IMPACT OF TEMPORAL FLUCTUATIONS IN POWER PLANT EMISSIONS ON AIR QUALITY FORECASTS

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1. INTRODUCTION

In recent years, three dimensional air quality models such as the Community Multiscale Air Quality (CMAQ) model are being used regularly to forecast daily air quality. The research group at the New York State Department of Environmental Conservation (NYSDEC), in collaboration with other partners, has been performing air quality forecast simulations using CMAQ since June 2005. The ability of a modeling system to accurately predict air quality is dependent, in part, on the quality of the emissions used and the associated uncertainties. In an air quality forecasting context, the anthropogenic emissions are usually annual average emissions that are then allocated to each hour based on typical temporal profiles for each source category. Some source categories, such as electric generating units (EGUs), may exhibit significant temporal variations in emissions in response to weather conditions. This study examines the sensitivity of model predictions of ozone (O_3) to such changes in the temporal variations of activity of EGUs.

2. MODEL AND OBSERVATIONAL DATABASE

2.1 Model Setup

In this study, archived meteorological forecast fields were used to drive the CMAQ photochemical model for May through September of 2007. The meteorological forecast consisted of the National Center for Environmental Prediction (NCEP) 12z WRF-NMM (Non-hydrostatic Mesoscale Model of the Weather Research and Forecasting System) weather forecasts that had been archived by NYSDEC. Model simulations were conducted for two sets of emissions scenarios: "Actual" and "Average." Both inventories were based on the recently developed "OTC 2007 proxy" emission inventory (OTC, 2010). The OTC proxy emission inventory uses the 2007 MANE-VU inventories for non-road, non-EGU and EGU point sources, the EPA-CHIEF 2005 platform (USEPA, 2010a,b) for non-EGU and EGU point sources for all other regions, and interpolated 2007 inventories for other source sectors/regions. The difference between the two scenarios is in the temporal profiles that were used to allocate annual emissions for EGU sources to month of the year, day of the week, and hour of the day. Other sources used identical temporal allocation profiles between the two scenarios.

For the 2007 "actual" emissions scenario, temporal allocation of EGU emissions was based on measured hourly emissions from Continuous Emissions Monitors (CEMs) for EGUs on unit by unit basis. For the MANE-VU states, 2007 unit-level hourly and annual total emissions were developed using hourly CEMs data, state-submitted emissions and cross-walk files. For the non-MANE-VU states, the 2005 annual emissions were temporally allocated by SMOKE using the 2007 hourly CEMs files obtained from EPA's CAMD website (USEPA, 2010c) and cross-referencing ORIS/boiler ID. For the 2007 "average" scenario, annual emission totals were allocated to specific hours using temporal profiles derived from the actual 2007 CEM data on a state-by-state basis. This is in line with the typical practice followed in developing temporal profiles for forecast-based modeling. Emissions from only those units that were in operation throughout the entire period from January through December 2007 were used in the calculation of the temporal profiles.

All emissions were processed using SMOKEv2.6 for the Carbon Bond-05 (CB05) mechanism. Biogenic emissions were estimated using BEIS3.14. CMAQv4.7.1 was used to perform the air quality simulations. The CMAQ simulation was started on May 2, 2007 using clean initial conditions. Simulations for every day thereafter were initialized using modeled concentration fields from the previous day. Time-invariant boundary conditions were used. The modeling domain

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covered almost the entire Eastern U.S with a 12 km horizontal grid resolution.

2.2 Observational Database

Hourly measured concentrations of O_3 were downloaded from the EPA AIRNOW system for monitors within the modeling domain. Daily maximum 1-hr and 8-hr average O_3 concentrations were then determined from the hourly data and used in the subsequent analyses.

3. DATA ANALYSIS, RESULTS AND DISCUSSION

The objective of this study was to examine the sensitivity of model predictions to differences in temporal allocation of EGU emissions. The analysis examined differences in the EGU emission profiles and the resulting differences in O_3 model predictions. First, for each scenario, hourly speciated and temporally processed emissions reported by SMOKE were added to determine monthly emissions for each State. Second, the average hourly emissions were calculated over the entire ozone season. Next, specific time series of emissions on high ozone days were also analyzed. Model predictions of O_3 from both scenarios were compared against each other and against observations in terms of 1-hr and 8-hr daily maximum concentrations. Most analysis presented here is focused on the MANE-VU region.

