Draft Final Report

MODEL PERFORMANCE EVALUATON FOR THE JUNE-JULY 2006 OZONE EPISODE FOR THE DENVER 8-HOUR OZONE STATE IMPLEMENTATION PLAN

Prepared for:

Regional Air Quality Council
1445 Market Street, Suite 260
Denver, Colorado 80202

Prepared by:

Ralph Morris
Ed Tai
Tanarit Sakulyanontvittaya
ENVIRON International Corporation
773 San Marin Dr. Suite 2115
Novato, CA 94998

Dennis McNally
Cyndi Loomis
Alpine Geophysics, LLC
7341 Poppy Way
Arvada, Colorado 80007

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EXECUTIVE SUMMARY

Due to violations of the 0.08 parts per million (ppm) 8-hour ozone National Ambient Air Quality Standard (NAAQS) based on 2005-2007 air quality data, in November 2007 the Denver Metropolitan Area (DMA) reverted to an 8-hour ozone nonattainment area. This requires the DMA to develop an 8-hour ozone State Implementation Plan (SIP) that demonstrates the area will achieve the 0.08 ppm 8-hour ozone NAAQS by 2010. The Denver Regional Air Quality Council (RAQC), in consultation with the Colorado Department of Health and Environment (CDPHE) Air Pollution Control Division (APCD) contracted with ENVIRON International Corporation and their subcontractor Alpine Geophysics, LLC to develop the photochemical modeling databases necessary to demonstrate that the DMA will achieve the 0.08 ppm 8-hour ozone NAAQS by 2010.

OVERVIEW OF APPROACH

The Comprehensive Air-quality Model with extensions (CAMx; www.camx.com) was set up for a June-July 2006 episode on a 36/12/4 km grid with the 4 km domain focused on Colorado. Meteorological inputs were prepared using the MM5 meteorological model whose results and evaluation are discussed by McNally and co-workers (2008). An initial emissions inventory was prepared using the SMOKE emissions modeling system and a preliminary 2006 base case was performed. A preliminary model performance evaluation was conducted and diagnostic sensitivity tests performed to identify an optimal model configuration for simulating ozone formation in the DMA (Morris et al., 2008b).

A revised CAMx 2006 base case (Run 17) simulation was conducted that included the following emission updates from the preliminary 2006 base case simulation reported by Morris and co-workers (2008):

- Corrections and enhancements to the 2006 emissions for Colorado provided by the CDPHE/APCD.
- Application ConCEPT MV mobile source emissions modeling system that uses diurnally varying link-based Vehicle Miles Traveled (VMT), fleet mix and other data to provide more detailed on-road mobile source emissions in the DMA.
- Use of the WRAP Phase III oil and gas production emissions inventory for the Denver-Julesburg Basin.
- Biogenic emission estimates from the MEGAN biogenic emissions model (Guenther and Wiedinmyer, 2004).

This report presents the model performance evaluation for the final 2006 base case simulation performed as part of the Denver 8-hour ozone attainment demonstration modeling.

MODEL PERFORMANCE EVALUATION

The model performance evaluation of the Denver final 2006 base case simulation performed both an operational evaluation that evaluated how well the model predicted the ozone observations and a diagnostic evaluation that evaluated the model for ozone precursors, key indicator species, particulate matter (PM) and ozone aloft.

Operational Model Performance Evaluation

The operational model performance evaluation focused on how well the model predicted the observed surface ozone concentrations in the DMA and included graphical displays of model performance as well as statistical evaluation metrics and comparisons with model performance goals.

Comparison against Model Performance Goals

One element of an ozone SIP model performance evaluation is to test how well the model reproduces the observed ozone concentrations. As part of this, statistical performance metrics are calculated that are compared against model performance goals as a method to gauge model performance, compare it against other studies and to assist in determining whether the model is getting the right answer. EPA's latest modeling guidance (EPA, 2007) emphasizes using graphical and diagnostic evaluation techniques to assure that the photochemical rid model is capturing the correct chemical regimes and emissions sources that lead to the high ozone (i.e., assuring that the model is getting the right answer for the right reason).

EPA's 1991 1-hour ozone guidance included three performance goals that have been used for over two decades to assist in evaluating ozone models as part of the ozone SIP modeling process:

- Unpaired Accuracy of the Peak ≤±20%;
- Normalized Mean Bias ≤±15%; and
- Normalized Mean Gross Error ≤35%.

The Mean Normalized Bias and Gross Error statistical measures are calculated using all predicted and observed hourly ozone pairs matched by time and location for which the observed ozone is 60 ppb or greater.

Figure ES-1 compares the Denver final 2006 base case CAMx hourly ozone model performance against these three EPA model performance goals for each day during the June-July 2006 episode. The CAMx final 2006 base case simulation achieves the Unpaired Accuracy of the Peak performance goal of ≤±20% for 58 of the 60 simulation days of the episode (i.e., 97% of the modeled days). There are 58 days with bias and error comparisons during the episode as two days had no observed ozone greater than 60 ppb so no statistics could be calculated. Of these 58 days, 50 of them (86%) achieved EPA's ≤±15% performance for Mean Normalized Bias and all of them achieves EPA's performance goal for Mean Normalized Gross Error.

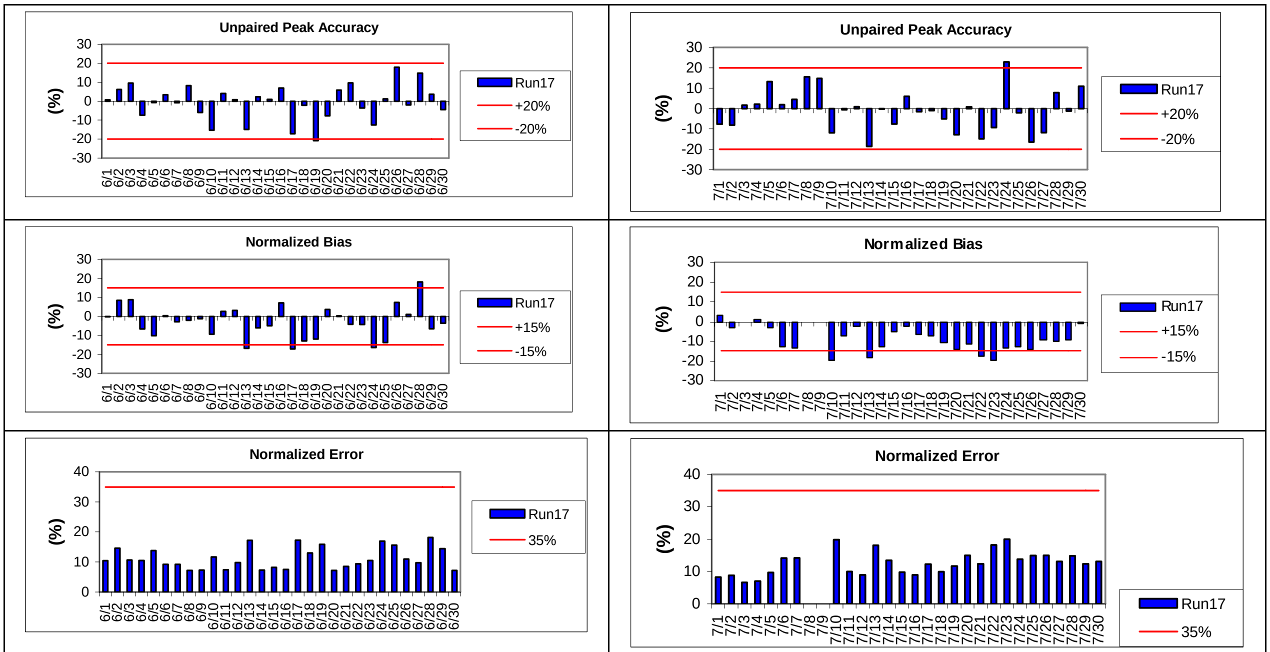

Figure ES-1. Hourly ozone performance statistics for June (left) and July (right) 2006 and Unpaired Peak Accuracy (top), Mean Normalized Bias (middle) and Mean Normalized Gross Error (bottom) and comparison against EPA's model performance goals (red lines).

EPA's draft 1999 8-hour ozone modeling guidance has a performance goal for daily maximum 8-hour ozone concentrations that the predicted value near the monitor be within ±20% on most monitor-days. This is a particularly important performance metric as it is these exactly same predicted daily maximum 8-hour ozone concentrations near the monitor that are used to make future year ozone projections. By "near the monitor" we used the same 7 x 7 array of 4 km grid cells centered on the monitor as used in the ozone projections and have made this analysis three ways by selecting the Maximum predicted value in the array, the predicted value Closest to the observed value, and the predicted value Co-Located at the monitor, with this last comparison being a particularly stringent test of model performance. Table ES-1 summarizes the results of this performance test, with a scatter plot of the predicted and observed daily maximum 8-hour ozone concentrations Co-Located at the monitor shown in Figure ES-2. Using the Maximum, Closest and Co-Located predicted daily maximum 8-hour ozone concentration near the monitor we see that the model achieves the within ±20% of the observed value performance goal 76%, 89% and 82% of the monitor-days. Thus, the Denver final 2006 base case CAMx simulation (Run 17) daily maximum 8-hour ozone predictions achieves EPA's ≤±20% of the observed value on most monitor-days performance goal.

Table ES-1. Percent of the monitor-days that the model predicted daily maximum 8-hour ozone concentrations near the monitor is within ±20% of the observed value (total monitor-days = 1008).

Maximum Near the Monitor		
Percent Difference	# Days	% Days
<-20	9	1%
-20% to +20	769	76%
> +20	230	23%
Closest Near the Monitor		
Percent Difference	# days	%
<-20	23	2%
-20% to +20	902	89%
> +20	83	8%
Co-Located At the Monitor		
Percent Difference	# days	%
<-20	48	5%
-20% to +20	829	82%
> +20	131	13%

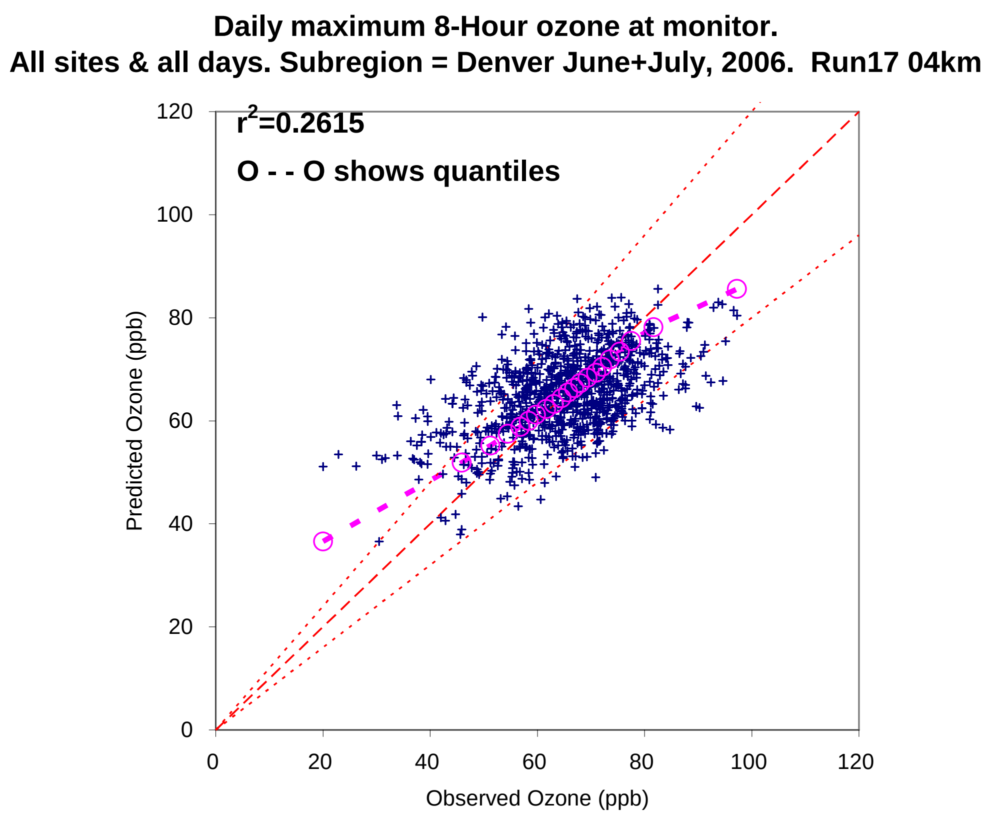

Figure ES-2. Comparison of predicted and observed daily maximum 8-hour ozone concentrations for the June-July 2006 modeling period and the final CAMx Run 17 2006 base case simulation using the Co-Located predicted value near the monitor.

Spatial and Temporal Evaluation of Ozone Model Performance

A detailed analysis of the ozone model performance was assessed by examining the ability of the model to predict the observed ozone concentrations for three 3-day episodes during the June-July 2006 modeling period when 7 of the 9 8-hour ozone exceedance days occurred. The detailed ozone model performance revealed that at some days the model failed to reproduce the elevated ozone concentrations and model performance was poor. Whereas, on other days the ozone model performance was quite good. In general, there were days with good model performance at the high southern (e.g., Chatfield) and northwestern (e.g., Rocky Flats North) ozone monitors, but there was a general underprediction bias at the northern Fort Collins West monitor. Figure ES-3 compares the spatial distribution of the predicted and observed daily maximum 8-hour ozone concentrations in the two highest days during the two month modeling period: July 14 and 29, 2006. On July 14th, the model is correctly predicting elevated ozone concentrations to the north-northwest of the DMA with the highest modeled values near the highest observed value at Fort Collins West monitor, although the modeled peaks are below the observed ozone peaks. On July 29, 2006 the model correctly predicts that the very highest ozone concentrations occur in and near the DMA with both the modeled and observed 8-hour ozone peaks in excess of 90 ppb. Time series of predicted and observed hourly ozone concentrations for the July 13-16 and July 27-29 periods and the two highest monitoring sites (RFNO and FTCW)are shown in Figure ES-4. In general the model underestimates the observed ozone peaks; the exception to this is at Rocky Flats North monitor for July 27-29, 2006 that exhibits very good ozone model performance.

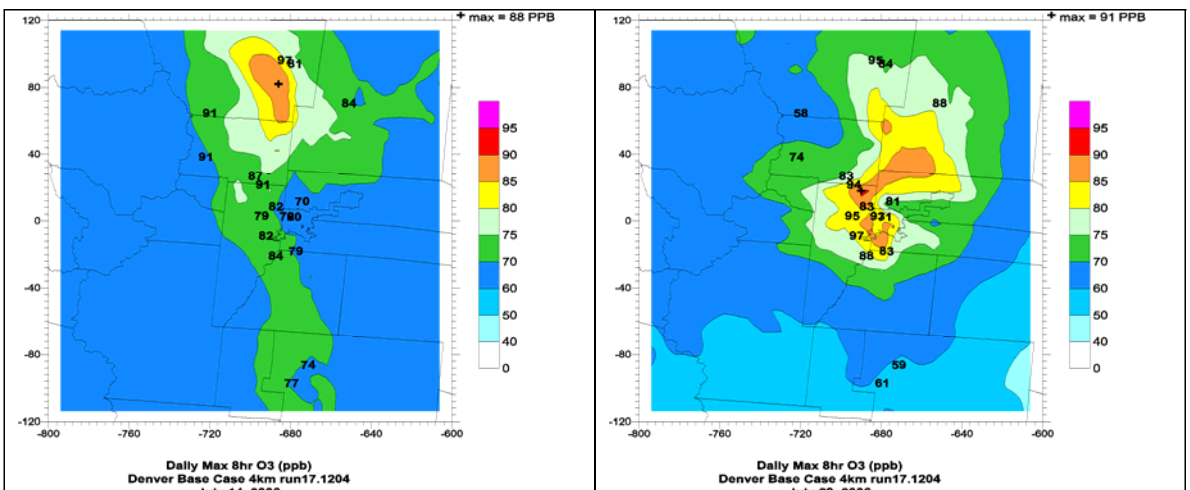

Figure ES-3. Comparison of the predicted and observed daily maximum 8-hour ozone concentrations on the two highest observed ozone days during the June-July 2006 modeling period using the final 2006 base case CAMx simulation (Run 17) results.

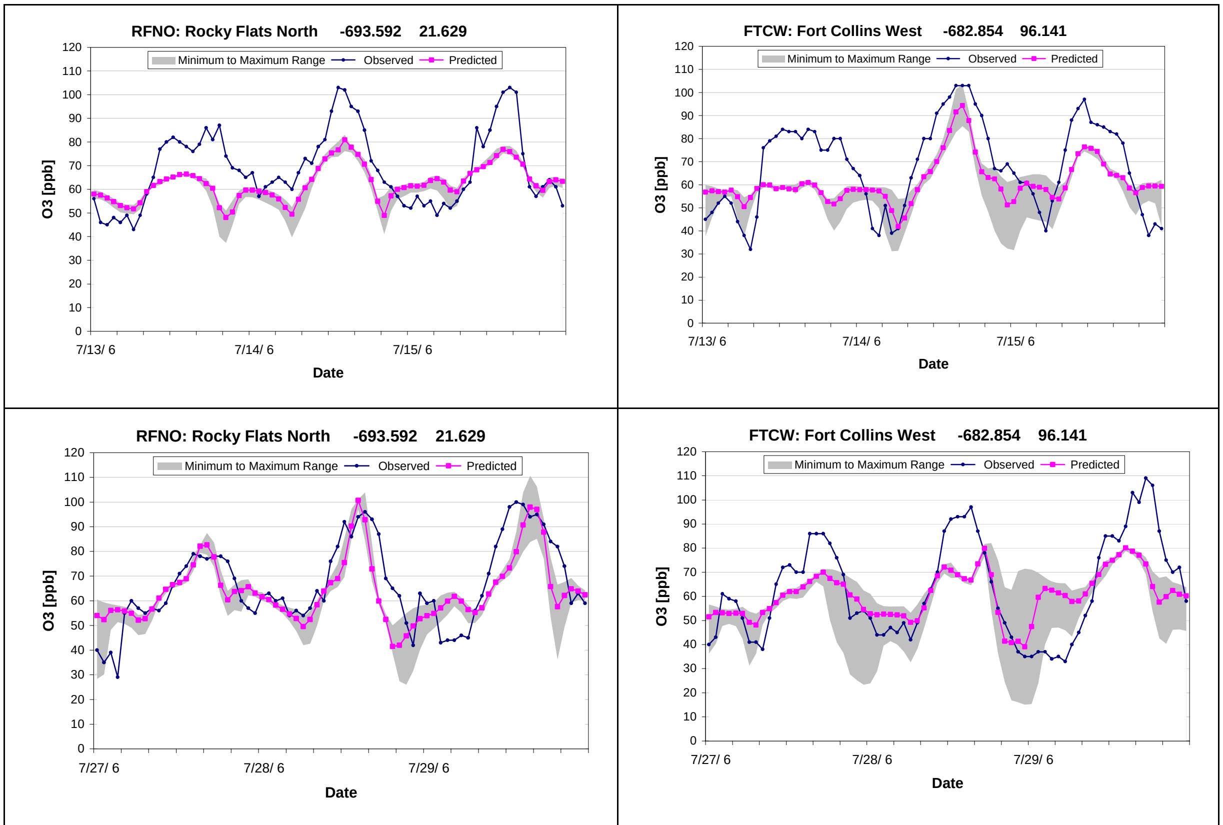

Figure ES-4. Predicted and observed hourly ozone concentrations at the Rocky Flats North (left) and Fort Collins West (eight) monitoring sites during July 13-16, 2006 (top) and July 27-29, 2006 (bottom) periods.

Diagnostic Model Performance Evaluation

In addition to the many diagnostic tests performed to test the sensitivity of the model to model inputs and options performed as part of the preliminary model performance evaluation discussed in previous reports (Morris et al., 2008b; McNally, et al., 2008), the diagnostic model performance evaluation also included comparisons against ozone precursors, key indicator species, PM species and ozone aloft.

