications. This meteorological data set needs to be used to simulate ozone and particulate matter in 2005 before a final determination may be made as to whether or not the meteorological model performance is good enough to appropriately simulate ozone and PM2.5 in 2005.

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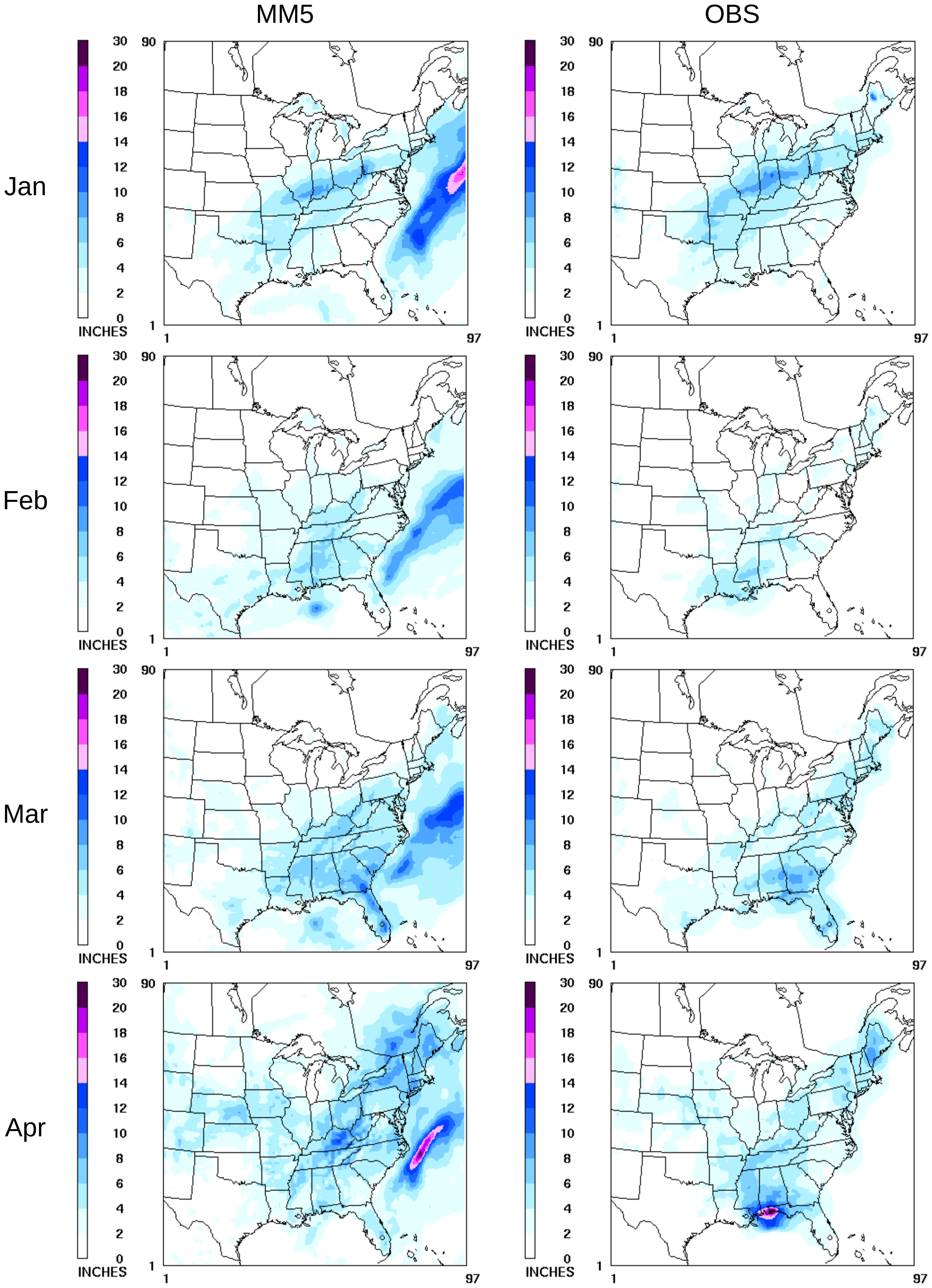
APPENDIX A

Total Rainfall


MM5
OBS
Jan
Feb
Mar
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14