3.1 Emissions

Monthly NO_x emissions for the two scenarios agreed reasonably with each other for the MANE-VU states and were within ±6% for those states with emissions greater than 2000 tons/month. For the other regions, the monthly emissions between the two scenarios differed by more than 10% and varied widely among the states. Part of this large difference might be due to the way the temporal profiles were developed, wherein only those units that were operational throughout the year were included. Temporary units, such as those operated during periods of peak electricity demand, may have not been included.

On a daily basis, the emissions between the two scenarios are expected to differ. This is because the "average" profile uses an average day of week profile for each month. Consequently, it does not account for high electric demand days, when the generation, and hence the emissions, may be higher than normal. Figure 1 shows a stacked bar plot of the net difference between the "actual" and the "average" emissions scenarios for the whole MANE-VU region for each day from May 1 to September 30, 2007. Note that each bar consists of multiple stacks representing the emission differences in each of the 13 states in the MANE-VU region.

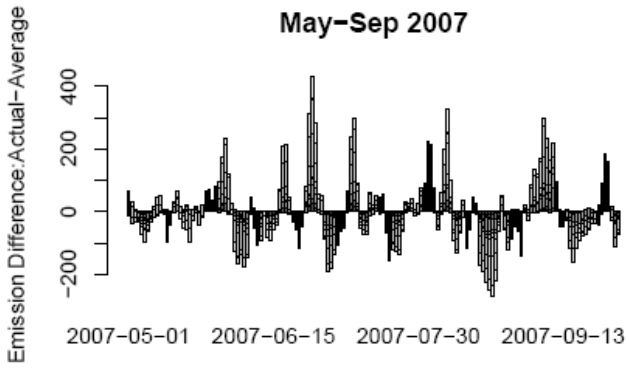

Figure 1. Stacked bar plot of the net difference in daily EGU NO_x emissions ("Actual" – "Average", tons/day) across the whole MANE-VU region from May through September 2007. .

As shown in Figure 1, the "actual" and "average" emissions differ on a daily basis. Except for the days in early September 2007, the time periods when the "actual" emissions were larger than the "average" emissions (i.e., positive difference) usually coincided with days leading to high ozone concentrations and the "actual" emissions from these days mostly exceeded the 90th percentile of the emissions on a state by state basis. The effect of such differences in emissions and its temporal variation on O_3 predictions is the intent of this study.

Average diurnal emissions over the whole period (May-September) were calculated for each state. For illustration, average diurnal EGU emissions in NY, PA and VA are shown in Figure 2. On average, the hourly profiles tracked each other. However, the average emissions appeared to increase rapidly during the early morning hours until about 10 am and then stabilized until about 6 pm and then began to decrease. The actual emissions profile increased at a slower rate than the average emissions, and reached a maximum peak around 3 pm, a little later than the average profile. Consequently, the average emissions are larger than the actual emissions during the early morning hours, and lower than actual in the afternoon.

3.2 Ozone Concentrations

Model predictions of O_3 were compared between the two scenarios. Daily 1-hr and 8-hr maximum concentrations were determined for each scenario. The difference between the two scenarios ("actual" minus "average") in the 1-hr and 8-hr daily maximum concentrations was calculated for each day.

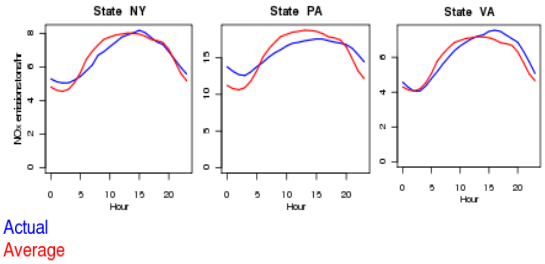

Figure 2. Average diurnal EGU emissions in NY, PA and VA for "actual" (blue) and "average" (red) emission scenarios, from May through September 2007.