Ozone Precursor and Indicator Species Comparisons

The CDPHE/APCD collected 3-hour VOC samples at several sites during a few days of the June-July 2006 modeling period. Figure ES-5 displays the example comparisons of ozone precursor and their ratios at the downtown Denver CAMP monitoring site. In these comparisons, the observed VOC species were converted to the CB05 lumped VOC species that is the chemical mechanism used in CAMx. Then the modeled and observed CB05 species were summed to get the total predicted and observed VOC concentrations, respectively. Note that ethane (ETHA) was not included in the total VOC species when summing the CB05 lumped species. Also note that since the VOC sampling did not collected measurements for methanol and ethanol, those species were also not accounted for when summing the CB05 species.

The model is systematically underpredicting the observed VOC concentrations at the CAMP monitoring site, whereas for NOx and CO there are days with underpredictions and days with overpredictions, although on average NOx is underpredicted as well. The CAMP monitor is located in downtown Denver where we would expect VOC, NOx and CO emissions to be dominated by on-road mobile sources. Thus, these comparisons provide a good evaluation of the on-road mobile source emissions. However, there are incommensurability differences between the observed point measurements at the 4 km grid cell average model predictions. Thus, a better indication of the accuracy of the on-road mobile source emissions are the VOC/NOx and CO/NOx key indicator ratio comparisons. Comparison of the predicted and observed VOC/NOx ratios also provide an indication of whether the model is reproducing the correct chemical regime in the DMA. Of the 15 days with morning VOC/NOx comparisons, very good comparisons are seen on 11 (73%) of the days. Of the four days in which the model is underpredicting the observed VOC/NOx ratio one is July 4th that has atypical traffic patterns that were not simulated in the CONCEPT modeling. Two of the other VOC/NOx ratio overprediction days were weekend days, although on two other weekend days we saw good performance. The CO/NOx ratios appear to be slightly overpredicted on most days which may indicate that MOBILE6 is overestimating the on-road mobile source CO emissions, which has also been noted by Pollack and co-workers (2004). Ethane (ETHA) is underpredicted by approximately a factor of 10 at the CAMP monitor with observed values of ~25 ppbC and predicted values of ~2.5 ppbC. The underprediction of ethane is even greater at the two Weld County monitoring sites where the CB05 paraffin species is also underpredicted. As ethane is primarily associated with natural gas, its underprediction could indicate that organic emissions from natural gas related and oil and gas development sources are understated in the inventory.

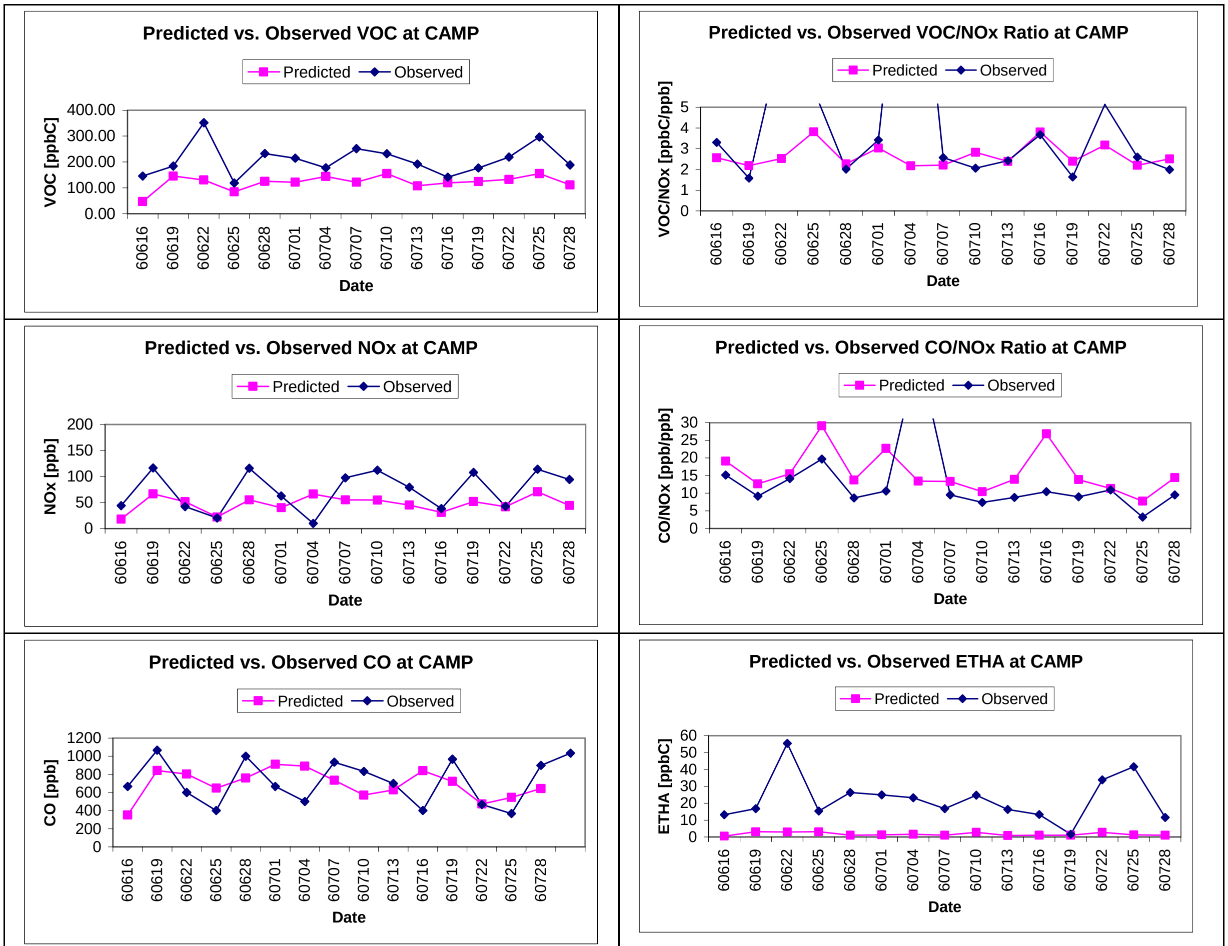

Figure ES-5. Comparison of predicted and observed early morning (5-8am MST) VOC, NOx and CO concentrations and VOC/NOx and CO/NOx ratios at the CAMP monitoring in downtown Denver.

In addition to the underestimation of observed ethane and paraffin VOC species noted above, carbonyl VOC species were also systematically underpredicted by the model. The underprediction of acetaldehyde may be due in part to the SMOKE VOC speciation profile for on-road mobile sources not accounting for ethanol blended gasoline whose combustion produces higher acetaldehyde than conventional gasoline. However, the reasons for the large underprediction of formaldehyde are less clear and since formaldehyde is an important VOC species that initiates the radical cycle its underprediction may help explain why the model tends to form ozone too slowly and does not obtain as high ozone peaks as observed. A review and evaluation of the VOC speciation profiles in the Denver modeling is recommended.

Ozone Aloft

During six days of the June-July 2006 modeling period, ozonesondes were released from Boulder that obtained a measured vertical ozone profile in the atmosphere. One hypothesis for the conceptual model on ozone formation in the DMA is that on some days there is a reservoir of ozone above the ground that is entrained and mixed to the ground as the mixing height rises. The comparison of the modeled vertical ozone profile with the ozonesonde measurements would provide an indication of whether the model is capturing this phenomenon. As the ozonesonde rises it will move downwind with the prevailing wind. In these comparisons we used the modeled vertical ozone profile in the grid cell at the time of the ozonesonde launch, so did not account for the horizontal and temporal displacement of the ozonesonde measurements from its launch point and start time. Figure ES-6 displays two of the comparisons of the predicted and observed vertical ozone profiles for June 15 and July 21, 2006. In general, the model does a better job reproducing the observed vertical ozone profiles for the three June days than the three July days. For example, on June 15 the model and observed ozone agree well in the lowest 2 km of the atmosphere and then deviate from each other. On the other hand, on July 21, 2006 the model is underpredicting the observed ozone in the lowest 2 km of the atmosphere by 20 ppb.

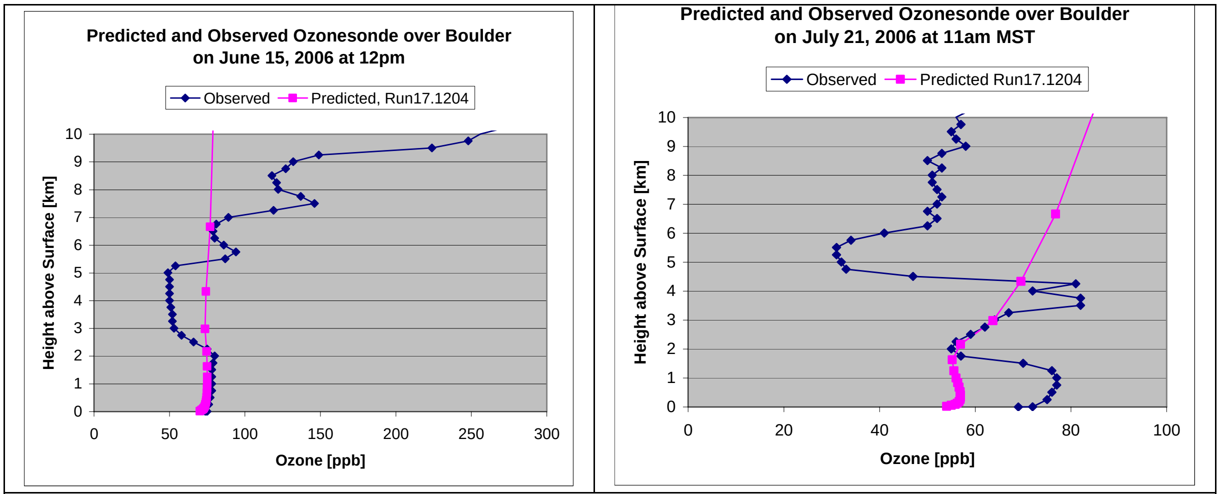

Figure ES-6. Comparison of predicted and observed vertical ozone profiles at Boulder for June 15 and July 21, 2006.

PM Performance

The Denver June-July 2006 photochemical modeling database was developed for demonstrating attainment of the 8-hour ozone standard. Consequently, the focus was on ozone and ozone precursor performance. Thus, no effort was spent on optimizing model performance for particulate matter (PM) species. In particular, the CDPHE/APCD only provided complete ozone precursor emissions (i.e., VOC, NOx and CO) for the state of Colorado. When modeling many sources categories, such as on-road mobile using SMOKE-MOBILE6 and CONCEPT MV models and processing the CEM data for point sources, we pick up the PM precursor emissions. However, for area and non-road mobile source emissions for sources in Colorado we only have ozone precursor emissions so are missing many PM related species (e.g., SO2, primary PM and ammonia). Thus, we expect to underpredict PM mass and PM species in the model performance evaluation.

Figure ES-7 displays an example evaluation for total PM2.5 mass from the more urban-oriented FRM and more rural-oriented IMPROVE monitoring networks. As expected, PM2.5 is underestimated most of the time. This underprediction is prevalent across all PM species with the lowest underprediction for SO4 and highest for NO3. These results are consistent with missing PM precursor emissions from area and non-road sources that would affect NO3 the most.

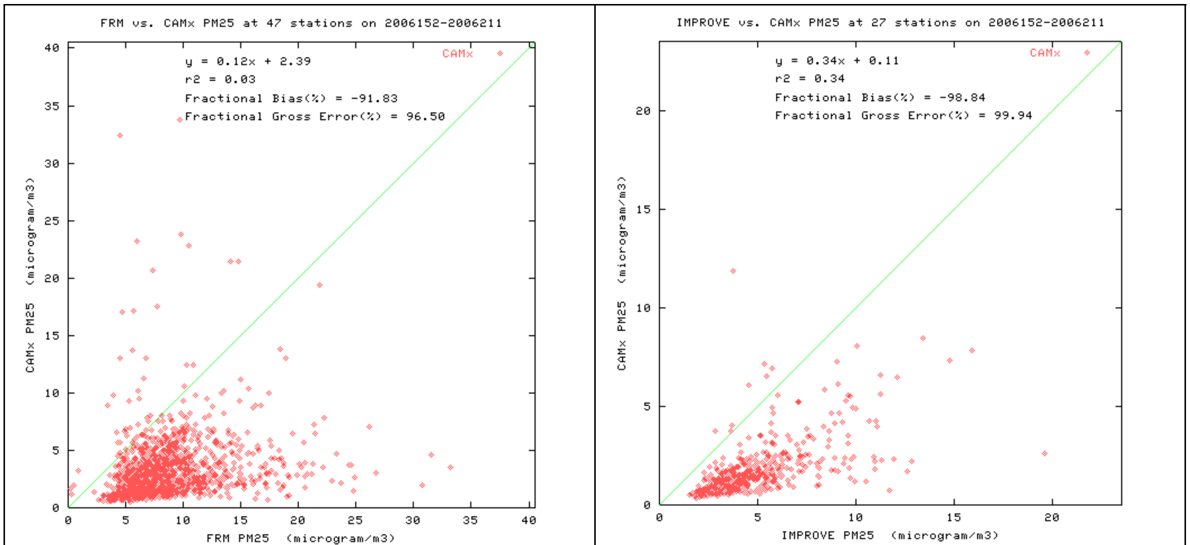

Figure ES-7. Comparison of predicted and observed total $PM_{2.5}$ mass model performance at FRM (left) and IMPROVE (right) sites in the 12 km modeling domain.

CONCLUSIONS OF MODEL PERFORMANCE EVALUATION

As noted in EPA's latest air quality modeling guidance, "by definition, models are simplistic approximations of complex phenomena" that "…contain many elements that are uncertain". Consequently, achieving perfect model performance is unattainable and some uncertainties will always exist. The Denver final 2006 base case (Run 17) CAMx simulation achieves EPA's performance goals on a vast majority of days during the June-July 2006 modeling episode. The model is also exhibiting very good agreement for VOC/NOx ratios in Denver on most days, suggesting that the model is simulating the correct chemical regimes. The model performance is as good as or better than past ozone SIP modeling in the Denver and many other areas whose SIPS have been approved by EPA. Based on the model performance evaluation presented in this report, we conclude that the model is performing well enough to reliable project future-year ozone concentrations within the normal uncertainties of photochemical grid modeling. Although care should be taken that the ozone projections are not unduly affected by the few poor performing days.

The model performance evaluation has identified several areas of future research that could improve model performance including a focus on VOC speciation and the presence of aldehydes in the inventory, improvements in oil and gas emissions and other sources of natural gas related emission sources and better simulation of ozone aloft.

1.0 INTRODUCTION

1.1 BACKGROUND

Ozone air quality in the Denver Metropolitan Area (DMA) has been near the 8-hour ozone National Ambient Air Quality Standard (NAAQS) of 0.08 ppm (exceedance defined by values of 85 ppb or higher) for several years. Based on 2005-2007 measured air quality, the DMA violated the 0.08 ppm 8-hour ozone NAAQS so is required to prepare an 8-hour ozone State Implementation Plan (SIP) that demonstrates attainment by 2010. This report presents the 2006 base case modeling and model performance evaluation element of the DMA 2010 attainment demonstration modeling.

1.1.1 Denver EAC 8-Hour Ozone SIP

In December 2002, the Denver Regional Air Quality Council (RAQC) and Colorado Department of Health and Environment (CDPHE) Air Pollution Control Division (APCD) and others entered into an 8-hour ozone Early Action Compact (EAC) with the U.S. Environmental Protection Agency (EPA). EPA's EAC allows an area to submit an enforceable 8-hour ozone State Implementation Plan (SIP) by March 2004 that demonstrates attainment of the 8-hour ozone NAAQS by 2007. In return, EPA will defer the classification of an area as nonattainment until 2007. The RAQC and APCD contracted with ENVIRON International Corporation with their subcontract of Alpine Geophysics, LLC to perform the photochemical modeling necessary for the Denver 8-hour ozone EAC SIP. At the outset of the EAC modeling, the DMA was in attainment of the 8-hour ozone NAAQS. However, the monitored ozone concentrations during the summer of 2003 resulted in violations of the 8-hour ozone standard. Because of the EAC, EPA classified the DMA as "nonattainment deferred", with final designation to be determined after the 2007 ozone season. More details on the Denver 8-hour EAC SIP are available at: http://www.raqc.org/ozone/EAC/ozone-eac.htm

Ozone attainment is based on 8-hour ozone Design Values (DVs) that are defined as the three-year average of the fourth highest 8-hour ozone concentration during a year at a monitor. Based on measured ozone concentrations during the 2005-2007 three-year period, the maximum 8-hour ozone DV in the DMA was 85 ppb at the Rocky Flats North (RFNO) monitoring site, which exceeds the 8-hour ozone NAAQS. Consequently, in November 2007 the DMA reverted to an 8-hour ozone nonattainment area and the RAQC/APCD is charged with developing a new 8-hour ozone SIP emissions control plan that demonstrates the DMA will achieve attainment of the 0.08 ppm 8-hour ozone NAAQS by 2010.

1.1.2 New 8-Hour Ozone NAAQS

On March 12, 2008, EPA promulgated a new primary ozone NAAQS that has the same form as the 0.08 ppm 8-hour ozone NAAQS, but lowers the threshold from 0.08 ppm (85 ppb) to 0.075 ppm (75 ppb). Of the ~14 ozone monitors in the greater DMA, half have 2005-2007 8-hour ozone DVs that are 75 ppb or higher. The current Denver 8-hour ozone SIP modeling effort addresses the 0.08 ppm 8-hour ozone NAAQS. The designations of 8-hour ozone nonattainment areas under the new 0.075 ppm 8-hour ozone NAAQS will be made in 2010 based on 2007-2009 observed ozone concentrations with subsequent SIPs due in 2013. Attainment of the new 8-hour ozone NAAQS will be required by 2016 (moderate) to 2030 (extreme) depending on the nonattainment area classification.

1.2 PURPOSE

With the Denver region needing to quickly develop an 8-hour ozone attainment control strategy for the SIP, ENVIRON and Alpine were reenlisted to prepare the photochemical modeling databases necessary to develop a control plan that demonstrates attainment of the 8-hour ozone standard by 2010. The ENVIRON/Alpine Modeling Team are employing the fifth generation Mesocale Model (MM5) meteorological model (Anthes and Warner, 1978; Dudhia, 1993), the Sparse Matrix Operating Kernel Emissions (SMOKE) modeling system (Coats, 1996) and the Comprehensive Air-quality Model with extensions (CAMx) photochemical grid model (ENVIRON, 2008) to model ozone in the Denver area for a June-July 2006 modeling period for the purposes of demonstrating attainment of the 8-hour ozone standard by 2010. The 8-hour ozone modeling activities being performed by the ENVIRON/Alpine Modeling Team consists of the following activities:

- Development of a Denver 8-hour ozone SIP attainment demonstration Modeling Protocol (Morris et al., 2007; http://www.ozoneaware.org/documents/DraftFinalProtocolDenver8-HourOzoneNov282007.pdf);
- Development of a preliminary 36/12/4 km photochemical modeling database for the June-July 2006 episode, the DMA, and initial model performance evaluation, sensitivity test modeling and identification of optimal model configuration for simulating ozone in the DMA (Morris et al., 2008);
- Final base case modeling and model performance evaluation for the June-July 2006 DMA episode (this document);
- 2010 base case modeling, emission sensitivity tests and ozone source apportionment modeling (in progress); and
- 2010 control strategy modeling (in progress).

A previous report documented the results of the preliminary application and evaluation of the photochemical modeling system for the June-July 2006 period using the initial model configuration and includes results of diagnostic tests designed to improve model performance and recommendations for a final optimal model configuration for the 8-hour Denver ozone SIP (Morris et al., 2008). This report presents the final 2006 base case modeling and model performance evaluation for the June-July 2006 episode.