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INCHES
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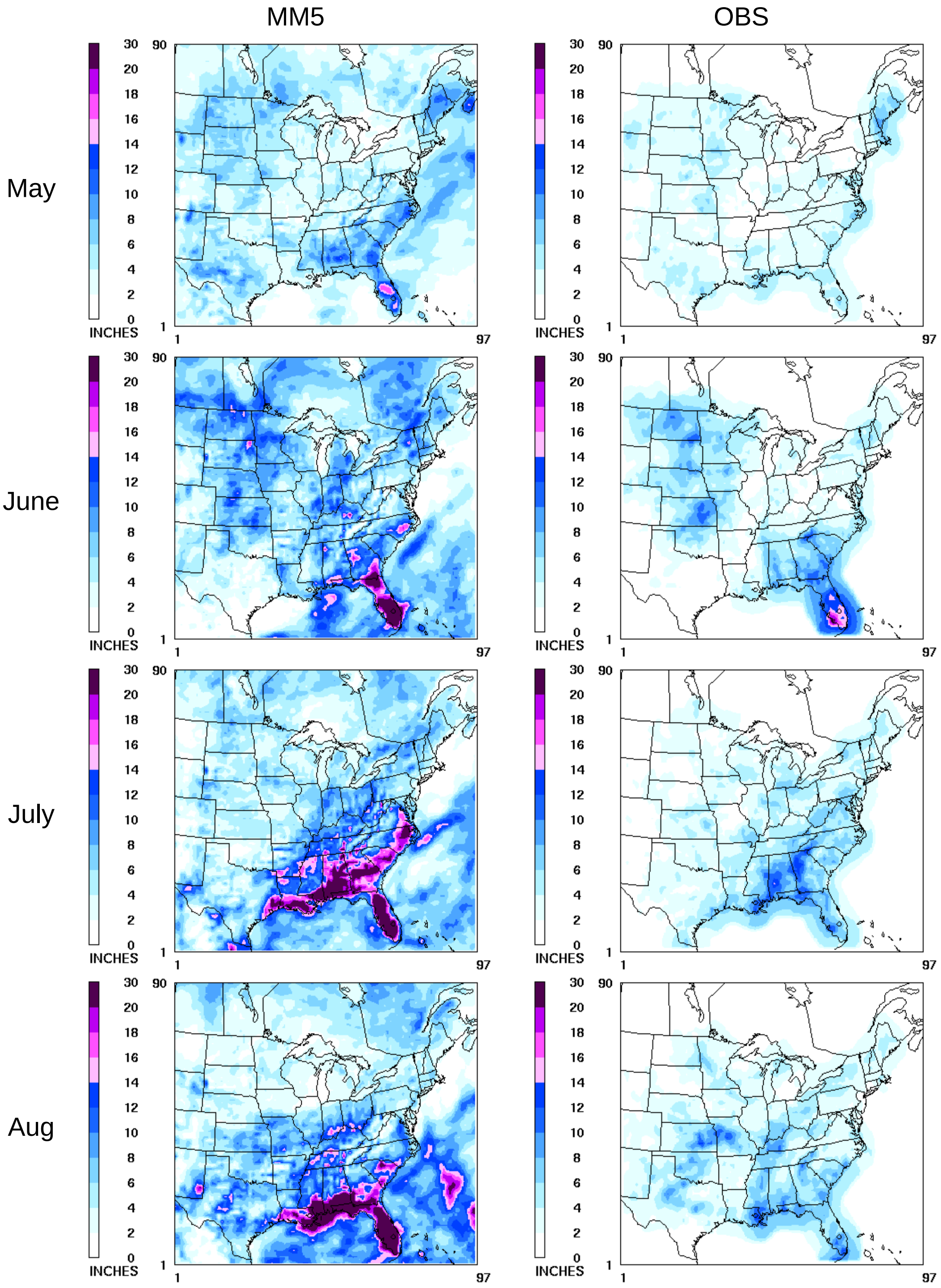
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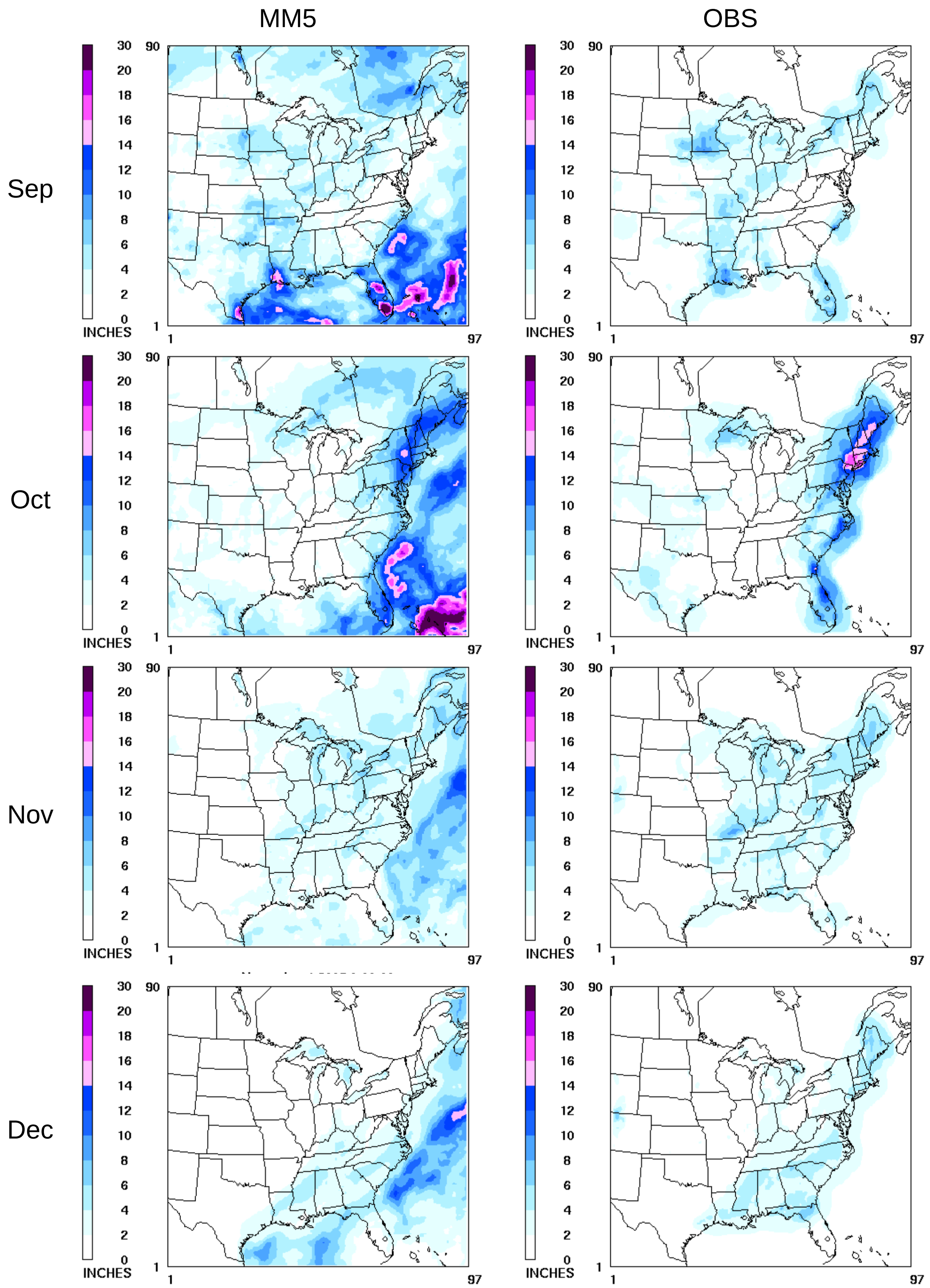
MM5
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APPENDIX B

Soil Moisture

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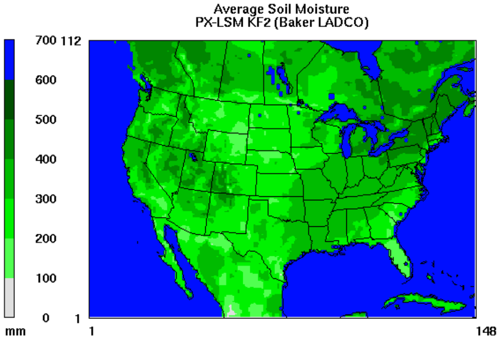
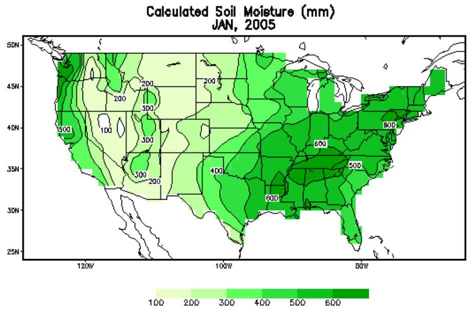
<tr><td>Jan</td><td>
</td><td>