Figure 3 shows, for each grid cell, the maximum and the minimum value over the entire period (unpaired in time) of the daily difference in the 1-hr and 8-hr daily maximum O_3 between the two emissions scenarios. A positive value indicates higher O_3 concentrations using "actual" emissions than "average" emissions. The maps show ±5 ppb or more difference in O_3 between the two scenarios in both 1-hr and 8-hr daily maximum concentrations. The largest maximum difference was as much as 18 and 13 ppb for the 1-hr and 8-hr O_3, respectively, while the largest minimum difference was -25 (1-hr) and -14 ppb (8-hr), at some point in the domain. The grid cells with large differences were located downwind of the EGU point sources. It is apparent from Figure 3, that the impact at each grid cell could be positive or negative. In order to convey the total daily variability in the model predictions between the two emission scenarios, the following approach was used: the maximum and the minimum difference in the hourly O_3 were determined for each grid cell for each day. Next, the difference between these daily maximum and minimum differences gives the total variability in model predictions for each day. Figure 4 shows the maximum of the daily variability over the entire period. As seen, more than 10 ppb variability in the hourly O_3 was noted in the grid cells along the Ohio River valley, and in parts of Western TN and the NC-VA border, near power plants, and a widespread 4-8 ppb variability engulfing the above regions.

In order to examine the effect of differences in the emissions on model predictions specifically at the monitor locations, similar analysis was conducted at the monitors in the MANE-VU region. Differences in daily maximum 1-hr and 8-hr average O_3 concentrations between the two emission scenarios were determined at each monitor. Next, at each monitor, the extreme (maximum, minimum) tendencies of these differences were determined over all days. The mean effect (average of these differences) was determined for four cases: a) for the entire period from May through September 2007; b) days when the observed 1-hr (for 1-hr daily max differences) and 8-hr average values (for 8-hr daily max differences) exceeded 75 ppb; c) days when the daily "actual" emissions exceeded the 90th percentile of the emissions in the state in which the monitor is located; and d) days when the daily "actual" emissions were in the lower 10th percentile of the emissions in the state in which the monitor is located.

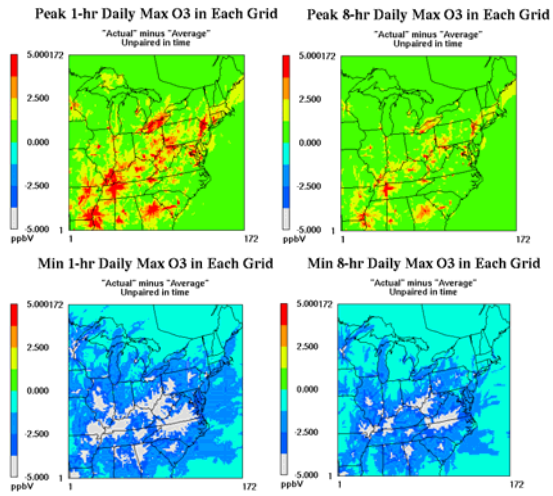

Figure 3. Maximum (top row) and minimum (bottom row) (unpaired in time) of the grid-specific daily difference in 1-hr (left column) and 8-hr (right column) daily max O_3 over the period from May through September 2007

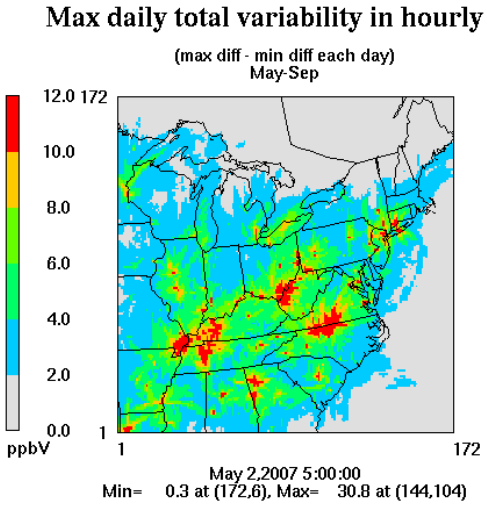

Figure 4. Maximum (unpaired in time) of the daily total variability in model predictions during May-September 2007.

The hourly emissions were first summed each day to get total daily emissions for each state. The 90th and 10th percentiles of the state-specific daily emissions between May and September were used

as cut-off to determine those days for case c) and d) in the above analysis. Cases b) and c) are representative of episodic days with high O_3 concentrations and high temperatures.