1.3 OVERVIEW OF MODELING APPROACH

The Denver 8-Hour ozone SIP modeling includes emissions, meteorological and ozone simulations using a nested 36/12/4 km grid with the 4-km grid focused on the state of Colorado including the DMA and vicinity. The procedures for conducting the Denver SIP ozone modeling are outlined in a Modeling Protocol (Morris et al., 2007). The Denver 8-hour ozone modeling approach was to develop an initial 36/12/4 km modeling database for the June-July 2006 episode using the MM5 meteorological, SMOKE emissions and CAMx photochemical grid models that is described by Morris and co-workers (2008). The preliminary photochemical modeling identified an optimal model configuration for the final 2006 base case that is described in this report. The emissions were also updated for the final 2006 base case modeling. In addition to obtaining revised and corrected emissions from the APCD for Colorado, the following two additional emission inventory enhancements were made for the final 2006 base case emissions inventory:

- Generation of refined on-road mobile source emissions using the CONCEPT emissions model and link-based Vehicle Miles Travelled (VMT) data from the Denver Regional Council of Government (DRCOG) Travel Demand Model (TDM); and
- Use of the WRAP Phase III oil and gas (O&G) emissions for the Denver-Julesburg Basin.

Below we provide an overview of the modeling approach and summarize emission updates performed for the final 2006 base case modeling. Details on the meteorological modeling, SMOKE emissions modeling and other aspects of the development of the June-July 2006 modeling database are presented in the preliminary modeling report (Morris et al., 2008).

1.3.1 Modeling Domains

Figure 1-1a displays the MM5 (red) and CAMx (blue) 36/12/4 km modeling domains used in the Denver 8-hour ozone modeling study. These modeling domains are based on a Lambert Conformal Project (LCP) using the parameters given in Table 1-1. The MM5 modeling domains are defined slightly larger than the CAMx domains in order to allow the MM5 model to eliminate any boundary artifacts that occur as the MM5 model brings the meteorological variables specified in the boundary conditions into dynamic balance with each other. Details on the Denver June-July 2006 MM5 meteorological modeling are provided in a companion report to this one (McNally et al., 2008).

The SMOKE, ConCEPT, MEGAN and GloBEIS emissions models use the same modeling domains as CAMx. Table 1-2 lists the number of rows and columns and the definition of the X and Y origin (i.e., the southwest corner) for the 36/12/4 km domains used by MM5, CAMx and the SMOKE, CONCEPT and MEGAN emissions models. In Table 1-2 “Dot” refers to the grid mesh defined at the vertices of the grid cells while “Cross” refers to the grid mesh defined by the grid cell centers. Thus, the dimension of the dot mesh is equal to the cross mesh plus one.
Figure 1-1b displays the SMOKE/CAMx 12/4 km modeling domains. The CAMx model was first applied to the 36 km continental U.S. domain using boundary conditions (BCs) from a global climate air quality model (Figure 1-1a). The CAMx 2006 base case modeling results from the 36 km continental U.S. domain simulation are then processed to generate BCs for the CAMx 12/4 km domain (Figure 1-1b). The CAMx 2006 base case simulations for the 12/4 km domains were run using two-way interactive grid nesting (i.e., pollutants can flow back and forth between the 12 km and 4 km domains to account for recirculation).

Table 1-1. Lambert Conformal Projection (LCP) definition for the Denver 36/12/4 km modeling grids.

Parameter	Value
Projection	Lambert-Conformal
1st True Latitude	33 degrees N
2nd True Latitude	45 degrees N
Central Longitude	-97 degrees W
Central Latitude	40 degrees N

Table 1-2. Grid definitions for MM5, Emissions and CAMx modeling domains.

MODEL	COLUMNS DOT(CROSS)	ROWS DOT(CROSS)	XORIGIN (KM)	YORIGIN (KM)
MM5				
36 km grid	165 (164)	129 (128)	-2952.0	-2304.0
12 km grid	187 (186)	157 (156)	-1836.0	-936.0
4 km grid	151 (150)	136 (135)	-984.0	-324.0
Emissions/CAMx				
36 km grid	(148)	(112)	-2736.0	-2088.0
12 km grid	(167)	(92)	-1704.0	-624.0
4 km grid	(119)	(119)	-940.0	-940.0

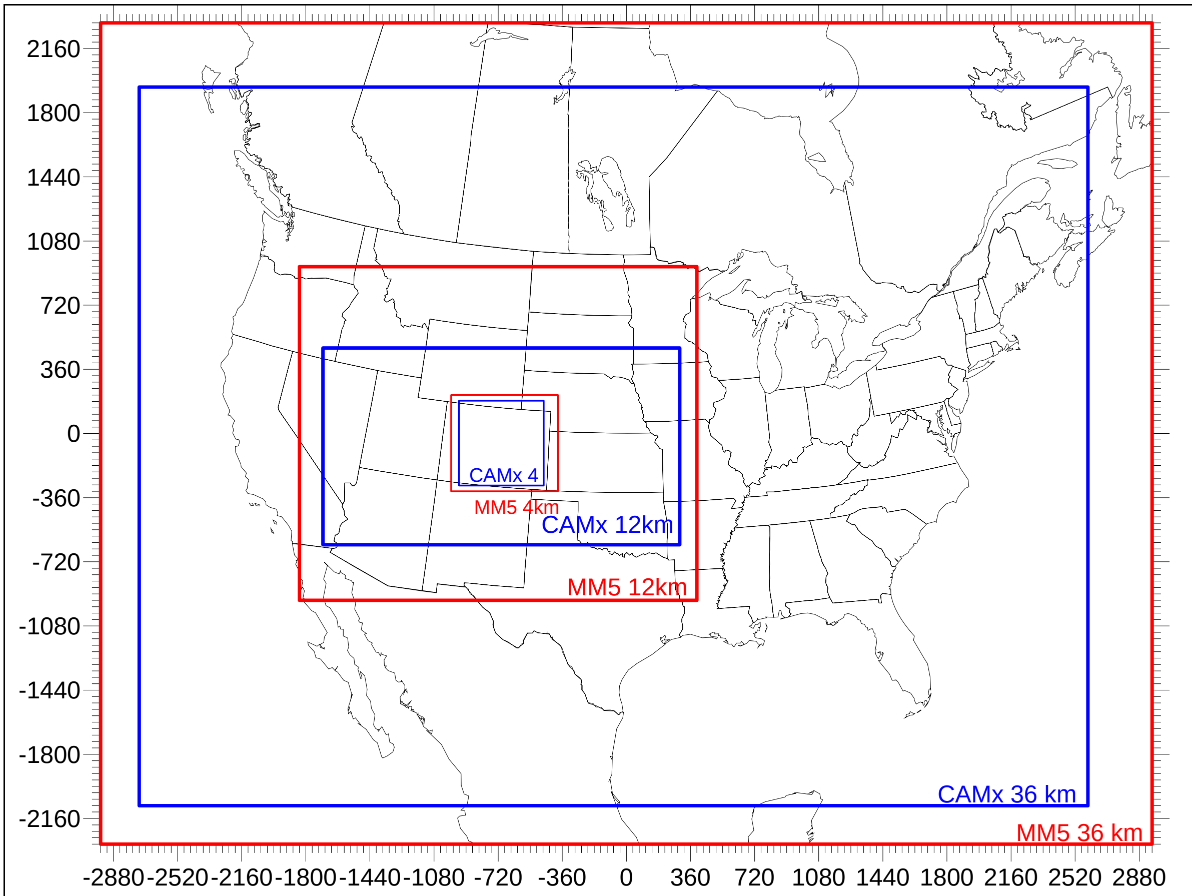

Figure 1-1a. Nested 36/12/4 km modeling domains for the Denver 8-hour ozone modeling study. Blue line domains are for CAMx/SMOKE domains that are nested in the MM5 red line domains.

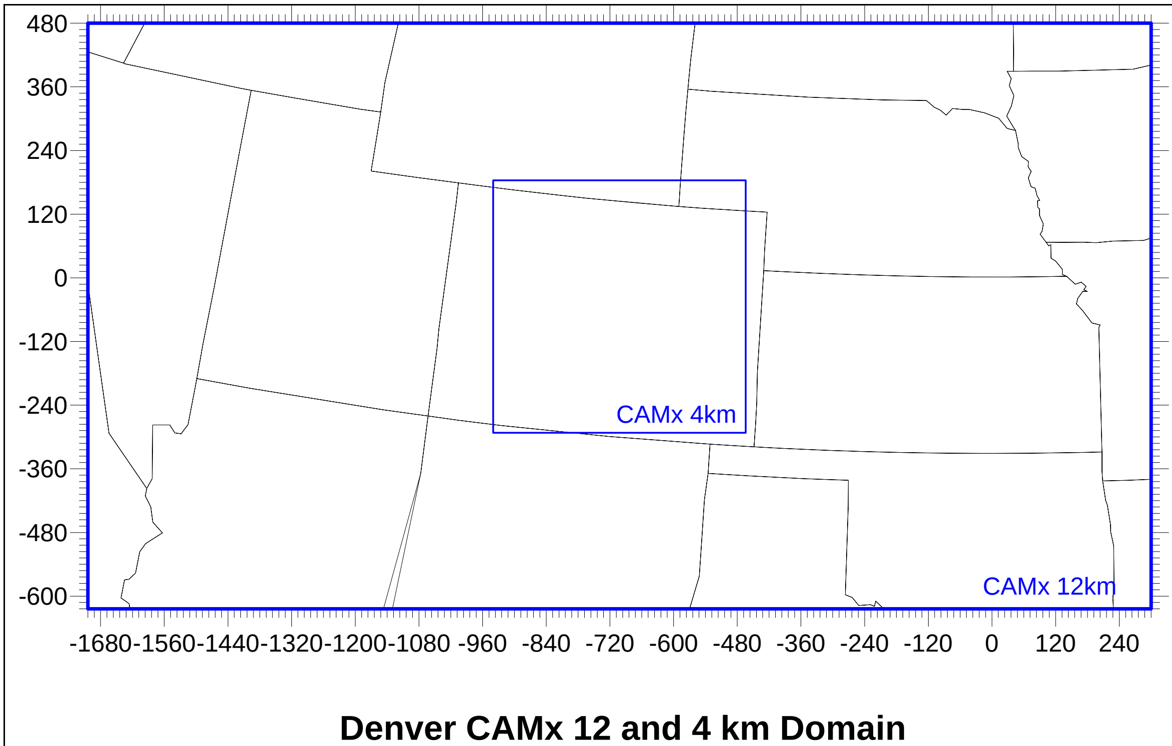

Figure 1-1b. Nested 12/4 km modeling domains for the Denver CAMx air quality and SMOKE emissions modeling.

1.4 EMISSIONS MODELING APPROACH

The emission inputs for the Denver June-July 2006 8-hour ozone modeling episode were prepared in two phases. In the first phase, a Fast Track model-ready emissions inventory was developed in late 2007 using the SMOKE emissions model for all anthropogenic emissions and the GloBEIS model for biogenic emissions (Morris et al., 2008). The CDPHE/APCD provided 2006 emissions for Colorado counties with the rest of the region using the WRAP and other RPO 2002 emissions projected to 2005. The Fast Track emissions inventory was used for initial diagnostic testing and model performance evaluation of the CAMx model (Morris et al., 2008). The CDPHE provided revised 2006 base case emissions for Colorado that contained several updates and corrections. In addition, emissions for on-road mobile sources in the DMA and oil and gas sources were updated as described below.

1.4.1 SMOKE Emissions Modeling Approach

CAMx-ready emissions were generated using the Sparse Matrix Operator Kernel Emissions (SMOKE) emissions modeling system (Coats, 1996) for all anthropogenic emissions categories except on-road mobile sources in the DMA, which used the Consolidated Community Emissions Processing Tool (ConCEPT) modeling system (Loomis et al., 2005). The final 2006 base case biogenic emissions were based on the Model of Emissions of Gases and Aerosols from Nature (MEGAN) biogenic emissions model (Guenther and Wiedinmyer, 2004).

Emissions inventory development for episodic 8-hour ozone modeling must address several source categories including: (a) stationary point sources; (b) area sources; (c) on-road mobile sources; (d) non-road mobile sources; (e) biogenic sources; and (f) fire sources. For this analysis, these estimates were developed for the June-July 2006 modeling period, the 36, 12 and 4 km grids (Figure 1-1) and the CB05 chemical mechanism.

CAMx requires two emission input files: (1) low-level gridded emissions that are emitted directly into the first layer of the model from sources at the surface with little or no plume rise; and (2) elevated point sources (stacks) with plume rise calculated from stack parameters and meteorological conditions.

1.4.1.1 SMOKE Configuration

The CAMx-ready emission files for anthropogenic emissions and the Fast Track emissions modeling were prepared using the SMOKE emissions modeling system. The SMOKE emissions model performs the following tasks:

> Temporal Adjustments: Adjust emission rates for seasonal, day-of-week and hour-of-day effects. The temporal allocation factors used are standard SMOKE adjustment factors, supplemented with state and county specific adjustments developed during the RPO modeling process.
>
> Chemical Speciation: Emission estimates for total VOC are converted to the more detailed chemical speciation used by the Carbon Bond 5 (CB05) chemical mechanism in CAMx. Total unspeciated NOx emissions are allocated to NO and NO2 components. The SMOKE emission model includes default speciation profiles by SCC codes.
>
> Spatial Allocation: Area and non-road mobile sources are estimated at the county level, and are allocated to the grid cells within each county based on spatial surrogates (e.g., population and economic activity). On-road mobile source emissions are also allocated to grid cells, using spatial surrogates based on roadway locations and population. The latest spatial surrogates available from EPA, dated April 2004, and were used in the emissions modeling. (http://www.epa.gov/ttn/chief/emch/spatial/newsurrogate.html)
>
> Quality Assurance: SMOKE includes quality assurance (QA) and reporting features to keep track of the adjustments at each processing stage and ensure that data integrity is not compromised.

The outputs from the emissions model are called the “model-ready” emissions, and are day-specific, gridded, speciated and temporally (hourly) allocated. SMOKE performs all of the processing steps for the anthropogenic emissions. The biogenic emissions were prepared using the MEGAN model using hourly MM5 meteorological data and gridded biomass type and density information.

The configuration used in the SMOKE emissions modeling for the final Denver 2006 base case simulation is shown in Table 1-3. More details on the SMOKE emissions modeling is provided in the preliminary evaluation and sensitivity modeling report (Morris et al., 2008).

Table 1-3. Summary of SMOKE configuration parameters and data inputs.

Emissions Component	Configuration	Details
Model Code	SMOKE Version 2.2	www.cmascenter.org
Horizontal Grid Mesh	36/12/4 km	
36 km grid	148 x 112 cells	
12 km grid	167 x 92 cells	
4 km grid	119 x 119	
Area Source Emissions	2006 CDPHE/APCD for Colorado 2005 projected from 2002 RPO outside Colorado	SMOKE processing
On-Road Mobile Sources	SMOKE-MOBILE6	County HPMS VMT and SMOKE-MOBILE6 In DMA replaced by CONCEPT link-based VMT mobile source emissions
Point Sources	2006 day-specific CEM Projected 2002 RPO outside Colorado	Use 2006 day-specific hourly CEM for actual and processed CEM for Typical 2006 emissions
Off-Road Mobile Sources	2006 CDPHE/APCD for Colorado Projected 2002 RPO outside Colorado	
O&G Sources	WRAP Phase III for D-J Basin WRAP Phase II outside of D-J	Bar-Ilan et al., 2008
Emissions Data Sources	2006 CDPHE/APCD for Colorado	
	2002 Plan02b WRAP States	Projected to 2005
	2002 Base G CENRAP States	Projected to 2005
	2002 Base M MRPO States	Projected to 2005
	2002 Base G VISTAS States	Projected to 2005
	2006 HPMS for outside Colorado	Process with SMOKE-MOBILE6
	Acid Rain Database for CEM data	Large stationary source NOx and SO2
	O&G WRAP Phase III for D-J Basin	
Biogenic Sources	MEGAN	Use day-specific hourly MM5 meteorology
Wildfires	2006	From NCAR
Temporal Adjustments	Seasonal, day, hour	Based on latest collected information updated for RPO modeling
Chemical Speciation	Revised CB05 Chemical Speciation	EPA updated in 2007
Gridding	Spatial Surrogates based on landuse	EPA updated in 2004
Quality Assurance	QA Tools in SMOKE and CONCEPT; PAVE plots; Summary reports	

1.4.2 Updated WRAP Phase III O&G Emissions for the D-J Basin

The Independent Petroleum Association of Mountain States (IPAMS) is sponsoring the development of a Phase III regional oil and gas emission inventory for the inter-Mountain West jointly with the Western Regional Air Partnership (WRAP), to build on the WRAP Phase I and Phase II inventory projects (WRAP Phase III O&G Project). This effort is focused on creating a comprehensive criteria pollutant emissions inventory for all activities associated with oil and gas field operations in the basins throughout the study region for year 2006 as well as future projection years; that includes all point and area sources related to the oil and gas industry.

The initial region of interest for the WRAP Phase III O&G emission inventory is the Denver-Julesburg (D-J) Basin, which includes the Denver and Northern Front Range 8-hour ozone nonattainment areas. The 2006 baseline inventory consists of two primary categories: sources subject to Air Pollution Emission Notice (APEN) reporting requirements, and sources exempt from APEN reporting. The WRAP Phase III project has completed the O&G emissions development for the 2006 base and 2010 future year (Bar Ilan et al., 2008a,b) and the reports are available on the WRAP website at:

- http://www.wrapair.org/forums/ssjf/documents/eictts/OilGas/2008-04_'06_Baseline_Emissions_DJ_Basin_Technical_Memo_(04-30).pdf
- http://www.wrapair.org/forums/ssjf/documents/eictts/OilGas/2008-04_'10_Projection_Emissions_DJ_Basin_Technical_Memo(04-30).pdf

In general, the inventory was developed using a combination of well count and production activity from a commercially available database of oil and gas data maintained by IHS Corporation ("the IHS database"), the State of Colorado's database of permitted sources including APENs sources and Regulation 7 reports, and detailed survey responses of oil and gas activity from several major participating companies that operate in the D-J Basin. Some additional data sources were also used, including American Petroleum Institute (API) technical literature, the US Environmental Protection Agency's (EPA) AP-42 emissions factor technical guidance, the US EPA's NONROAD emissions model, and the US EPA's Natural Gas Star program technical guidance.

1.4.2.1 Temporal and Geographic Scope

The WRAP Phase III D-J O&G emissions inventory considers a base year of 2006 for purposes of estimating emissions, consistent with the June-July 2006 modeling episode for the Denver 8-hour ozone SIP modeling. All data requested from participating companies were for these companies' activities in the calendar year 2006. Similarly, all well count and production data for the basin obtained from the IHS database were for the calendar year 2006. Emissions from all source categories are assumed to be uniformly distributed throughout the year except for heaters and pneumatic pumps, which are assigned seasonality fractions as they are typically used primarily in winter.

The geographic scope of this inventory is the D-J Basin, whose boundaries as defined by the US Geological Survey (USGS) were used. The USGS boundaries for the D-J Basin were intersected with the State of Colorado boundaries so that only the portion of the D-J Basin within Colorado was considered for this inventory. The following counties were wholly contained within the boundaries of the D-J Basin in this inventory:

- Adams
- Arapahoe
- Boulder
- Broomfield
- Crowley
- Denver
- Douglas
- Elbert
- El Paso
- Fremont
- Jefferson
- Kit Carson
- Larimer
- Lincoln
- Logan
- Morgan
- Phillips
- Pueblo
- Sedgwick
- Teller
- Washington
- Weld
- Yuma

Figure 1-2 shows the boundaries of the D-J Basin, with the 2006 well locations extracted from the IHS database overlaid.