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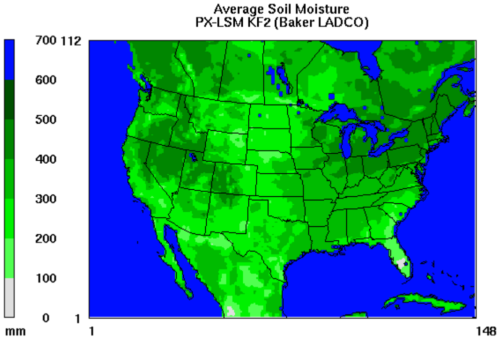
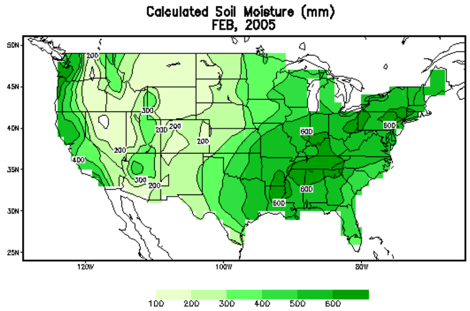
<tr><td>Feb</td><td>
</td><td>
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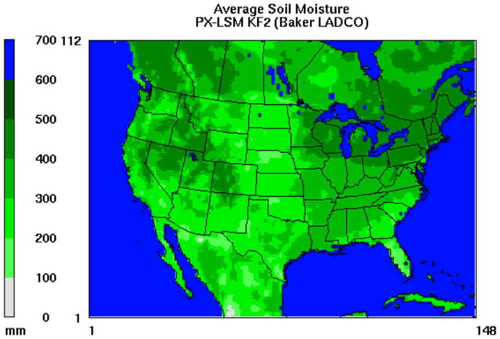
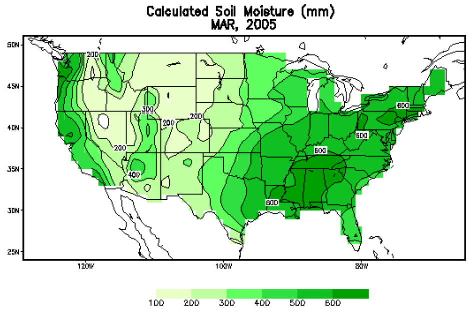
<tr><td>Mar</td><td>
</td><td>
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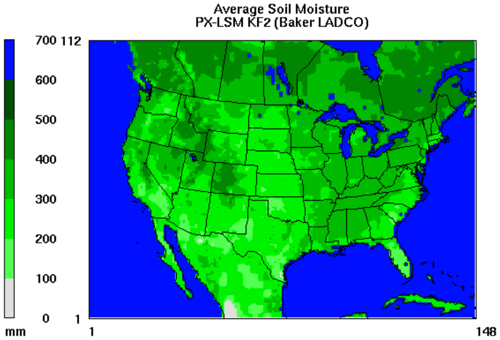
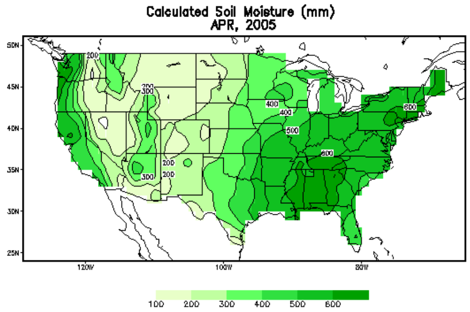
<tr><td>Apr</td><td>
</td><td>