The distributions of the maximum and the minimum differences across all monitors in the MANE-VU region for all days are shown as boxplots in Figure 5. As seen, the maximum difference at the MANE-VU monitors ranged from near zero to 12 ppb for 1-hr daily max, while it ranged from near zero to 8 ppb for 8-hr daily max when considering all days from May through September. At 50% of the monitor locations (i.e., median of boxplot), the peak difference was only ~ 1.5 ppb in 1-hr daily max and ~ 1 ppb in 8-hr daily max between the 2 emission scenarios. The minimum difference reached as much as -10 ppb for 1-hr daily max, and ~ -7.4 for 8-hr daily max. Here again, the minimum difference at 50% of the monitor locations was -1.8 ppb and -1.3 ppb, for the 1-hr and 8-hr daily max, respectively. The max/min difference was less than ±3ppb at 75% of the sites. These differences between model predictions are similar in magnitude to variability arising from differences in meteorology or emissions (Hogrefe et al., 2008; Doraiswamy et al., 2009).

Figure 6 shows the distribution of the average difference across the monitors in the MANE-VU region for all 4 cases. The median was distributed similar to the distribution of the average difference, and hence is not shown. The average difference over all days (case (a)) ranged less than ±1.8 ppb at the monitors, with 50% of the locations having near zero difference. The distribution was similar when the analysis was restricted to just days with observed O_3 greater than 75 ppb or days when the daily emissions total exceeded the 90th percentile. The noticeable difference was the wider inter-quartile range (IQR) for cases (b) and (c) (0.35-0.36 ppb) than case (a) (0.16 ppb) as shown by the 25th and the 75th percentiles. For case (d) (emissions in the lowest 10th percentile), the IQR was even narrower (which was also true for the max/min distribution, not shown) than the other 3 cases, and a 50th percentile close to zero, indicating that the differences between the model simulations were negligible on non high-electric demand days.

Based on these results, the following can be inferred:

1. Differences in EGU emissions and their temporal profiles caused less than ±2 ppb maximum difference between the two model simulations in both the 1-hr and the 8-hr daily maximum O_3 concentrations at 50% of the monitor locations in the MANE-VU region, and < ±3 ppb at 75% of the sites.
2. At certain sites, the maximum impact in modeled O_3 concentrations could be more than ± 8 to ±10 ppb in 1-hr and 8-hr daily maximum O_3, as shown by the outlying points in the box plots.
3. The impact could be both positive and negative. The average impact over the time period was near zero with 75% of the sites having < ±0.5 ppb difference in the MANE-VU region.

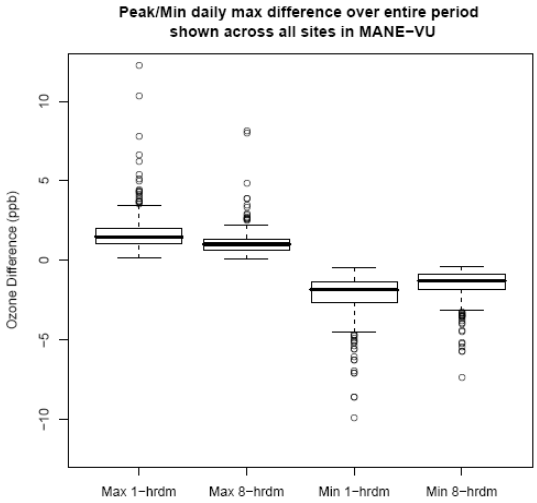

Figure 5. Distribution of the maximum and minimum difference of 1-hr (1-hrdm) and 8-hr (8-hrdm) average daily max O_3 predictions at locations of monitors, across all monitors in the MANE-VU region for all days from May through September. The box represents the 25th, 50th and 75th percentiles. The upper (or lower) whiskers represent the largest (or the lowest) data that is less than or equal to the 75th percentile plus 1.5 times the interquartile range [IQR] (or greater than or equal to the 25th percentile minus 1.5 times IQR). Data that fall outside the whiskers are shown as outlying points.

Figure 7 presents a time series of the hourly, and the 1-hr and 8-hr daily max O_3 predictions on the left ordinate, and the differences in emissions and O_3 predictions on the right ordinate for two selected monitors. These two monitors were chosen to illustrate the nature of the impact. The NY site (360050110) is an urban site with high emission density, while PA (420070005) site is a rural agricultural site near the OH-PA border. At the NY site 360050110, the difference in the hourly O_3 concentrations are mostly negative suggesting that predictions using average emissions were greater than that from actual emissions profiles. On the other hand, at the PA site 420070005, the differences were mostly positive. Further, in both cases, differences were noticed mostly on days of high ozone concentrations (except September).