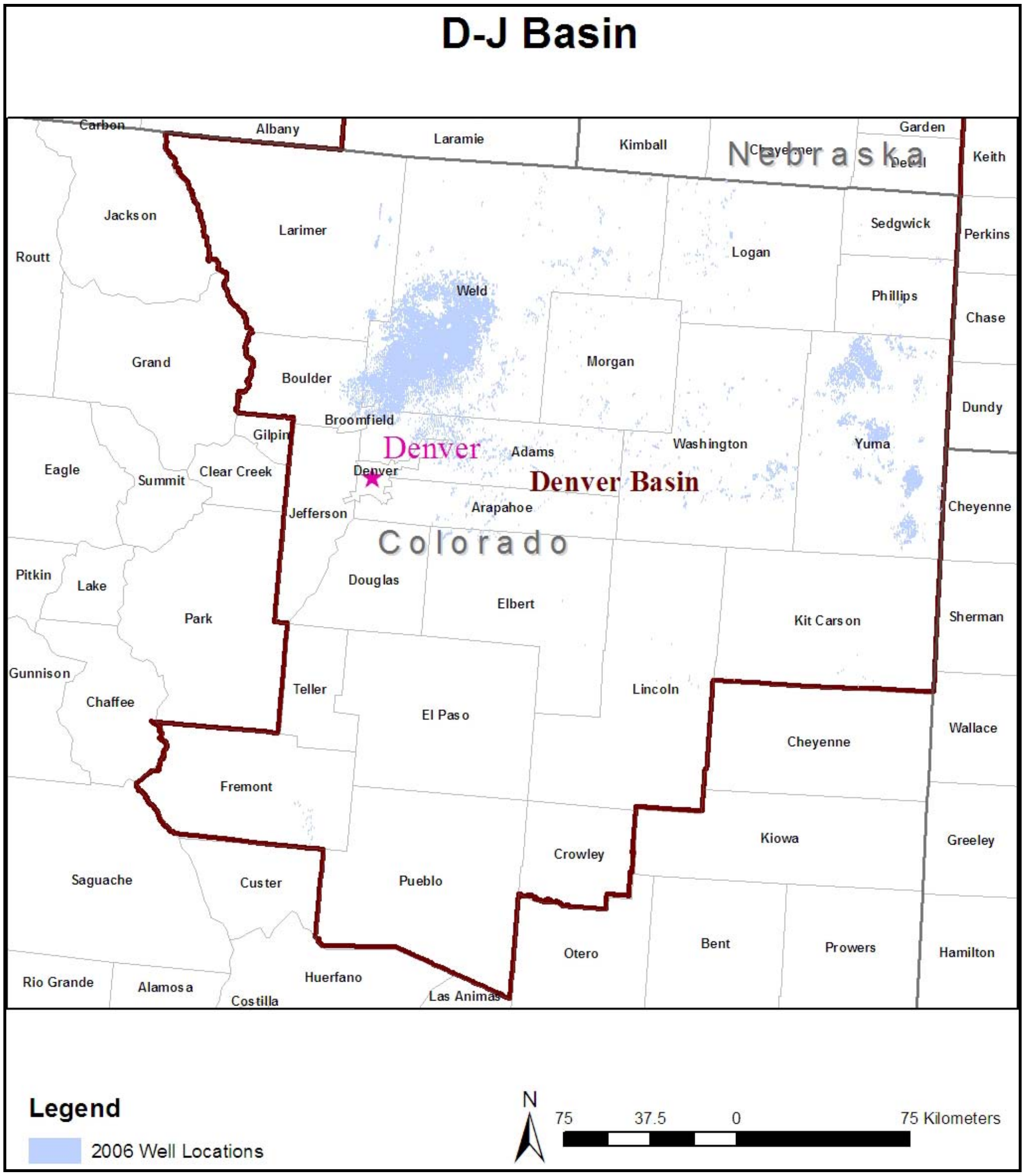

Figure 1-2. D-J Basin boundaries overlaid and 2006 oil and gas well locations.

1.4.2.2 Well Count and Production Data

Oil and gas related activity data across the entire D-J Basin were obtained from the IHS Enerdeq database queried via online interface. The IHS database uses data from the Colorado Oil and Gas Conservation Commission (COGCC) as a source of information for Colorado oil and gas activity. Two types of data were queried from the Enerdeq database: production data and well data. Production data includes information relevant to producing wells in the basin while well data includes information relevant to drilling activity ("spuds") and completions in the basin.

1.4.2.3 Sources Subject to APEN and Condensate Tanks Subject to Regulation 7

On October 31, 2007 a request was made to the APCD for the 2006 Colorado APEN database for all oil and gas related emission sources covered by the following SCC and SIC codes:

- All of the SCCs 202002*, 310*, 404003* (where * indicates all sub-SCCs for the SCC)
- And only those with the following SICs: 13*, 492*, 4612.

APEN data for the D-J basin were extracted and sorted by operator. Company specific APEN source data were forwarded to participating operators for a completeness review that included the following three issues:

1) Source Categories that were missing from the APEN database,
2) Specific sources missing from the database, and
3) Sources within the database known to be no longer operating.

Following the completeness review and the addition or deletion of sources as appropriate, emission rates were reviewed. Emission rates were updated to reflect 2006 actual emissions in cases where supporting data were available. Actual emission updates provided by operators followed the APCD calculation methodologies from existing permits or required Operation and Maintenance Plans. The APCD methodologies are used to update Annual Emission Calculations (Minor Sources) and 12-Month Rolling Emission Totals (Synthetic Minor and Major Sources).

A separate request was made to APCD for a copy of the 2006 Regulation 7 atmospheric storage tank reports for year 2006. Within the Ozone Control Area, data from the Regulation 7 reports was utilized in place of the APEN data to represent stock tank emissions as the Regulation 7 reports best reflected actual emissions. The Regulation 7 reports for condensate tanks were in the form of monthly reports of condensate throughput for each tank, and emissions for each tank, for all companies operating condensate tanks subject to Regulation 7 in the ozone non-attainment area. A macro was written in EXCEL to process the reports in such a way that monthly condensate throughput (bbl) and emissions (lb-VOC) could be extracted and summed. Confirmation was obtained that CDPHE's annual Regulation 7 condensate tank emissions summary for 2006 was in reasonable agreement with the extracted emissions from the monthly Regulation 7 reports.

GIS analysis was used to intersect the boundary of the ozone non-attainment area with the latitude/longitude coordinates of all APENs sources. Those sources falling within the ozone non-attainment area were filtered to remove any sources that were condensate tanks, based on SCC and SCC description. For purposes of summing all permitted oil and gas sources' emissions in the D-J Basin, emissions from the remaining APENs sources (excluding condensate tanks in the ozone non-attainment area) were added to the summary emissions from all Regulation 7 condensate tank reports.

1.4.2.4 APEN Exempt Sources

Survey forms consisting of 11 Excel spreadsheets were forwarded to participating operators in the D-J basin. Each spreadsheet contained a request for specific data related to one of the following APEN exempt source categories:

- Well blowdowns
- Well completions
- Drilling rigs
- Exempt engines
- Fugitive emissions
- Heaters
- Gas composition analysis for the basin
- Pneumatic devices
- Pneumatic pumps
- Water tanks
- Workover rigs

The companies participating in the survey process for the D-J Basin represented 50% of well ownership in the basin, 63% of gas production in the basin, and 58% of oil production in the basin. This represented a sufficiently large percentage of oil and gas activity in the basin that it was felt that the responses obtained from the participating companies would be representative of all oil and gas operations in the basin.

In addition to the source categories listed above, emissions from three additional APEN exempt source categories were estimated based on additional information requests from the participating companies:

- APEN exempt atmospheric storage tanks
- Truck loading activities
- Flaring from condensate tanks

1.4.2.5 WRAP Phase III D-J Basin O&G Summary Results

Results from the combined permitted sources (APENs sources excluding condensate tanks in the ozone non-attainment area, and condensate tanks in the ozone non-attainment area from the Regulation 7 reports), and the combined unpermitted sources are presented below on a county level and as summaries for the entire D-J Basin as a series of pie charts and bar graphs.

Figure 1-3 shows that NOx emissions are primarily concentrated in Weld and Yuma counties, which is not surprising given that it is the areas of large concentrations of well locations. Figure 1-4 shows that VOC emissions are primarily concentrated in Weld county only. Production activity in Yuma County is mostly dry gas, and therefore a smaller proportion of total VOC emissions occur in Yuma County.

Figure 1-4 shows that compressor engines and drilling rigs combined account for almost 80% of NOx emissions. Similarly, Figure 1-5 shows that permitted and unpermitted condensate tanks and pneumatic devices account for approximately 81% of VOC emissions. Table 1-4 summarizes the WRAP Phase III emissions for the D-J Basin and 2006 base case by county. A majority of the VOC (78%) and NOx (59%) D-J Basin O&G emissions come from Weld County.

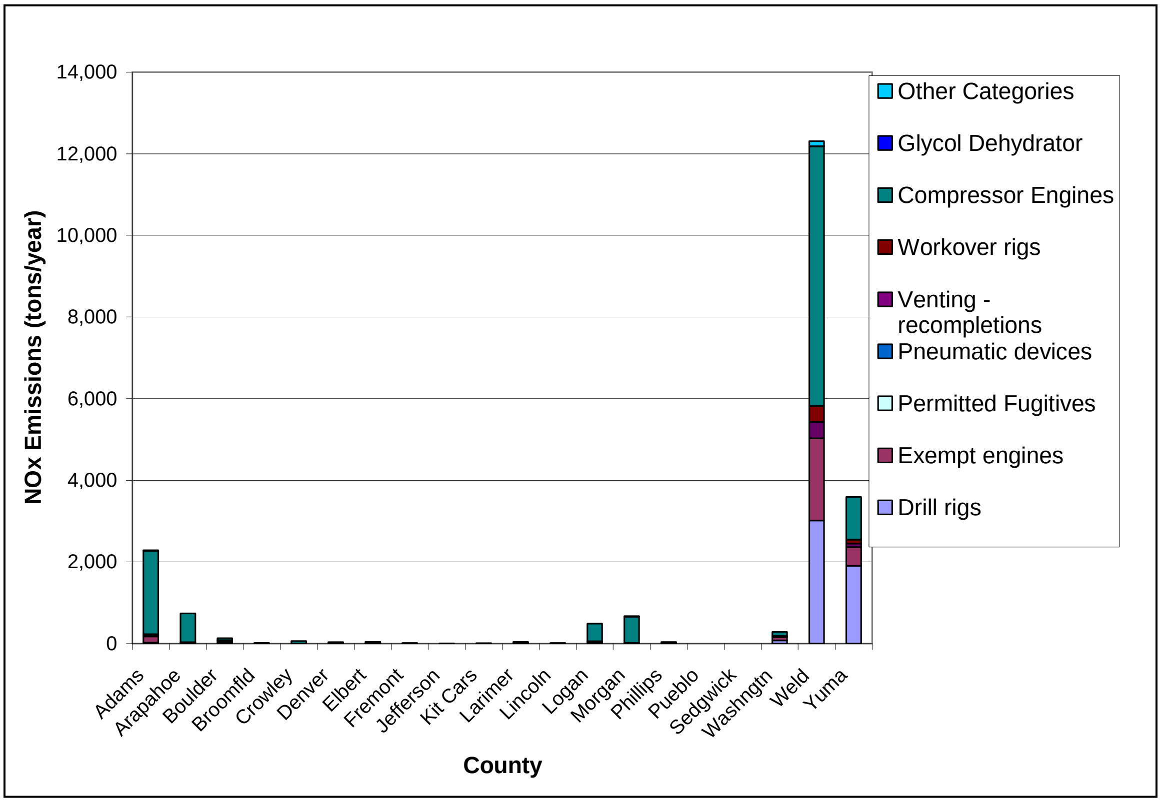

Figure 1-3. 2006 NOx emissions by source category and by county in the D-J Basin.

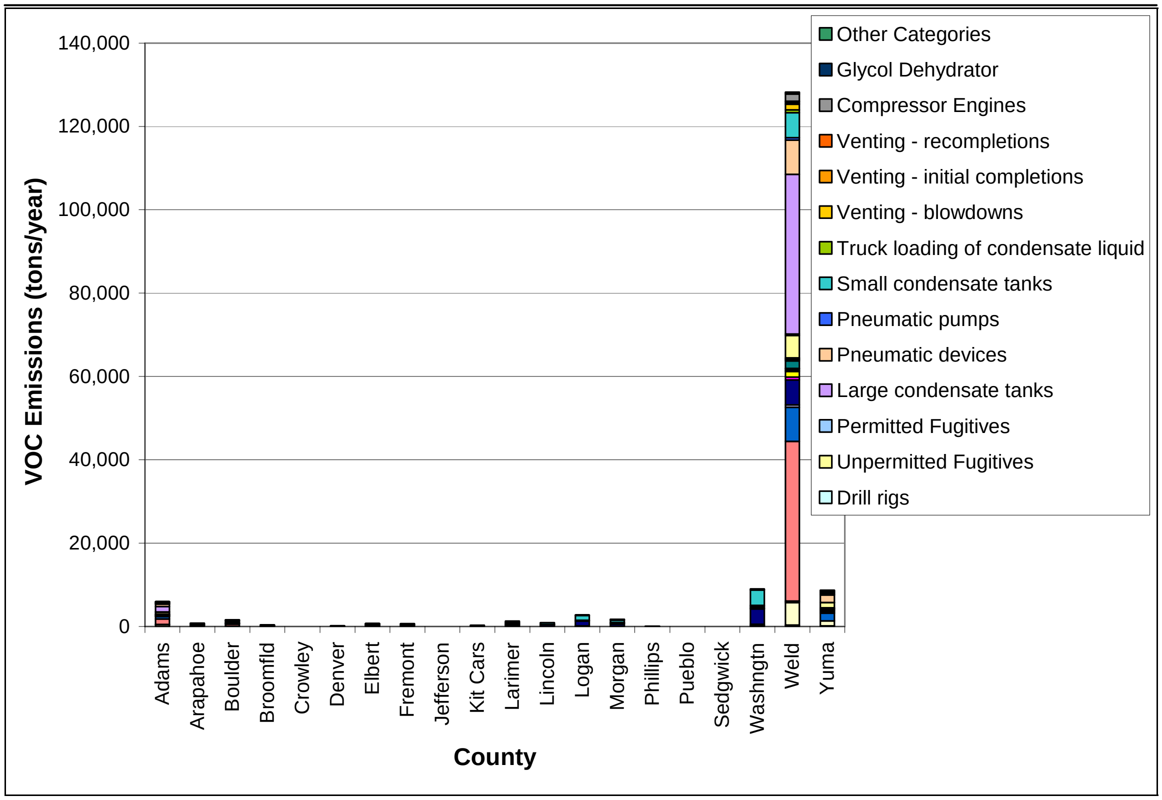

Figure 1-4. 2006 VOC emissions by source category and by county in the D-J Basin.

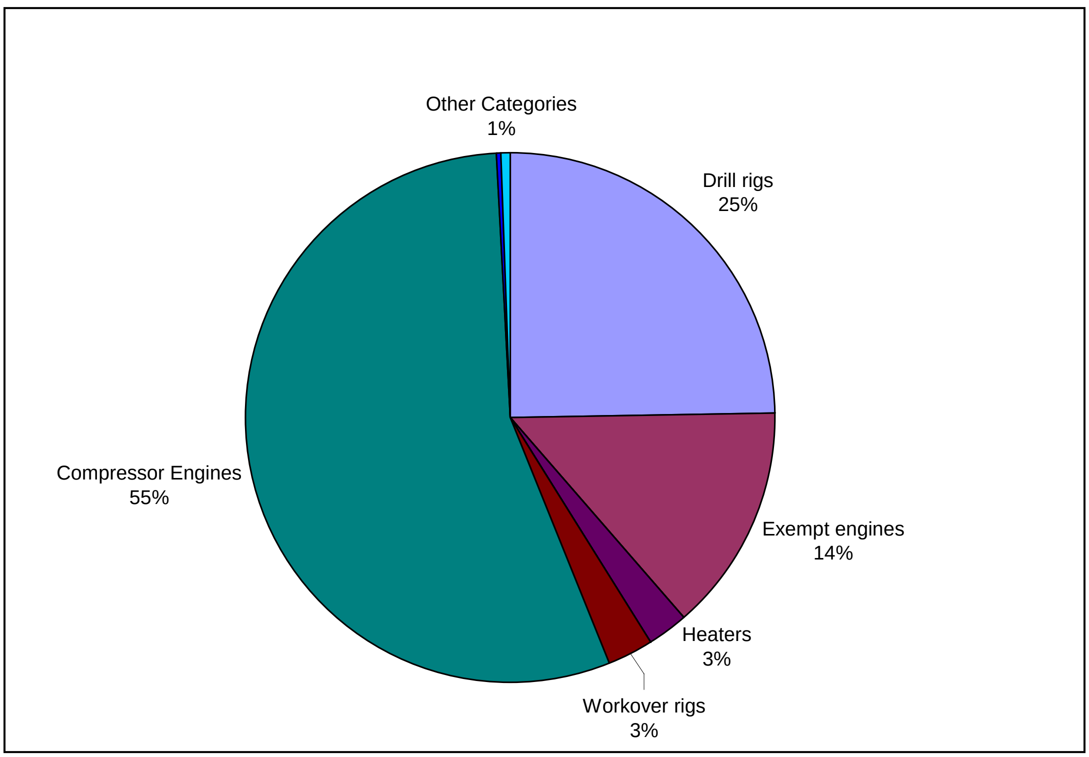

Figure 1-5. D-J Basin NOx emissions proportional contributions by source category.

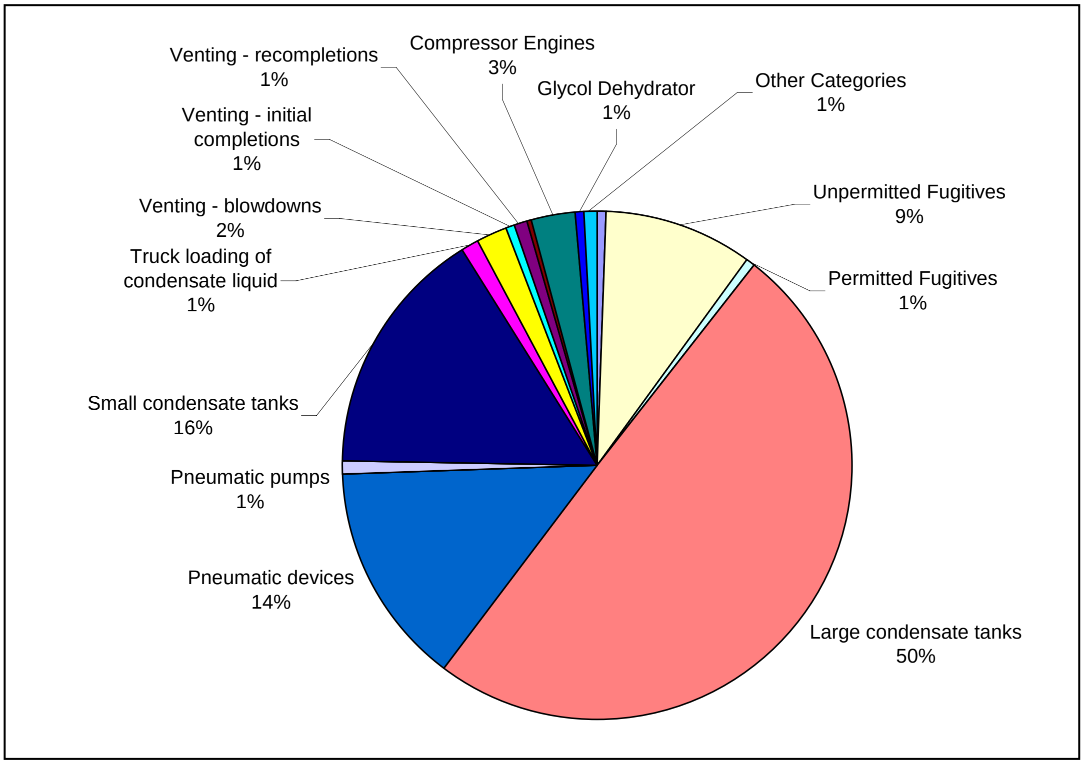

Figure 1-6. D-J Basin VOC emissions proportional contributions by source category.