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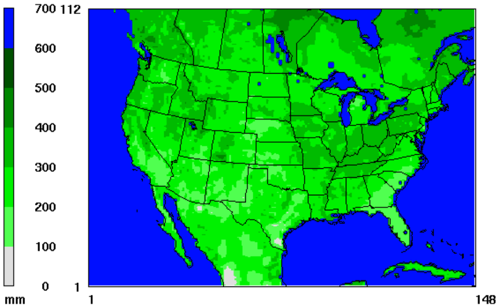
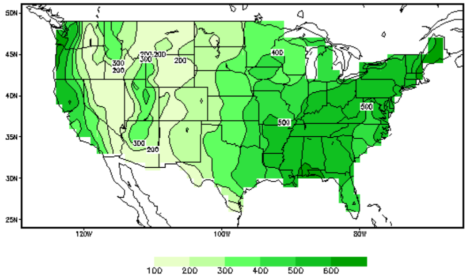
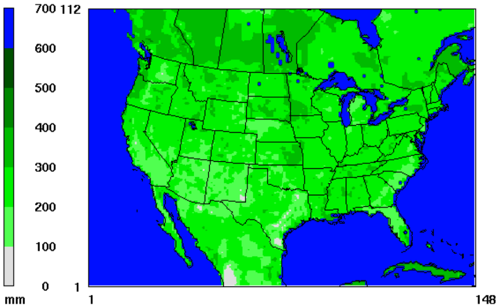
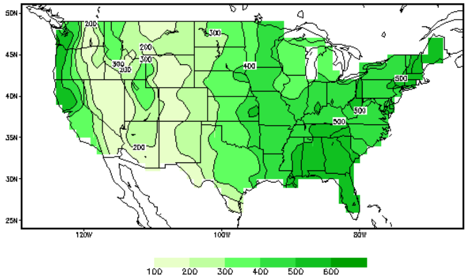
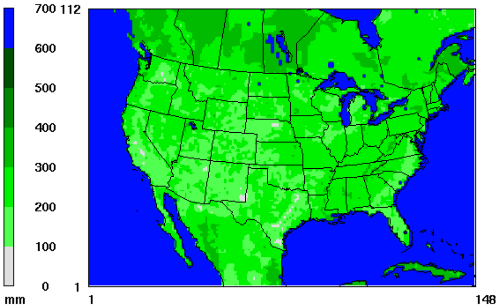
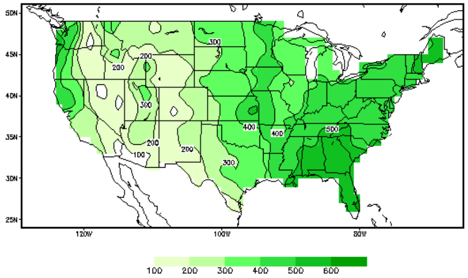
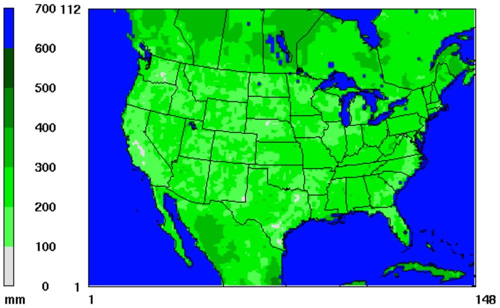
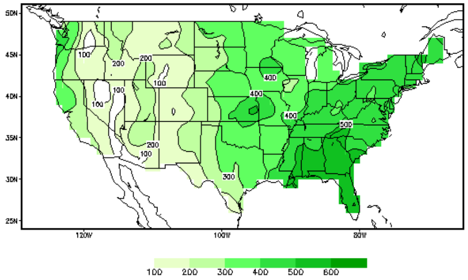
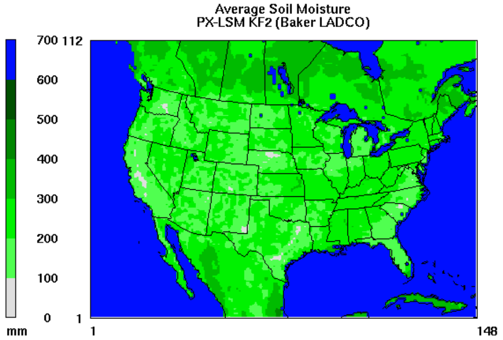
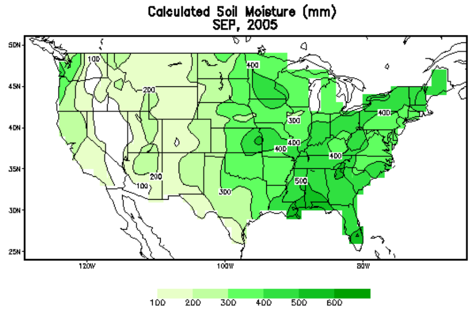
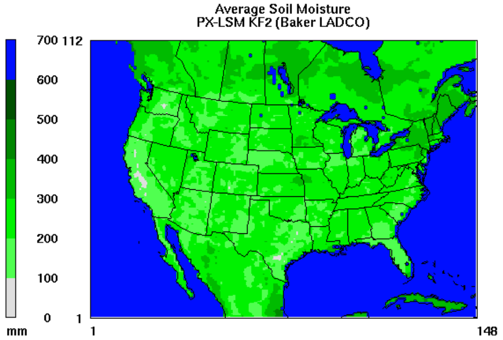