These are further apparent from the plots for the 1-hr and 8-hr daily max. On these plots, differences in the statewide EGU NO_x emissions between the two scenarios have also been included. The periods with positive changes in emissions mostly coincided with the negative changes in O_3 at the NY site, while showing positive O_3 changes for the PA site. Thus, a higher "actual" emission causes different responses in O_3 depending on the nature of the site. The highly urbanized NY site was subject to scavenging of O_3 indicating a higher loading of NO_x. This suggests that the response is dependent upon the photochemical regime of the region and its distance from the source.

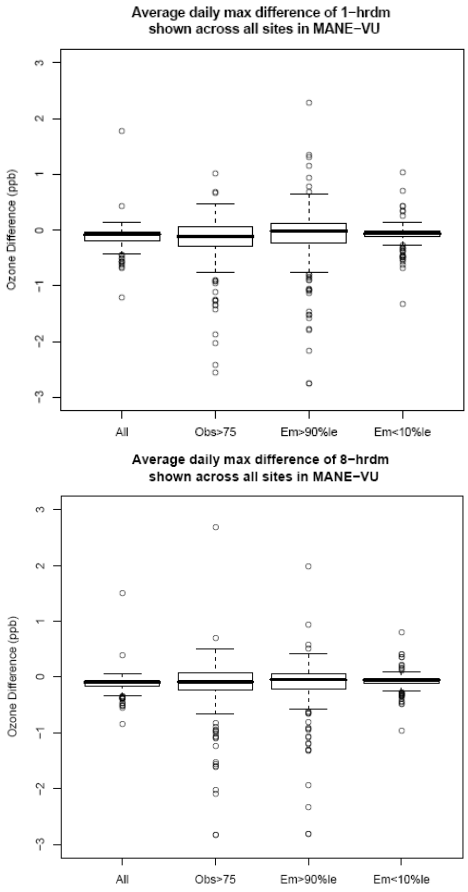

Figure 6. Distribution of the average difference of 1-hrdm and 8-hrdm O_3 predictions at locations of monitors, across all monitors in the MANE-VU region for four cases: a) all days from May through September ("All"); b) days when observed 1-hr or 8-hr O_3 exceeded 75 ppb ("Obs>75"); c) days when daily "actual" emissions exceeded the 90th percentile for the state in which the monitor is located ("Em>90%le"); and d) days when daily "actual" emissions were less than the 10th percentile ("Em<10%le"). One outlying data point (7.4 ppb) is not shown for Obs>75.

Emission differences were noticed in September at both sites, although no ozone exceedances were observed at that time. The above-stated impacts on O_3 during September also coincide with emission changes.

When compared to observed O_3 concentrations, both model predictions showed similar biases. For example, Figure 8 shows the normalized mean bias (NMB) of 8-hr average daily maximum model predictions compared to observations for both scenarios between May and September 2007. In general, model predictions were within ±10% of observations, except for few sites that showed greater than 20% NMB. Between the two scenarios, both showed similar biases. Only about 40 out of 620 sites (6.5%) showed biases that fell into a different bin in Figure 8.

4. CONCLUSIONS

This study examined the effect of differences in EGU emissions and their temporal allocation on model predictions of O_3. Two sets of emissions scenarios based on "actual" and "average" temporal profiles were used to drive the CMAQ model simulations. The analysis focused on the MANE-VU region. Analysis of daily emissions shows that the emissions typically varied on a daily basis between the two scenarios. "Actual" NO_x emissions were typically greater than "average" emissions on days that led to high O_3 concentrations.

The impact of these differences in emissions on O_3 predictions varied by location. The largest impact was noted at the grid cells adjacent to the point source. Depending on the location of the grid cell or the monitor, these differences in emissions caused either an increase or a decrease in O_3 and appeared to be dependent on the photochemical regime of the region. The maximum difference in 1-hr or 8-hr daily max was typically greater than 4 ppb around the Ohio River valley, and less than 2.5 ppb in general. The maximum total daily variability was more than 10 ppb along the Ohio River valley, and in parts of Western TN and the NC-VA border near location of power plants. In other regions, the variability was between 4 and 8 ppb.