Table 1-4. 2006 emissions of all criteria pollutants by county for O&G emissions in the D-J Basin.

County	NOx [tons/yr]	VOC [tons/yr]	CO [tons/yr]	SOx [tons/yr]	PM [tons/yr]
Adams	2,286	3,005	939	13	19
Arapahoe	742	408	253	0	4
Boulder	129	803	76	1	4
Broomfield	14	193	10	0	0
Crowley	63	1	85	0	1
Denver	32	103	19	0	2
Douglas	0	0	0	0	0
Elbert	43	363	27	0	1
El Paso	0	0	0	0	0
Fremont	16	329	9	0	1
Jefferson	6	0	10	0	0
Kit Carson	10	139	6	0	1
Larimer	37	651	23	0	1
Lincoln	14	462	11	0	0
Logan	491	1,382	183	2	9
Morgan	672	883	672	132	4
Phillips	40	47	26	0	1
Pueblo	0	0	0	0	0
Sedgwick	1	11	0	0	0
Teller	0	0	0	0	0
Washington	284	4,509	207	1	9
Weld	12,310	64,111	8,393	51	421
Yuma	3,592	4,359	1,993	24	158
Totals	**20,783**	**81,758**	**12,941**	**226**	**636**

1.4.3 ConCEPT On-Road Mobile Source Emissions for the DMA

CONCEPT is an emissions model that performs the three key features of emissions processing: temporal allocation of the emissions (to hourly), spatial allocation of the hourly emissions to the grid cells in the modeling domain, and emissions speciation to develop emissions for species used by the air quality model. CONCEPT MV runs MOBILE6 to generate on-road mobile emissions in a very detailed manner. The basic steps in the calculation of on-road emissions using CONCEPT MV are as follows (additional details in Table 1-5):

- <u>Activity Data Preparation</u>. CONCEPT estimates and grids link-level emissions using the output from Transportation Demand Models (TDMs). The TDM Transformation Tool, or T3, to processes the traffic demand model vehicle types, road networks, and vehicle activity to the file formats required by CONCEPT.
- <u>Temporal Allocation</u>. Transportation demand model (TDM) data are typically provided for multi-hour periods. CONCEPT uses the total VMT hourly, daily, and monthly temporal profiles to split the multi-hour volumes to hourly volumes per link.
- <u>Speed Adjustment</u>. CONCEPT calculates hourly volume/capacity ratios and applies adjustments to the free-flow speeds to account for congestion.
- <u>Spatial Allocation</u>. The vehicle activity data for each link for each hour are spatially allocated to grid cells using an overlay of the link network on the model grid.
- <u>VMT Mix Profiles</u>. VMT data are split into eight vehicle classes using the vehicle mix temporal profiles that vary by hour of day, day of week, and month of year.
- <u>Execute MOBILE6</u>. MOBILE6 is executed by CONCEPT-MV for each link in each grid cell using the link-specific speed and grid-specific temperature and humidity from the MM5 modeling data files, and county-specific MOBILE6 model inputs.
- <u>Calculate link-level emissions</u>. Emissions for each vehicle class, emission type, and pollutant for each link in each grid cell are estimated as the product of the emission factor and the VMT for each vehicle class.
- <u>Speciate the Emissions</u>. CONCEPT MV applies the appropriate speciation profiles by pollutant and emission mode to generate the speciated emissions and create model-ready files for CMAQ or AERMOD.

Table 1-5. Summary of CONCEPT parameters and data inputs.

Emissions Component	Configuration	Details
Activity data preparation	T3 used to format TDM data	TransCAD output from DRCOG
Temporal allocation	Total volume and vehicle mix profiles generated from automated traffic counter data in the DMA	The traffic counter data was provided by the Department of Transportation. A discussion of the traffic counter data analysis is provided in Appendix A.
Speed adjustment	BPR volume-delay applied by road type	Curve coefficients provided by DRCOG
Spatial allocation	Links gridded to the 4km nest by CONCEPT	
VMT mix profiles	Vehicle mix profiles generated from automated traffic counter data in the DMA	The traffic counter data was provided by the Department of Transportation
Execute MOBILE6	MOBILE6 inputs provided by CDPHE	CONCEPT uses a customized version of M6 (developed by Air Improvement Resource [AIR] under contract to LADCO) that summarizes the database output across model years within vehicle classes, and into the eight MOBILE5 vehicle classes employed in CONCEPT
Speciate emissions	The CB05 speciation profiles were developed for EPA	
QA	Output reports from both T3 and CONCEPT. Comparison with county totals generated by Alpine Geophysic's application of the SMOKE model	T3 summaries of VMT by county and time period provided to CONCEPT. CONCEPT reports of emissions (in tons) by county, emissions by vehicle type and emissions mode, summaries of M6 runs, total emissions in tons, hourly VMT, and summaries of adjusted and unadjusted speeds.

The transportation demand model (TDM) data used in the CONCEPT modeling were provided by the Denver Regional Council of Governments (DRCOG) from their Integrated Regional Model. The activity data included:

- Link Characteristics: Start and end node coordinates, link length, free-flow speeds, roadway type, hourly capacity, and county.
- Link Volumes: Period-level directional total weekday average volumes for the following ten time periods: 630 – 700, 700 – 800, 800 – 900, 900 – 1130, 1130 – 1500, 1500 – 1700, 1700 – 1800, 1800 – 1900, 1900 – 1900 – 2300, 2300 – 630. The period-level volume was pre-processed to whole hours, and then CONCEPT further disaggregated the volumes to hourly values using the temporal profile inputs.
- Speed Adjustment: Bureau of Public Roads (BPR) speed adjustment curve coefficients

A plot of the 2005 transportation network is presented in Figure 1-7.

ALPINE GEOPHYSICS

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ENVIRON

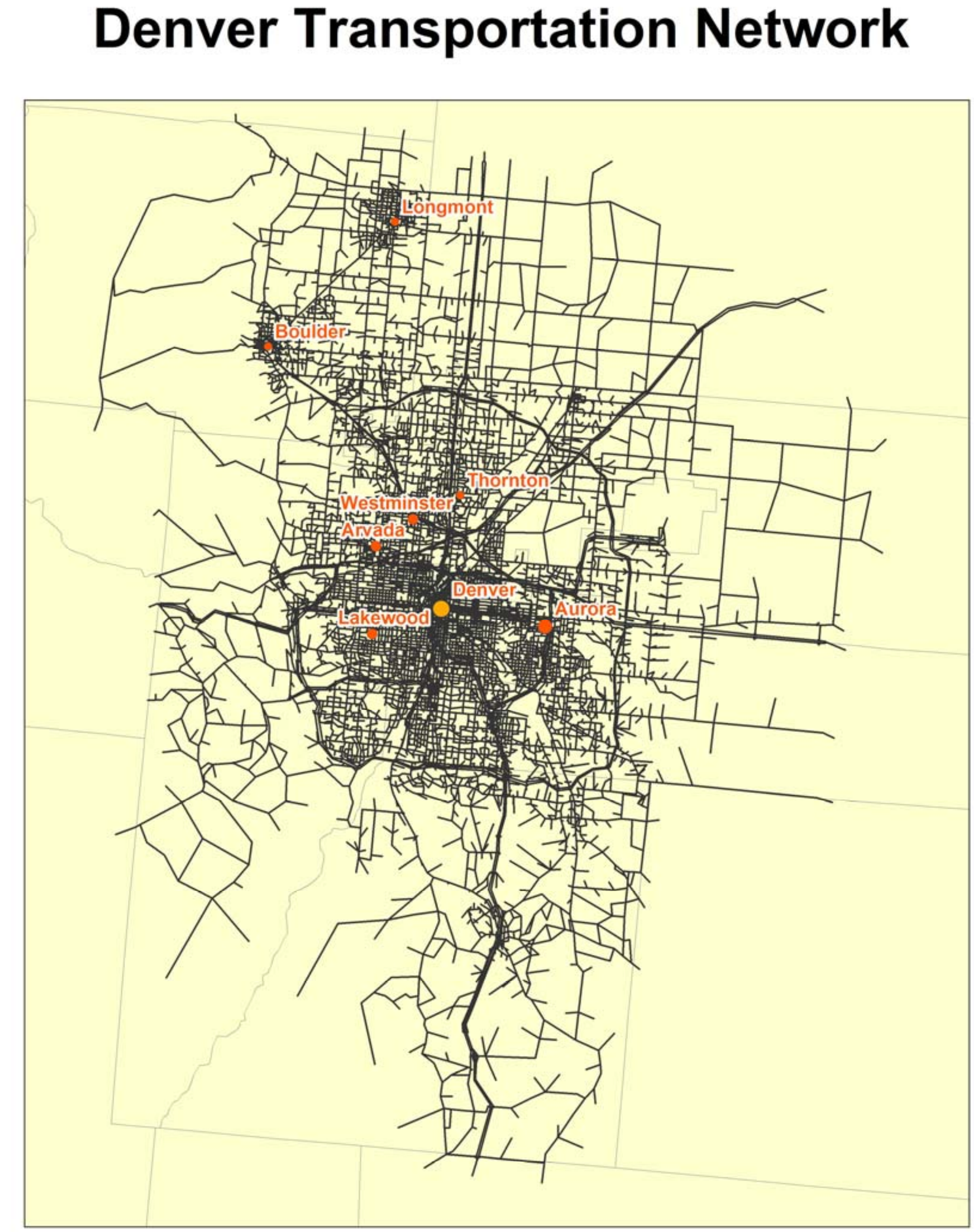


Figure 1-7. DRCOG link-based transportation network used in the CONCEPT on-road mobile source emissions modeling.

Area Type

The area types in the TDM output were represented by numeric codes that were translated as follows:

Code	Description	Urban/Rural
1	CBD	Urban
2	Fringe	Urban
3	Urban	Urban
4	Sub-Urban	Urban
5	Rural	Rural

Roadway Type

The TDM functional classes were provided as numeric codes that were translated to HPMS roadway types as follows:

Code	Urban/Rural	Functional Class	HPMS Type (Code)
1	Rural	freeway	Principal Arterial - Interstate (01)
2	Rural	major regional arterial	Principal Arterial - Other (02)
3	Rural	principal arterial	Principal Arterial - Other (02)
4	Rural	minor arterial	Minor Arterial (06)
5	Rural	collector	Major Collector (07)
6	Rural	ramp	Ramp (added to CONCEPT for modeling purposes) (03)
8	Rural	zone connector	Local System (09)
1	Urban	freeway	Principal Arterial - Interstate (11)
2	Urban	major regional arterial	Principal Arterial - Other Freeways or Expressways (12)
3	Urban	principal arterial	Principal Arterial - Other (14)
4	Urban	minor arterial	Minor Arterial (16)
5	Urban	collector	Collector (17)
6	Urban	ramp	Ramp (added to CONCEPT for modeling purposes) (13)
8	Urban	zone connector	Local System (19)

The VMT was calculated as the volume times the link length. Note that the VMT from the TDM centroid connectors was included as local road VMT.

Growth

DRCOG provided TDM output for 2005, 2015, and 2020. The 2005 transportation data were grown to 2006, and the 2015 data were back casted to 2010 using the county-level growth and back casting factors interpolated between the 2005 and 2015 county-level VMT.

The county total VMT from the TDM and the 2006 and 2010 interpolated totals are presented in Table 1-6.

Table 1-6. Annual county-level total average weekday VMT from the TDM.

County	2005	2006 Interpolated	2010 Interpolated	2015	2020
Adams	10,922,773	11,289,709	12,757,453	14,592,132	16,440,119
Arapahoe	10,931,247	11,253,596	12,542,993	14,154,738	15,673,382
Boulder	5,737,221	5,824,590	6,174,064	6,610,906	7,014,825
Broomfield	2,006,314	2,040,202	2,175,753	2,345,192	2,620,702
Clear Creek	36,082	38,101	46,175	56,267	70,371
Denver	14,430,681	14,731,101	15,932,782	17,434,883	18,292,519
Douglas	7,877,685	8,144,715	9,212,837	10,547,989	11,777,265
Gilpin	14,933	15,170	16,119	17,305	18,872
Jefferson	13,148,925	13,385,173	14,330,163	15,511,400	16,614,625
Weld	2,746,625	2,879,718	3,412,088	4,077,550	4,651,258
Total	**67,852,486**	**69,602,074**	**76,600,424**	**85,348,362**	**93,173,938**

Speed Adjustment

After CONCEPT disaggregated the total volumes into hourly values, the free-flow speeds were adjusted to congested speeds as appropriate using the most common volume-delay function (the Bureau of Public Roads curve, or BPR curve). The general form of this function is defined as:

$$S_a = \frac{S_{ff}}{1 + \left[A * \left(V/C \right)^B \right]}$$

where:

S_a = actual link speed (mph)

S_{ff} = reported link free flow speed (mph)

V = total link volume (vehicles OR vehicles per hour)

C = total link capacity (vehicles OR vehicles per hour)

A, B = curve calibration coefficients

The A and B coefficients employed were the revised coefficients in DRCOG's Highway Skimming and Assignment Documentation, December 2004. The roadway-specific coefficients are presented in Table 1-7.

Table 1-7. BPR speed adjustment coefficients used in estimating congested speeds.

A coefficients					
Area Type	**Freeway**	**Major Arterial**	**Principal**	**Minor Arterial**	**Collector**
CBD	0.70	0.10	0.20	0.20	0.20
Fringe	0.70	0.10	0.30	0.30	0.30
Urban	0.40	0.25	0.40	0.40	0.40
Suburban	0.40	0.25	0.40	0.40	0.40
Rural	0.40	0.40	0.40	0.40	0.40
B Coefficients					
CBD	5.50	7.50	5.00	5.00	5.00
Fringe	5.50	7.50	5.00	5.00	5.00
Urban	7.50	7.50	5.50	5.50	5.50
Suburban	7.50	7.50	5.50	5.50	5.50
Rural	5.00	5.00	5.00	5.00	5.00

The speeds of local roads were not adjusted.

Weekday/weekend Temporal Adjustment

CONCEPT disaggregates period-level VMT into hourly values by assigning the relative proportion of VMT for a given hour within a period based on the hourly temporal profiles. Because the TDM data are reflective of weekday volumes, we generated a second set of inputs to CONCEPT for the weekend day simulations where the period-level VMT were summed to create a daily total. This daily total was then fed to CONCEPT, which then disaggregated the VMT according to a true weekend temporal distribution.

Additional Temporal Adjustments

We received from the Colorado Department of Transportation 2005 and 2006 total volume and vehicle classification data in the DMA from automated traffic counters. The volume data consisted of the total number of vehicles counted on a roadway by day and hour. The vehicle mix profiles were generated using vehicle classification data provided by CDOT that counted the number of vehicles of each different class by day and hour. Data from both years was merged together in the temporal analysis; in other words, no distinction was made by year.

All the observation sites in the total volume and vehicle classification data were assigned to a Federal Highway Administration (FHWA) roadway function class. The cross-reference between the CDOT roadway classifications and FHWA classifications are presented in Table 1-8.

Table 1-8. FHWA Roadway functional classification.

CDOT Road Type	FHWA Classification and Code
Collector	Urban Collector (17)
Freeway	Urban Interstate (11)
Interstate	Urban Interstate (11)
Major Regional	Urban Principal Arterial - Other Freeways or Expressways (12)
Minor Arterial	Urban Minor Arterial (16)
Other Principal Arterial	Urban Principal Arterial - Other Freeways or Expressways (12)
Principal	Urban Major Arterial (14)
Principal Arterial	Urban Major Arterial (14)

The vehicle classes in the classification data are somewhat different than the vehicle classes in MOBILE5 or MOBILE6. They are presented in Table 1-9.

Table 1-9. Vehicle classifications.

FHWA Class	VTRIS Vehicle Type
1	Motorcycle
2	Passenger cars
3	Other 2-axle, 4-tire single unit vehicles
4	Buses
5	2-axle, 6-tire single-unit vehicles
6	3-axle, 6-tire single-unit vehicles
7	4+ axle single-unit vehicles
8	4 or less axle combination vehicles
9	5-axle combination vehicles
10	6+ axle combination vehicles
11	5-axle multi-trailer vehicles
12	6-axle multi-trailer vehicles
13	7+ axle multi-trailer vehicles
14	Unclassified
15	Unclassifiable

The estimated fraction of each FHWA vehicle class assigned to the MOBILE5 vehicle classes is shown in Table 1-10.

Table 1-10. Fractional Allocation of FHWA Vehicle Classes to MOBILE5 Vehicle Classes.

FHWA Class	LDGV	LDGT1	LDGT2	HDGV	LDDV	LDDT	HDDV	MC
1	0	0	0	0	0	0	0	1
2	0.52225	0.35340	0.11183	0.00748	0.00085	0.00180	0.00238	0
3	0.51365	0.34758	0.11956	0.00689	0.00084	0.00190	0.00957	0
4	0	0	0	0.16928	0	0	0.83072	0
5	0	0.24070	0.19405	0.12262	0	0.00287	0.43976	0
6	0	0.24070	0.19405	0.12262	0	0.00287	0.43976	0
7	0	0.24070	0.19405	0.12262	0	0.00287	0.43976	0
8	0	0.00031	0.00701	0.02044	0	0.00010	0.97214	0
9	0	0.00031	0.00701	0.02044	0	0.00010	0.97214	0
10	0	0.00031	0.00701	0.02044	0	0.00010	0.97214	0
11	0	0.00031	0.00701	0.02044	0	0.00010	0.97214	0
12	0	0.00031	0.00701	0.02044	0	0.00010	0.97214	0
13	0	0.00031	0.00701	0.02044	0	0.00010	0.97214	0

The CDOT data was read into a Microsoft SQL Server database. The total volume and vehicle classification data was processed in the following steps:

1) All counts across lanes in the same roadway direction were totaled. Different directions at site were treated separately.
2) All counts (either total volume or count for each vehicle class) were averaged for each site-direction pair by hour, day of week (i.e., Sunday through Saturday), month, and roadway classification. This means that at most five values were averaged together, corresponding to the total number of days in a week during one month. In other words, all Monday counts during January for hour 10 were averaged together at each site-direction pair. This averaging by site first was done so that sites that may not have had as long a period of observation would be weighted equally in the average across the sites.
3) The counts were averaged across the sites. These averages were calculated by roadway function class, vehicle class, month, day of week, and hour of the day.
4) Any holes in the data (where either data was missing or the data was not representative) were filled in.
5) The FHWA vehicle classes were mapped into MOBILE5 vehicle classes.

To calculate the temporal profiles, the total volume by roadway class was tallied for the year, month, and day of week. The monthly profile fractions were calculated by dividing the monthly totals by the yearly total. The day of week profiles were calculated by dividing the day of week totals by the monthly total for each month. Finally the hourly totals were calculated by dividing the hourly counts by the day of week totals (summed over all 24 hours) for each day of week and month. Each row in the temporal profiles sum to 1.

The vehicle mix profiles were calculated as the fractions contributed by each vehicle class to the total hourly volume. So for each roadway function class, month, day of week, and hour, the hourly vehicle mix profiles were calculated by dividing each vehicle class count by the total volume for that hour.