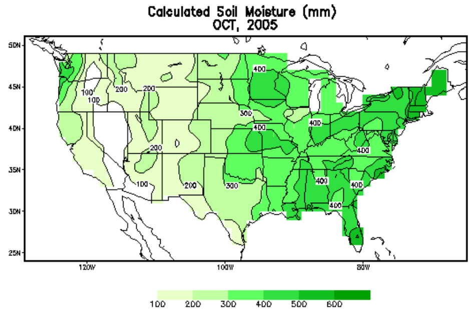
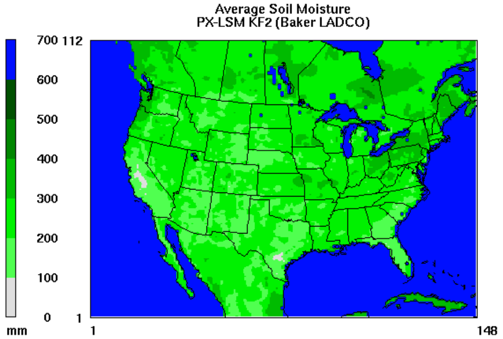
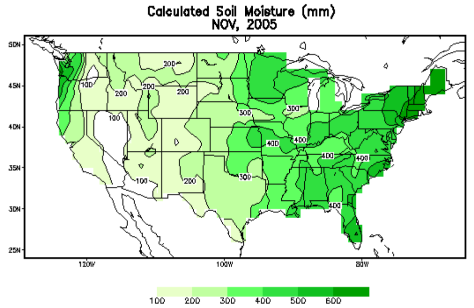
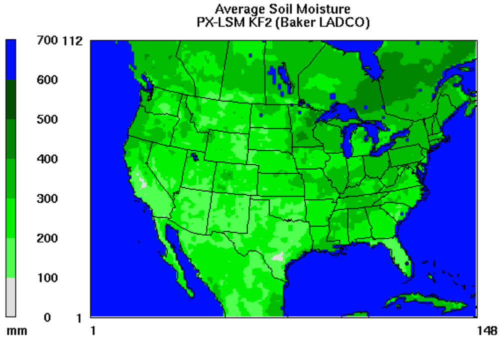
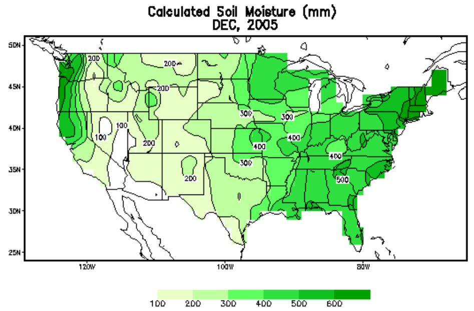
	MM5	CPC Estimate
May	Average Soil Moisture PX-LSM KF2 (Baker LADCO)  	Calculated Soil Moisture (mm) MAY, 2005 
Jun	Average Soil Moisture PX-LSM KF2 (Baker LADCO)  	Calculated Soil Moisture (mm) JUN, 2005 
Jul	Average Soil Moisture PX-LSM KF2 (Baker LADCO)  	Calculated Soil Moisture (mm) JUL, 2005 
Aug	Average Soil Moisture PX-LSM KF2 (Baker LADCO)  	Calculated Soil Moisture (mm) AUG, 2005 

	MM5	CPC Estimate
Sep	 Average Soil Moisture PX-LSM KF2 (Baker LADCO) 	 Calculated Soil Moisture (mm) SEP, 2005
Oct	 Average Soil Moisture PX-LSM KF2 (Baker LADCO) 	 Calculated Soil Moisture (mm) OCT, 2005
Nov	 Average Soil Moisture PX-LSM KF2 (Baker LADCO) 	 Calculated Soil Moisture (mm) NOV, 2005
Dec	 Average Soil Moisture PX-LSM KF2 (Baker LADCO) 	 Calculated Soil Moisture (mm) DEC, 2005