At the monitor locations, the average impact was less ±0.5 ppb across 75% of the monitors in the MANE-VU region. The maximum impact was less than ±3 ppb across 75% of the monitors in the MANE-VU. Differences as large as 8 to 10 ppb were noted at selected monitors. The maximum impact appeared to cover days other than just the high demand days. These differences are similar to the variability typically observed with differences arising from meteorology or emission inventories (Hogrefe et al., 2008; Doraiswamy et al., 2009). When compared to observed concentrations, both

model predictions showed biases within ±10% of the observed concentrations between May and September 2007. Except for ~6.5% of the sites, both model predictions showed similar biases in general, across the whole domain.

5. DISCLAIMER

This work was funded in part by NYSDEC and the New York State Energy Research and Development Authority (NYSERDA) under agreement #10599. The results presented here have not been reviewed by the funding agencies. The views expressed in this paper are those of the authors and do not necessarily reflect the views or policies of NYSDEC or the sponsoring agency.

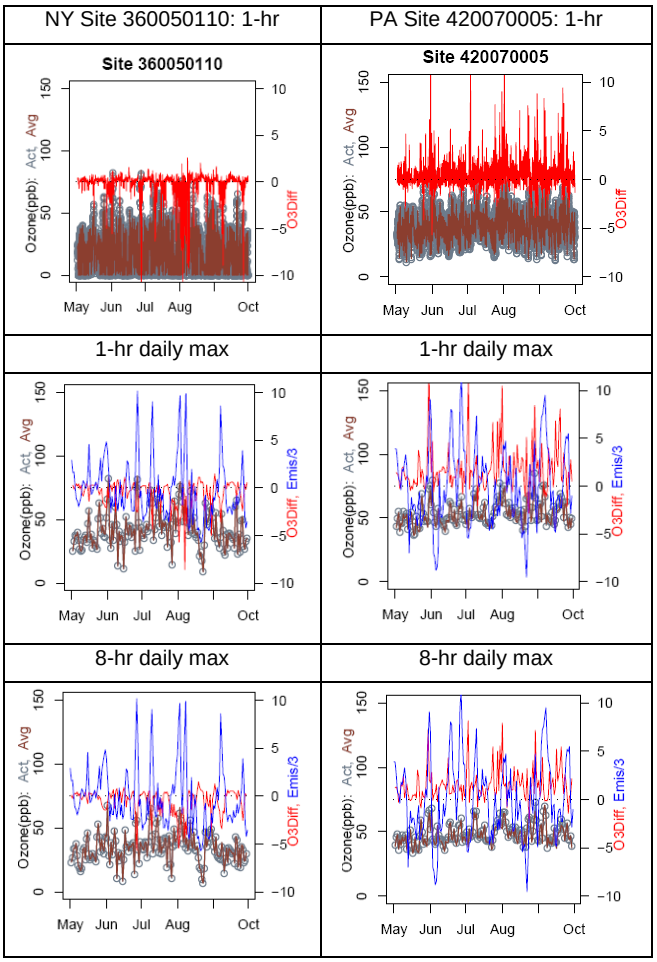

Figure 7. Time series of 1-hr, 1-hr daily max and 8-hr daily max model predictions (left ordinate) using "actual" (Act) and "average" (Avg) emissions, and difference in emissions (blue, right ordinate), and O_3 concentrations (red, right ordinate) from May through September, 2007 at two monitor locations. Emission differences have been divided by a factor of 3 and are in tons/day. O_3 is in ppb.

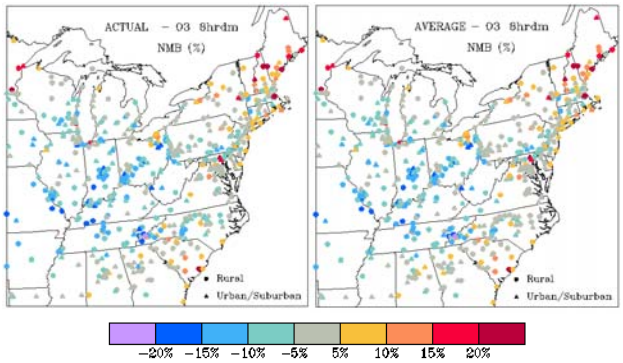

Figure 8. Normalized mean bias (NMB) of 8-hr daily maximum (8hrdm) model predictions of O_3 compared to observations from May through September 2007.

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