Before proceeding with the analysis, the following data was dropped to ensure the integrity of the profiles:

- Dropped 65 duplicate 2005 vehicle classification records corresponding to 10/29/2005 at sites 3, 103, 108, 124, 215, 245, 247, 256, 504, 507, 512, 609, 103608, 103694, 103712, and 11/13/2005 at site 107.
- Removed duplicated “05” records from the total volume data, where identical volume counts were recorded with the year “2005.”
- Replaced corrupted 2006 classification table stations 10, 12 & 103387 with corrected data, and dropped 144 records of other corrupted records in this dataset.
- Dropped the vehicle classification sites 7, 215 & 247 corresponding to FHWA facility class 16 (Minor Arterial) because according to CDOT, they were not representative of the Denver Area.
- Dropped all vehicle classification records for which the total hourly volume was less than 3.
- Dropped all records for which more than 25% of the hours in a day had zero volume.
- Dropped all records for which there were not 24 hours of observations in a day.
- Dropped sites for which there was not a complete week in a given month.

- For the total volume monthly profiles, dropped all sites for which there were not 12 months worth of data after incomplete weeks were dropped.

There was enough data to create profiles for the following facility classes:
01 – Rural Interstates
02 – Rural Principal Arterials – Other
06 – Rural Minor Arterials
11 – Urban Interstates
12 – Urban Principal Arterials – Other Freeways or Expressways
14 – Urban Principal Arterials – Other

We did not have enough data from the remaining classes:
07 (Rural Major Collector), 08 (Rural Minor Collector), 09 (Rural Local), 16 (Urban Minor Arterial), 17 (Urban Collector), or 19 (Urban Local). For the total volume profiles, we used the profiles generated for class 06 and applied them to classes 07, 08, and 09. We applied the total volume profiles from class 14 to classes 16, 17, and 19.

Figures 1-8 through 1-10 display the monthly, July day of week, and July urban interstate hourly total volume temporal profiles. Figures 1-11 and 1-12 display the vehicle mix hourly profiles for rural and urban interstates for a week in July.

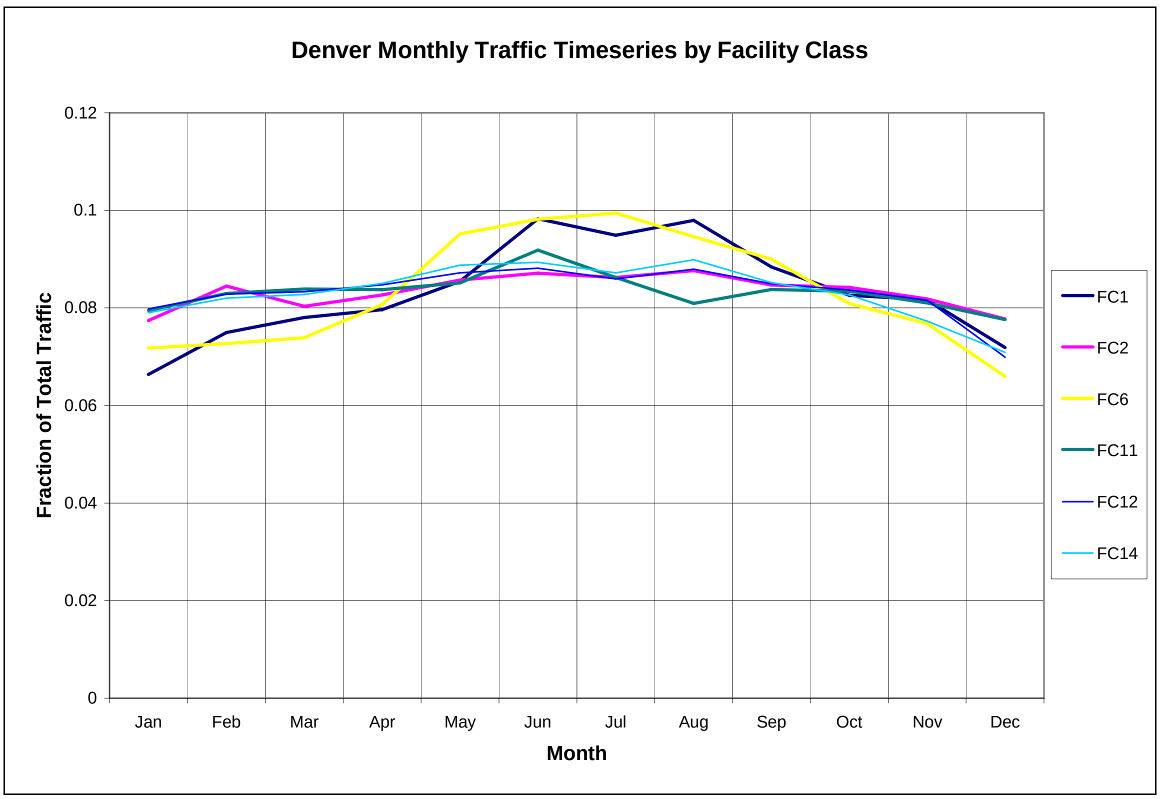


Figure 1-8. Monthly temporal profiles for facility classes 1 through 14.

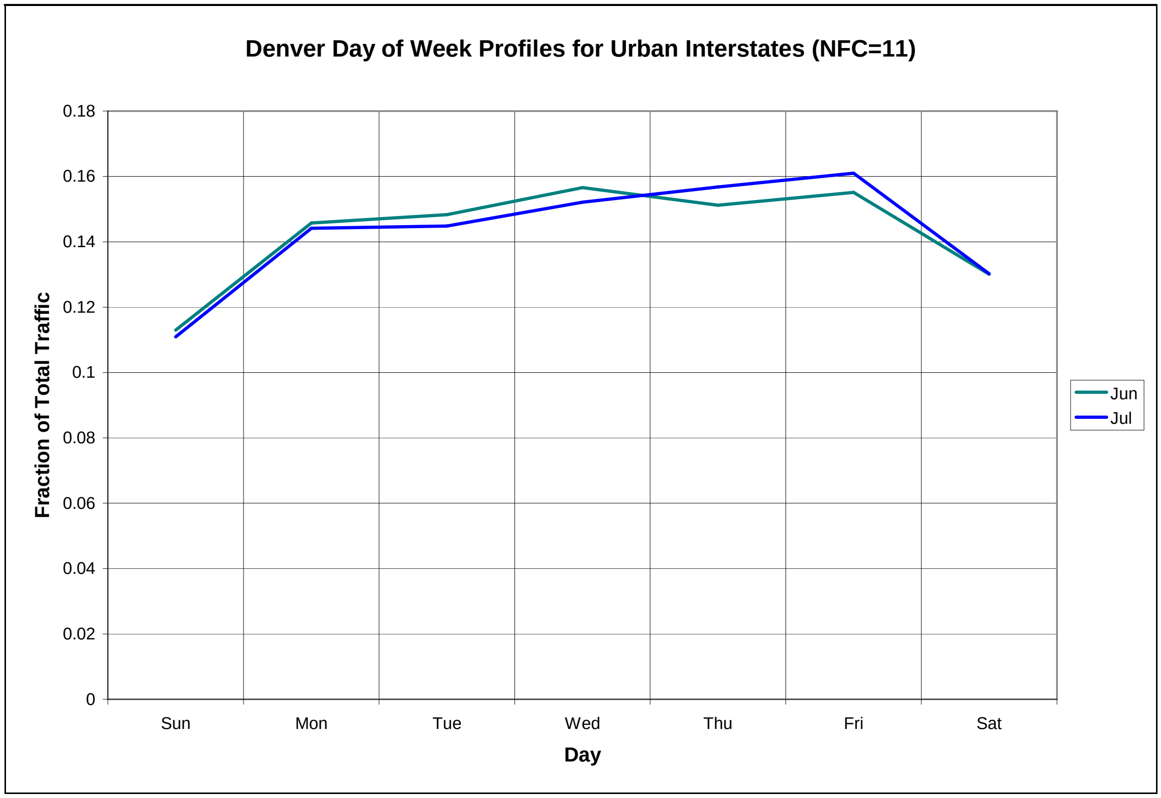


Figure 1-9. Day of week temporal profiles for June and July.

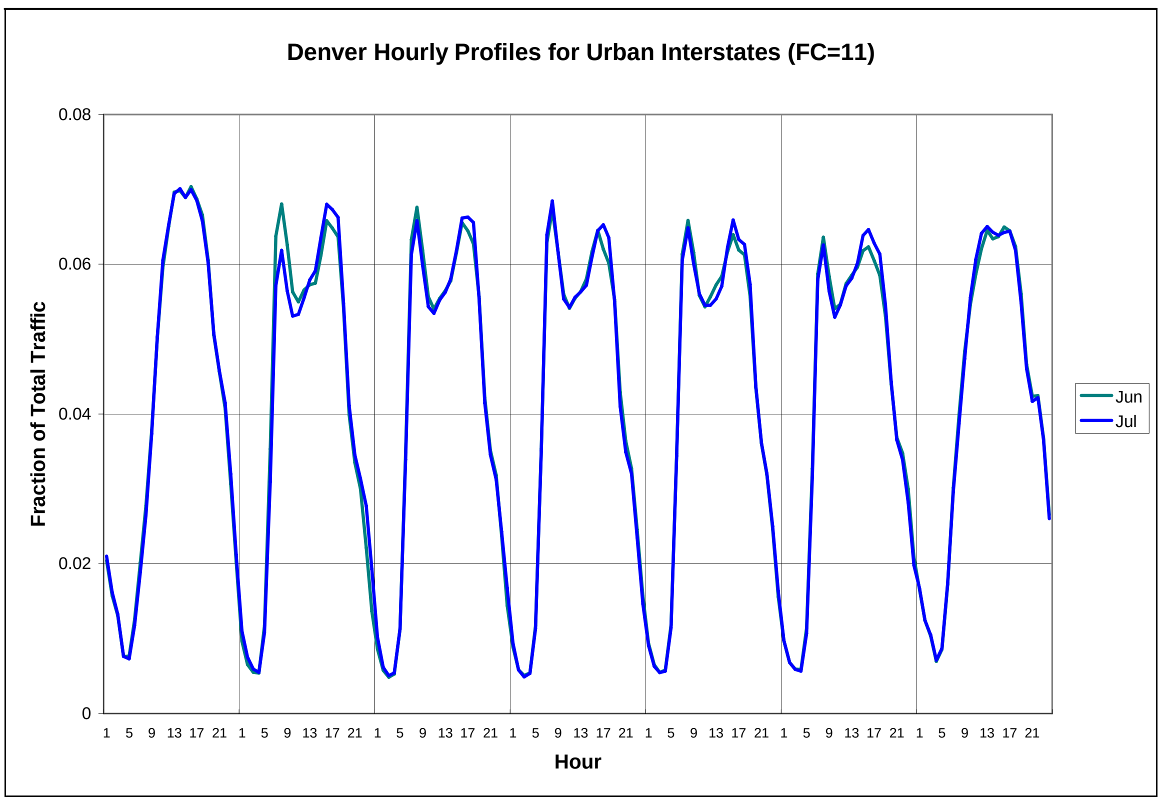


Figure 1-10. Hourly temporal profiles for urban interstates for a week in June and July.

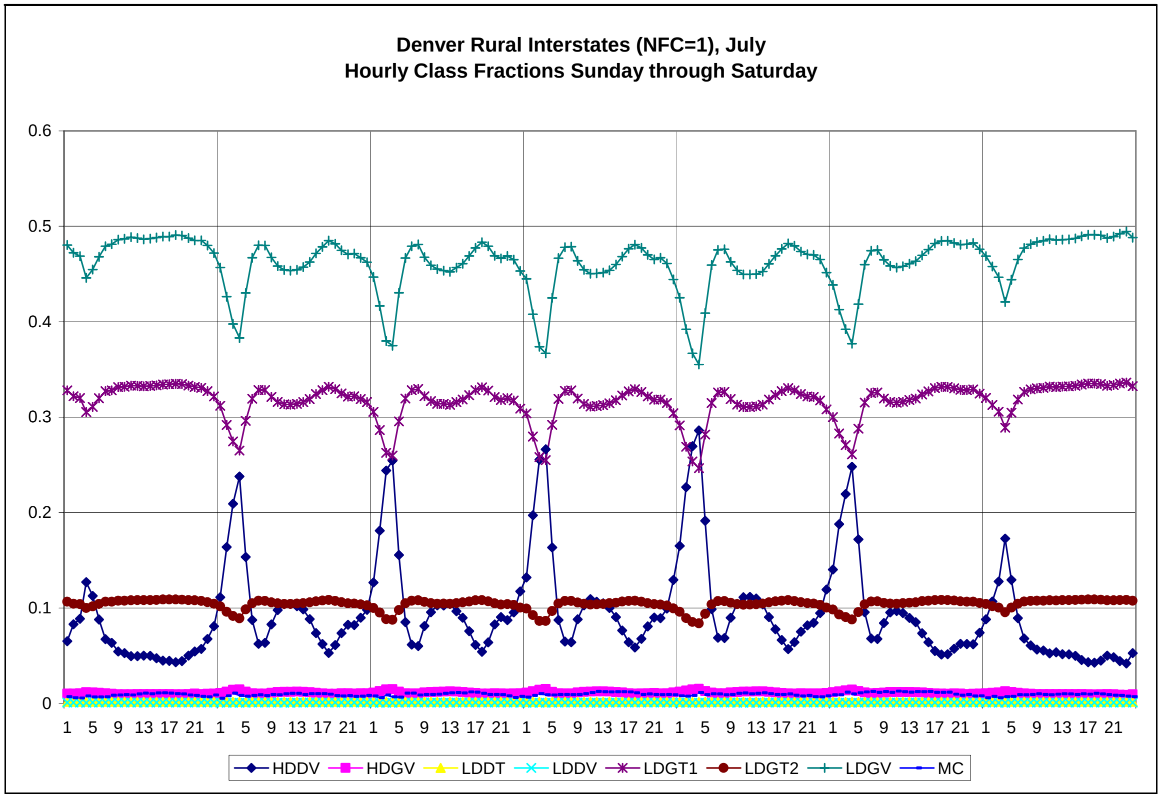


Figure 1-11. Vehicle mix hourly profile for rural interstates in July.

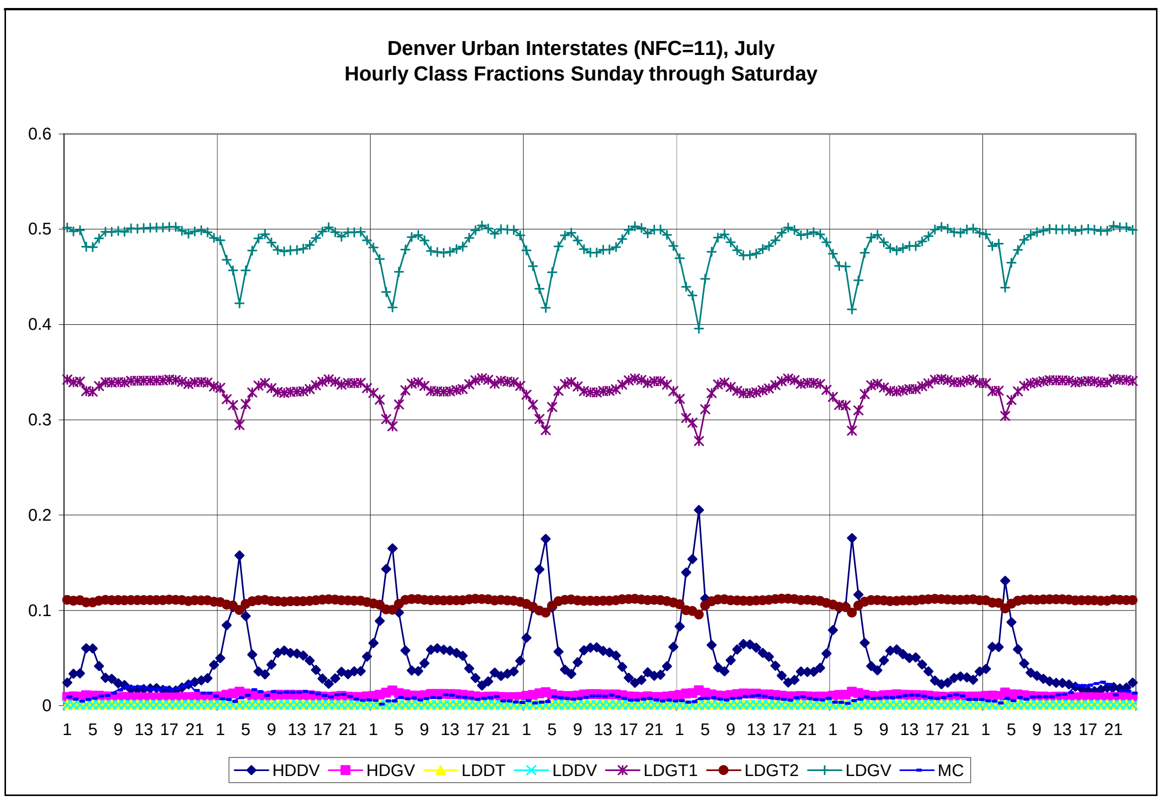


Figure 1-12. Vehicle mix hourly profile for urban interstates in July.

Combining ConCEPT DMA and SMOKE Colorado On-Road Mobile Emissions

The SMOKE-MOBILE6 and CONCEPT on-road mobile source emissions modeling both produced on-road mobile source emissions for the area covered by the DRCOG link-based VMT network. To avoid double counting on-road mobile source emissions in the DMA, a mask was developed that identified all 4 km grid cells that were covered by the DRCOG link-based network. The SMOKE-MOBILE6 on-road mobile source emissions in the area covered by the DMA mask were then eliminated so that they were replaced by the CONCEPT derived on-road mobile source emissions when the SMOKE-MOBILE6 and CONCEPT files were merged together.

2.0 OZONE OPERATIONAL MODEL PERFORMACE EVALUATION

2.1 INTRODUCTION

This Chapter describes the operational model performance evaluation for ozone and the final CAMx 2006 base case simulation (Run 17) of the June-July 2006 modeling period using the final model configuration. That is, the ozone operational model initial evaluation focuses on how well the model reproduces the observed surface ozone concentrations during the June-July 2006 modeling period. In Chapter 3 we present a diagnostic model performance evaluation that focuses on the model performance for ozone precursors (VOC, NOx and CO), ozone aloft and particulate matter (PM) species.

2.1.1 Purpose of the Model Performance Evaluation

The purpose of the model performance evaluation is to establish a reliable CAMx 8-hour ozone modeling database for the DMA that can be used for projecting future year 8-hour ozone concentrations. In general terms, this process consists of the following cycle:

- Exercise the modeling system for a series of base case simulations attempting to replicate the time and space behavior of the observed 1-hour and 8-hour ozone concentration fields as well as concentrations of precursor and product species;
- Identify sources of error and/or compensating biases, through evaluation of preprocessor models (MM5, SMOKE, CONCEPT, GloBEIS, MEGAN), air quality model inputs, concentrations aloft, mass budgets and conservation, process analysis, etc;
- Through a documented process of diagnostic and sensitivity investigation, pinpoint and correct the performance problems via model refinement, additional data collection and/or analysis, or theoretical considerations;
- Re-run the model for the refined base case and re-evaluate performance until adequate, justifiable performance is achieved or the modeling period is declared unsuited for further use based on documented performance problems.

In practice this process is limited by time and resource constraints. The preliminary model performance evaluation and diagnostic sensitivity tests performed most of the elements listed above (Morris et al., 2008b), whereas this document focuses on the last item; the documentation of the model performance of the final 2006 base case simulation and justification for its use in the 8-hour ozone attainment demonstration modeling.

2.1.2 Approach for the Operational Ozone Model Evaluation

The CAMx performance evaluations follows the procedures recommended in the EPA photochemical modeling guidance documents (EPA, 1991; 1999; 2005a; 2007). The evaluation was carried out in two sequential phases, beginning with the simplest comparisons of modeled and observed ground-level ozone concentrations presented in this Chapter follows by potentially more illuminating analyses presented in Chapter 3 (e.g., examination of available precursor and product species, comparisons of pollutant ratios and groupings, comparison against PM species, deposition and visibility). The CAMx evaluation will use most of the following six means for assessing photochemical model performance as specified in EPA's guidance are as follows:

- Use of computer generated graphics;
- Use of ozone metrics in statistical comparisons;
- Comparison of predicted and observed precursor emissions or species concentrations;
- Comparison of observed and predicted ratios of indicator species;
- Comparison of predicted source category contribution factors with estimates obtained using observational models as available; and
- Use of retrospective analyses in which air quality differences predicted by the model are compared with observed trends.

The Denver model performance evaluation focuses mainly on the first three of these elements for evaluating model performance, with some presentation of the fourth element that compares some predicted and observed indicator ratios presented in Chapter 3. The Denver ozone modeling did not perform any ozone source apportionment modeling for the 2006 base case, although such modeling was performed for the 2010 base case emissions scenario that is reported with the 2010 modeling. In addition, we did not perform any retrospective modeling to compare the modeling system's response to past changes in emissions. Although in hindsight, the Denver 8-hour ozone EAC SIP modeling of the June-July 2002 episode using essentially the same MM5/CAMx modeling system did perform some prospective modeling where the modeled changes in ozone between 2002 and 2007 compared favorable with the observed changes. The maximum 2007 projected 8-hour ozone Design Value predicted by the CAMx model using the 2002 EAC modeling database was 85 ppb at the Rocky Flats North monitor, which agreed exactly with the observed 2005-2007 8-hour ozone Design Value at that site.

2.1.2.1 Available Aerometric Data for the Evaluations

The model performance evaluation is limited by the availability of monitoring data in the region. Table 2-1 and Figure 2-1 display the ozone monitoring network in the DMA and vicinity. Also shown in Table 2-1 are the years of operation of the Denver ozone monitoring sites. Note that the Chatfield (CHAT) site was moved in 2004. The 2010 8-hour ozone Design Value projections will be based on current year Design Values from the 2005-2007 period, so only sites with ozone observations from those years will have monitor-specific Design Value projections. Although a two-year Design Value (2006-2007) was used for the Fort Collins West monitor that started in 2006.

Table 2-1. Ozone monitors operating within and near the DMA during 2002-2007.

ID Number	Site Name	Site ID	2002	2003	2004	2005	2006	2007	Lat	Long
080013001	Welby	WELB	x	x	x	x	x	x	39.838	-104.950
080050002	Highland	HIGH	x	x	x	x	x	x	39.568	-104.957
080130011	S. Boulder Creek	SBC	x	x	x	x	x	x	39.957	-105.238
080310002	CAMP	CAMP				x	x	x	39.751	-104.988
080310014	Carriage	CARR	x	x	x	x	x	x	39.752	-105.031
080350002	Chatfield #1	CHAT	x	x	x				39.538	-105.065
080350004	Chatfield #2	CHAT			x	x	x	x	39.534	-105.070
080410013	USAF Academy	ACAD	x	x	x	x	x	x	38.958	-104.817
080410016	Manitou Springs	MANI			x	x	x	x	38.853	-104.901
080590002	Arvada	ARVA	x	x	x	x	x	x	39.800	-105.100
080590005	Welch	WELC	x	x	x	x	x	x	39.639	-105.139
080590006	RFN	RFNO	x	x	x	x	x	x	39.913	-105.189
080590011	NREL	NREL	x	x	x	x	x	x	39.744	-105.178
080590012	Lookout Mountain	LOOK			x				39.727	-105.247
080690007	RMNP	RMNP	x	x	x	x	x	x	40.277	-105.545
080690011	FtC West	FTCW					x	x	40.593	-105.141
080691004	Ft. Collins	FTCO	x	x	x	x	x	x	40.577	-105.079
081230007	Greeley	GREE	x						40.416	-104.692
081230009	Weld Co. Tower	WCTO	x	x	x	x	x	x	40.386	-104.737

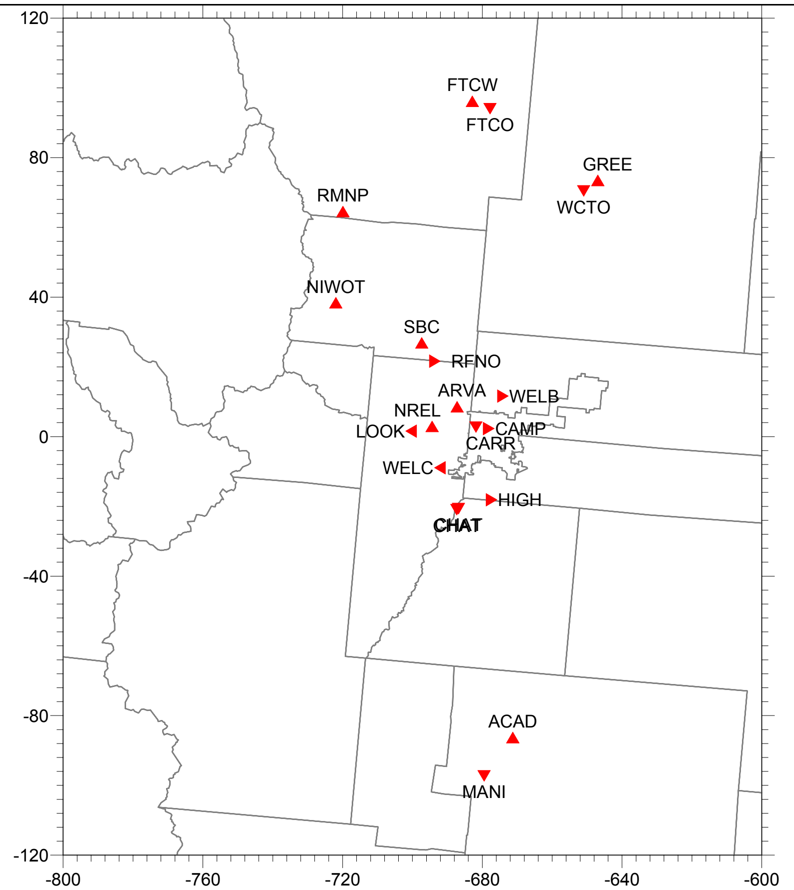


Figure 2-1. Location of ozone monitoring sites within and near the Denver Metropolitan Area (DMA) (triangle symbols point to monitor identifier).

During 2006, two of the routine monitoring sites (CAMP and WELB) also collected NO2 measurements in the DMA and 13 monitors collected CO as well.

We are aware of three "field study" campaigns in the general Denver area during 2006 that provides additional data to evaluate the modeling system:

- The CDPHE/APCD collected VOC samples during 2006 that will assist in evaluating this important ozone precursor. Most VOC samples were collected in the morning (6-9am MDT) with samples for the following sites available during some days of the June-July 2006 modeling episode:
  - CAMP
  - Welby
  - Fort Lupton
  - Platteville
  - Rocky Flats North
  - Fort Collins West
- During portions of the 2006 episode (end of July), NOAA launched daily ozonesondes at numerous sites throughout the U.S., including Boulder. The ozonesonde measurements will provide valuable information on the vertical structure of ozone concentrations, including the potential identification of an ozone reservoir aloft.
- Finally, the NPS and CDPHE collected special measurements as part of the ROMANS study during 2006.

The comparisons against these field study data are done in the Chapter 3 diagnostic evaluation section.

2.1.2.2 Model Performance Goals and Criteria

As discussed in the Denver Modeling Protocol (Morris et al., 2007) and preliminary model performance evaluation (Morris et al., 2008b), we are using several model performance goals and criteria based on EPA guidance documents and past studies to assist in gauging the 2006 base case model performance. The model performance goals and criteria are not meant to be pass/fail tests, but rather to help frame the model performance and put it into contact. EPA's 1-hour ozone modeling guidance presented three model performance goals for hourly ozone that are listed in Table 2-2.

Table 2-2. EPA's 1-hour ozone performance goals (EPA, 1991).

Performance Statistics	Performance Goal
Unpaired Peak Accuracy	<±20%
Mean Normalized Bias	<±15%
Mean Normalized Gross Error	<35%

EPA's 1999 draft 8-hour ozone modeling guidance presented a useful performance goal that compares the observed daily maximum 8-hour ozone concentrations with modeled values "near the monitor", with the goal being that most of the observed and modeled value near the monitor pairs be within ±20% of each other. This performance goal is particularly relevant because the modeled daily maximum 8-hour ozone concentrations near the monitor are the very values used in making the 8-hour ozone projections. As used in the Denver EAC SIP (Morris et al., 2003), we have developed three approaches for defining "near the monitor". For two of the approaches we define "near" as the same NX by NY array of cells centered on the monitor as used in EPA's 8-hour ozone attainment test (e.g., 7 x 7 for 4-5 km grid) and the two tests differ in only which estimated value is selected from this array of cells. For the third test, we select the estimated value at the monitor (i.e., spatially paired). The three methods for defining "near the monitor" are as follows:

Maximum: Select the maximum estimated daily maximum 8-hour ozone concentration near the ozone monitor for each day. This is the same approach used in EPA's 8-hour ozone attainment test.

Closest: Select the estimated 8-hour ozone concentrations near the monitor that matches the observed value best.

Spatially Paired: Select the estimated 8-hour ozone concentrations at the monitoring location.

Table 2-3 summarizes the performance goal for daily maximum 8-hour ozone concentrations using these three approaches for "near the monitor".

Table 2-3. 8-hour ozone model performance goal comparing observed daily maximum 8-hour ozone concentrations with predicted values "near the monitor" (EPA, 1999).

"Near The Monitor"	Threshold	Goal
Maximum modeled daily maximum 8-hour ozone concentrations within a 7 x 7 array of 4 km grid cells around monitor	<±20%	Most pairs within ±20%
Closest modeled daily maximum 8-hour ozone concentrations within a 7 x 7 array of 4 km grid cells around monitor to the observed value at the monitor.	<±20%	Most pairs within ±20%
Spatially Paired modeled daily maximum 8-hour ozone concentration at the location of the monitoring site	<±20%	Most pairs within ±20%

For PM species, several of the RPOs conducting regional haze modeling have adopted three levels of model performance goals and criteria for PM species fractional bias and gross error as listed in Table 2-4. Note that we are not suggesting that these performance goals be adopted as guidance. Rather, we are just using them to frame and put the PM model performance into context and to facilitate model performance intercomparison across episodes, species, models, sensitivity tests and studies.

Table 2-4. Model performance goals and criteria for components of fine particle mass.

Fractional Bias	Fractional Error	Comment
≤15%	≤35%	Goal for PM model performance based on ozone model performance, considered excellent performance
≤30%	≤50%	Goal for PM model performance, considered good performance
≤60%	≤75%	Criteria for PM model performance, considered average performance. Exceeding this level of performance indicates fundamental concerns with the modeling system and triggers diagnostic evaluation.

The above performance statistics are based use the Unpaired Peak Accuracy and normalized and fractional bias and gross error metrics. These statistical performance metrics are defined in Table 2-5.

Table 2-5. Definitions of statistical performance measures used in the model evaluation.

Statistical Measure	Shorthand Notation	Mathematical Expression	Notes
Accuracy of Paired Peak	A_p	$\frac{P - O_{peak}}{O_{peak}}$	Predicted value P is located at same monitor as observed peak
Unpaired Peak Accurcay	UPA	$\frac{P - O_{peak}}{O_{peak}}$	Predicted value P taken as the unpaired maximum anywhere in the local region
Mean Fractional Error	MFE	$\frac{2}{N}\sum_{i=1}^{N}\left\lvert\frac{P_i - O_i}{P_i + O_i}\right\rvert$	Reported as %
Mean Absolute Gross Error	MAGE	$\frac{1}{N}\sum_{i=1}^{N}\lvert P_i - O_i\rvert$	
Mean Normalized Gross Error	MNGE	$\frac{1}{N}\sum_{i=1}^{N}\frac{\lvert P_i - O_i\rvert}{O_i}$	Reported as %
Mean Bias	MB	$\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)$	Reported as concentration
Mean Normalized Bias	MNB	$\frac{1}{N}\sum_{i=1}^{N}\frac{(P_i - O_i)}{O_i}$	Reported as %
Mean Fractionalized Bias (Fractional Bias)	MFB	$\frac{2}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{P_i + O_i}\right)$	Reported as %

2.2 OVERVIEW OF MODEL PERFORMANCE EVALUATION APPROACH

The model performance evaluation of the final CAMx Run 17 2006 base case simulation of the June-July 2006 Denver ozone episode makes use of graphical, statistical and diagnostic evaluation tools. We first present a series of standard ozone model performance statistics for the entire June-July 2006 episode and compare them with the performance goals. Although such comparisons are not a comprehensive evaluation, they do identify if something is greatly wrong and provide a context for comparison model performance with other studies. The general CAMx ozone model performance over the entire episode is then discussed.

We then focus on the ozone model performance for three 3-day episodes when observed exceedances of the 8-hour ozone standard occurred in the Denver NAA. The details of the ozone model performance for these 3-day episodes are presented. Figure 2-2 displays the region-wide maximum 8-hour ozone concentration in the Denver NAA for the June-July 2006 modeling period, with the three 3-day episodes selected for more detailed analysis indicated by the red dotted lines at the 85 ppb ozone NAAQS level. These three 3-day episodes include 7 of the 9 8-hour ozone exceedance days during the June-July 2006 modeling period and are as follows:

- June 17-19, 2006

- July 13-15, 2006
- July 27-29, 2006

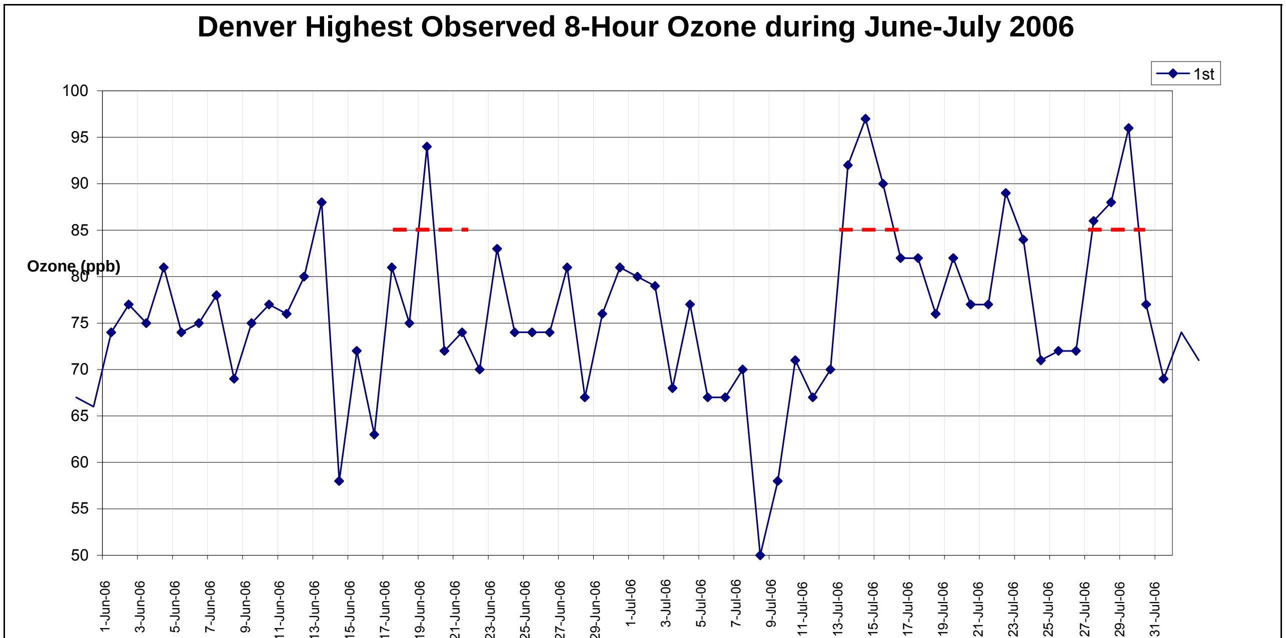


Figure 2-2. Maximum daily maximum 8-hour ozone concentration (ppb) observed during the June-July 2006 episode and three "mini episodes" selected for more detailed analysis: June17-19, July 13-15, and July 27-29.

2.3 OPERATIONAL OZONE MODEL PERFORMANCE FOR THE JUNE-JULY 2006 MODELING PERIOD

Figures 2-3 and 2-4 display the daily ozone modeling performance statistical metrics during June-July 2006 and the final CAMx Run 17 2006 base case simulation for, respectively, 1-hour and 8-hour ozone concentrations in the Denver NAA, and compares them with EPA's 1-hour ozone performance goals for Unpaired Peak Accuracy (≤±20%), Mean Normalized Bias (≤±15%) and Mean Normalized Gross Error (≤35%). EPA (1991) developed these ozone statistical performance goals for 1-hour ozone, but we have also applied them for 8-hour ozone performance for testing purposes as well. The ozone statistical performance measures are calculated using all ozone predicted and observed pairs (matched by time and location) for which the observed values is greater than a threshold values; a 60 ppb and 40 ppb observed threshold value was used for the 1-hour and 8-hour ozone performance measures, respectively.

There are five panels of daily ozone model performance presented in these figures for the June-July 2006 modeling period. The top panel presents the observed region-wide daily maximum 8-hour ozone concentration and the predicted value that is spatially paired at the same site. Not surprising, the modeled predicted daily maximum 8-hour ozone concentrations at the site with the observed maximum is almost always lower. The second panel presents the Unpaired Peak Accuracy metric and compares it to the ≤±20% EPA performance goal. The third panel is the Average Peak Paired Accuracy which is essentially the Normalized Mean Bias of predicted and observed daily maximum 8-hour ozone concentrations paired at each monitoring site. The fourth and fifth panels show the normalized bias and gross error statistical performance metrics that are compared to EPA's ≤±15% and ≤35% performance goals, respectively.

2.3.1 Ozone Performance Statistics for 1-Hour Ozone

The 1-hour ozone Unpaired Peak Accuracy performance metric achieves the ≤±20% performance goal for all days of the June-July 2006 modeling period except two days (second to top time series in Figure 2-3). On June 19, 2008 the modeled region-wide maximum 8-hour ozone concentrations is -20.8% below the observed value so just barely does not meet EPA's ≤±20% performance goal. And on July 24, 2006, the 1-hour ozone Unpaired Peak Accuracy is 22.9% that slightly exceeds the ≤±20% performance goal. The modeled unpaired peak on this day occurs to the southeast of Denver (see Appendix A) where no monitors exist so the presence of this higher modeled value can not be verified by the current monitoring network in the Denver NAA. In fact, more than two thirds of the time (73% of the days) the 1-hour ozone Unpaired Peak Accuracy metric achieves a more stringent ≤±10% performance goal (that is the final CAMx 2006 base case simulation modeled peak 1-hour ozone concentrations in the Denver NAA is within 10% of the observed peak on a vast majority of the days during the June-July 2006 modeling period).

The third daily time series panel in Figure 2-3 presents the 1-hour ozone Average Accuracy of the Peak performance measure. This is the Mean Normalized Bias for daily maximum 1-hour ozone concentrations across all sites in the Denver NAA matched by location and day (but may not match by time of day). There is no performance goal for this metric, but it appears most days during the June-July 2006 modeling period are within ±20%.

The bottom two panels in Figure 2-3 displays the daily Mean Normalized Bias and Mean Normalized Gross Error performance metrics for 1-hour ozone for which EPA has performance goals of within ≤±15% and ≤35%, respectively. The Mean Normalized Gross Error always achieves the ≤35% performance goal and, in fact, is always ≤20% and frequently ≤10%. These are quite good performance metrics for Mean Normalized Gross Error.

Of the 30 days during June 2006, 26 days achieve the <±15% performance goal for 1-hour ozone Normalized Bias (i.e., 87 percent of the days in June 2006 achieve the 1-hour ozone bias performance goal). Of the four days in June that do not achieve the bias performance goal, three are due to an underprediction bias of -16.8% (June 13), -17.2% (June 17) and -16.4% (June 24) and one is due to an overprediction bias of 18.1% (June 28).

The 1-hour ozone Mean Normalized Bias metrics for June are fairly balanced with days of both underprediction and overprediction bias (Figure 2-3a). However, in July a normalized bias undeprediction occurs on most days. Even with this underprediction bias in July, of the 28 days with normalized bias metrics, 24 days (86%) had normalized bias that achieves EPA's ≤15% performance goal. Note that normalized bias values were not calculated for July 8-9, 2006 because there were no observed hourly ozone concentrations above the 60 ppb threshold and July 31st was also missing because it was not simulated for the full day because it was at the end of the episode and meteorological data for the end of the day were not available due to the conversion from GMT to MST time; besides it was a low ozone day (all observed ozone < 70 ppb) so would not provide any additional data for the Design Value projections. The normalized bias on July 10, 13, 22 and 23 did not achieve the 1-hour ozone performance goal for normalized bias with normalized bias values of, respectively, -19.7%, -18.1%, -17.95% and -19.7%. The July 10th poor performance is not a concern since this is a low observed and modeled ozone day, however July 13, 22 and 23 are observed ozone exceedance or near exceedance days so the underprediction bias is a concern.

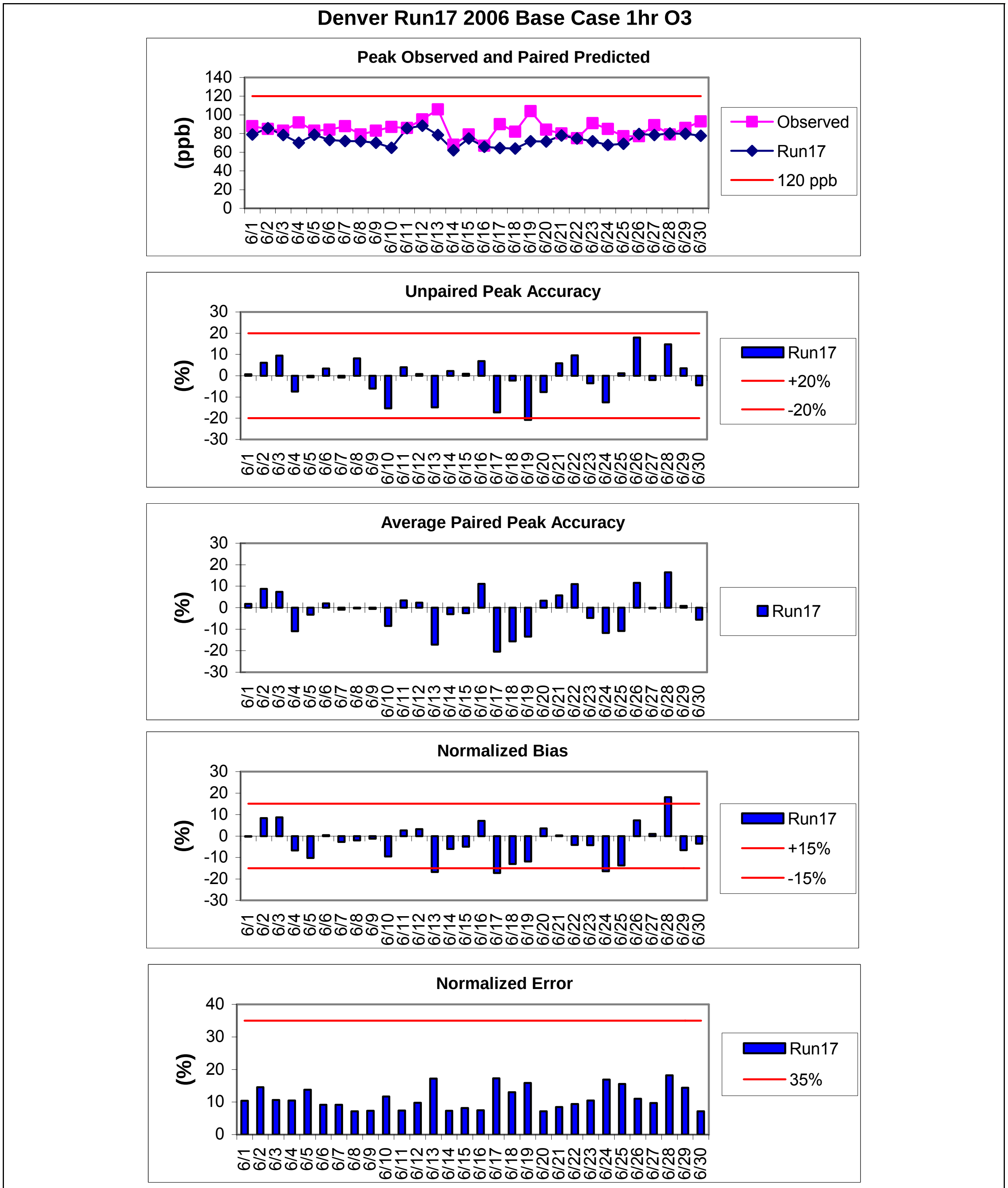


Figure 2-3a. Daily ozone model performance evaluation statistical performance measures in the Denver NAA and comparison with EPA performance goals for June 2006, the final CAMx Run17 2006 base case simulation and 1-hour ozone.

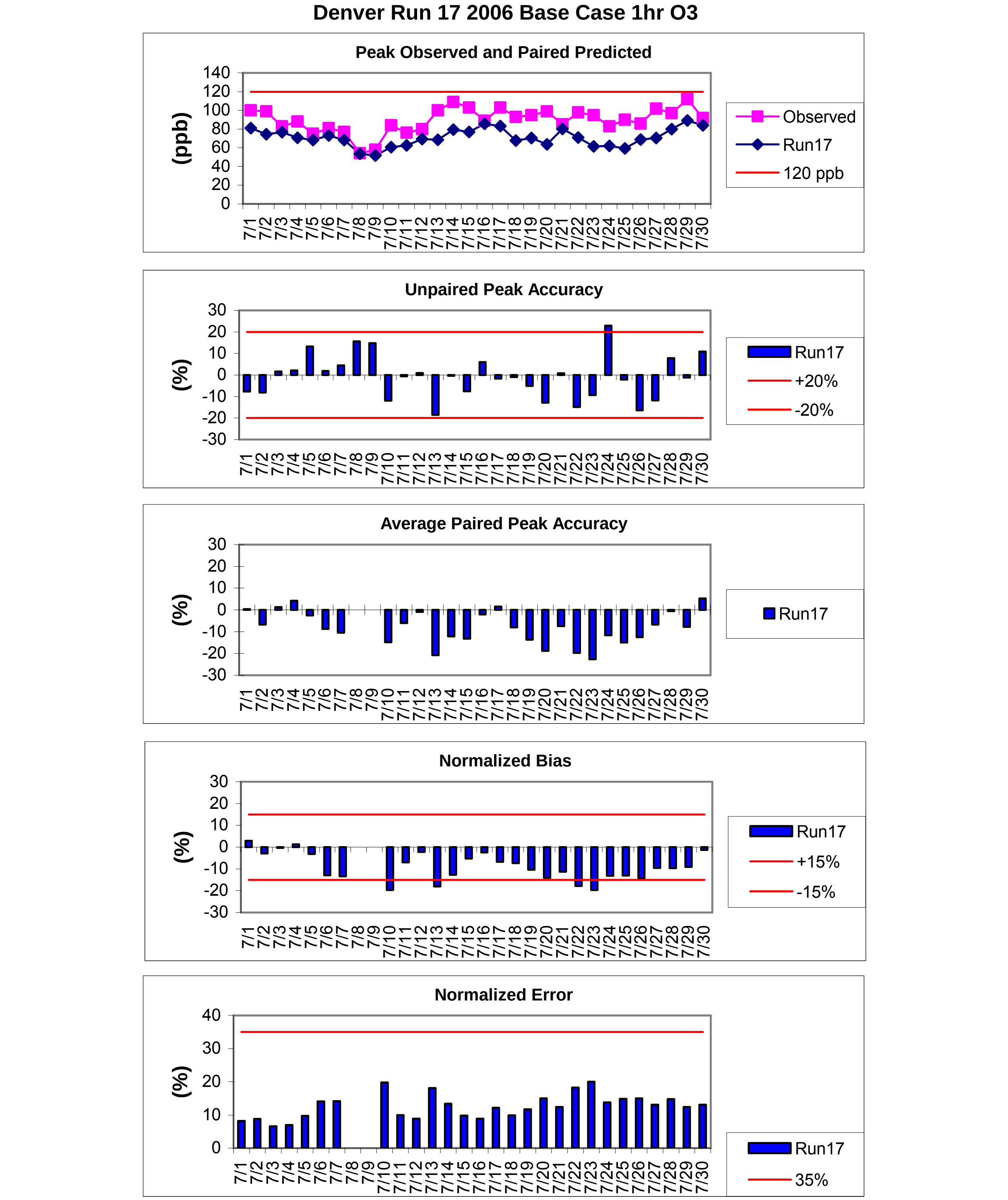


Figure 2-3b. Daily ozone model performance evaluation statistical performance measures in the Denver NAA and comparison with EPA performance goals for July 2006, the final CAMx Run17 2006 base case simulation and 1-hour ozone.

2.3.2 Daily Ozone Performance Statistics for 8-Hour Ozone Concentrations

Figure 2-4 displays the same daily statistical performance metric time series for running 8-hour ozone concentrations as shown for 1-hour ozone in Figure 2-3, only using a 40 ppb observed ozone cutoff instead of 60 ppb as used for the 1-hour ozone metrics. Also shown in Figure 2-4 are EPA's 1-hour ozone performance goals for Unpaired Peak Accuracy and Mean Normalized Bias and Gross Error that are compared to the 8-hour ozone statistics for reference. The Unpaired Peak Accuracy measure for 8-hour ozone achieves the ≤±20% performance goal on 27 of the 30 days (90% of the days) in June (Figure 2-4a). On June 19, 22 and 28 the 8-hour ozone Unpaired Peak Accuracy performance statistics were -23.8%, +20.6% and +26.1%, respectively. On June 19, 2006, the model predicts relatively low ozone (50-75 ppb) throughout the domain and completely fails to capture the observed ozone exceedances at RFNO (95 ppb), FTCW (88 ppb) and SBC (87 ppb). June 19, 2006 is a very poor performing day for the model. An examination of the maps comparing the predicted and observed spatial distribution of the 8-hour ozone concentrations on June 22, 2006 (Appendix A) reveals that there is a predicted cloud of elevated 8-hour ozone concentrations of 75-80 ppb that occurs south of Denver between the monitors in the DMA and Colorado Springs. Within the DMA, both the observed and modeled 8-hour ozone concentrations are between ~40 ppb and ~60 ppb. On June 28 the modeled 8-hour ozone peak is 86 ppb and occurs southeast of the DMA away from the ozone monitors; again within the DMA itself there is reasonable agreement between the predicted and observed daily maximum 8-hour ozone concentrations. The modeled high ozone southeast of the DMA is not supported by the observations in Colorado Springs, but its presence can not be confirmed or refuted by the current DMA ozone monitoring network. During July 2006, the CAMx Run 17 2006 base case simulations achieves EPA's ≤±20% performance goal on all 30 days of the month (Figure 2-4b).

With the exception of an overprediction bias on June 16 and 28, the Average Accuracy of the Peak performance metrics are less than ±20% for 28 days in June and less than ±20% for all 30 days in July (Figure 2-4). The 8-hour ozone Mean Normalized Bias values in June 2006 are characterized by an overprediction bias with 11 days exceeding the ≤±15% 1-hour performance goal. An examination of the time series plots of hourly ozone in Appendix C reveals that this overprediction bias is mainly due to overestimation of the nighttime low hourly ozone values.

Unlike for 1-hour ozone performance statistics, where June was performing better than July, for the 8-hour ozone performance statistics July is performing better (Figure 2-4b) than June (Figure 2-4a). All days in July the 8-hour ozone Unpaired Peak Accuracy meets the ≤±20% performance goal. With the exception of July 3 (+16.3%) and 12 (+16.2%) over 90% of the days in July exhibit normalized bias values for 8-hour ozone concentrations that achieve the ≤±15% 1-hour performance goal. As for June, all days achieve the gross error performance goal by a wide margin.

Denver Run 17 2006 Base Case 8hr O3

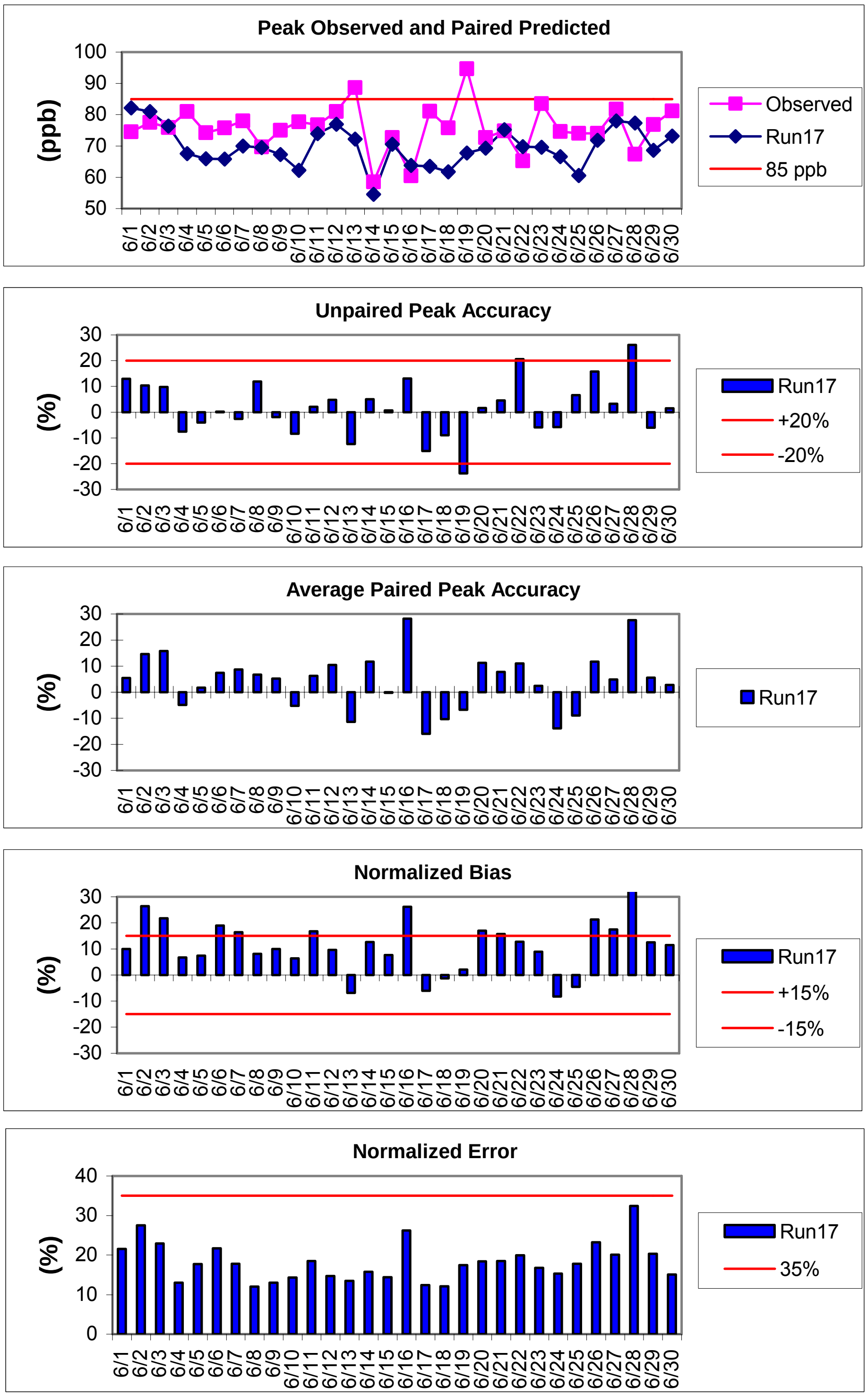


Figure 2-4a. Daily ozone model performance evaluation statistical performance measures in the Denver NAA and comparison with EPA performance goals for June 2006, the final CAMx Run17 2006 base case simulation and 8-hour ozone.

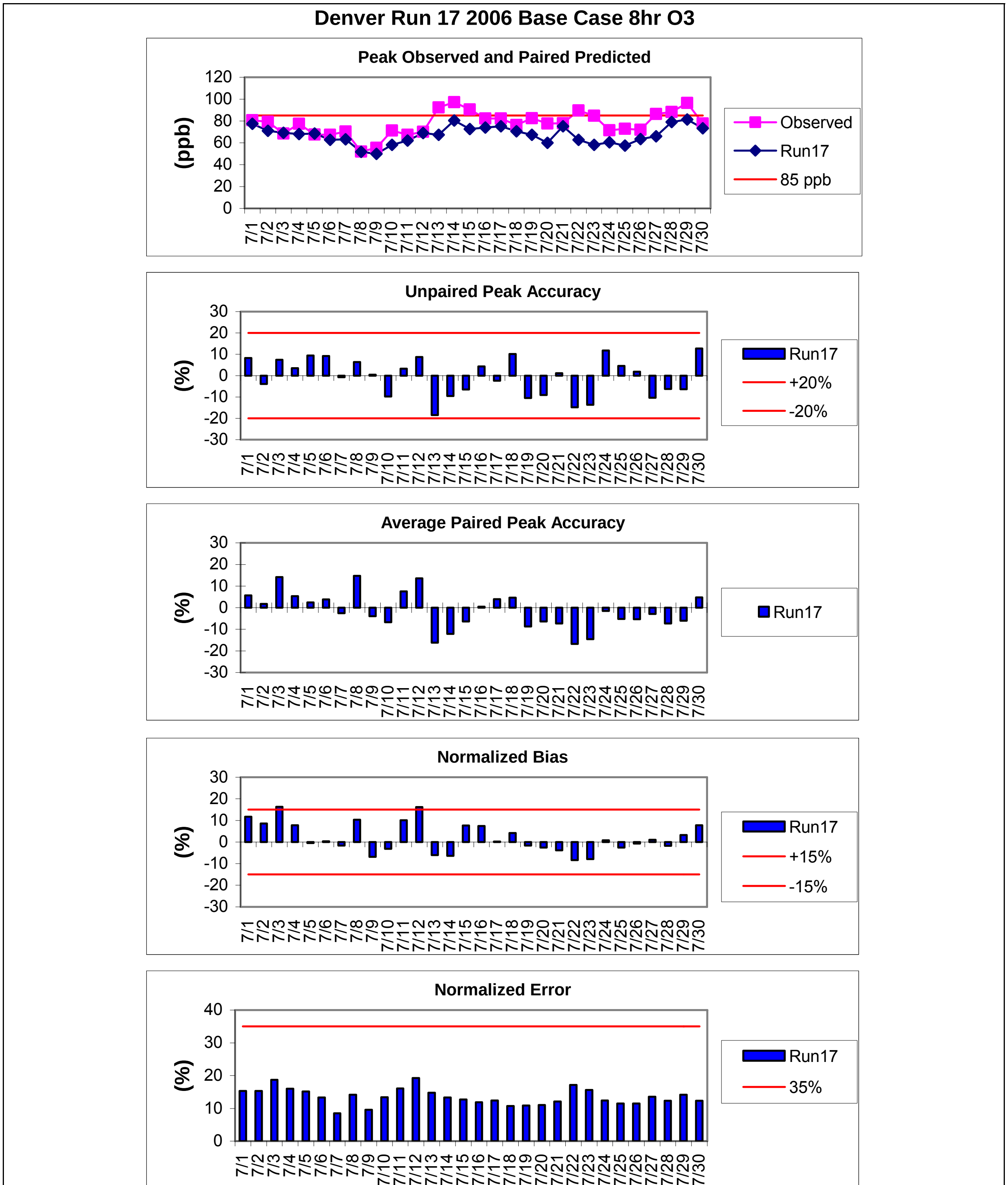
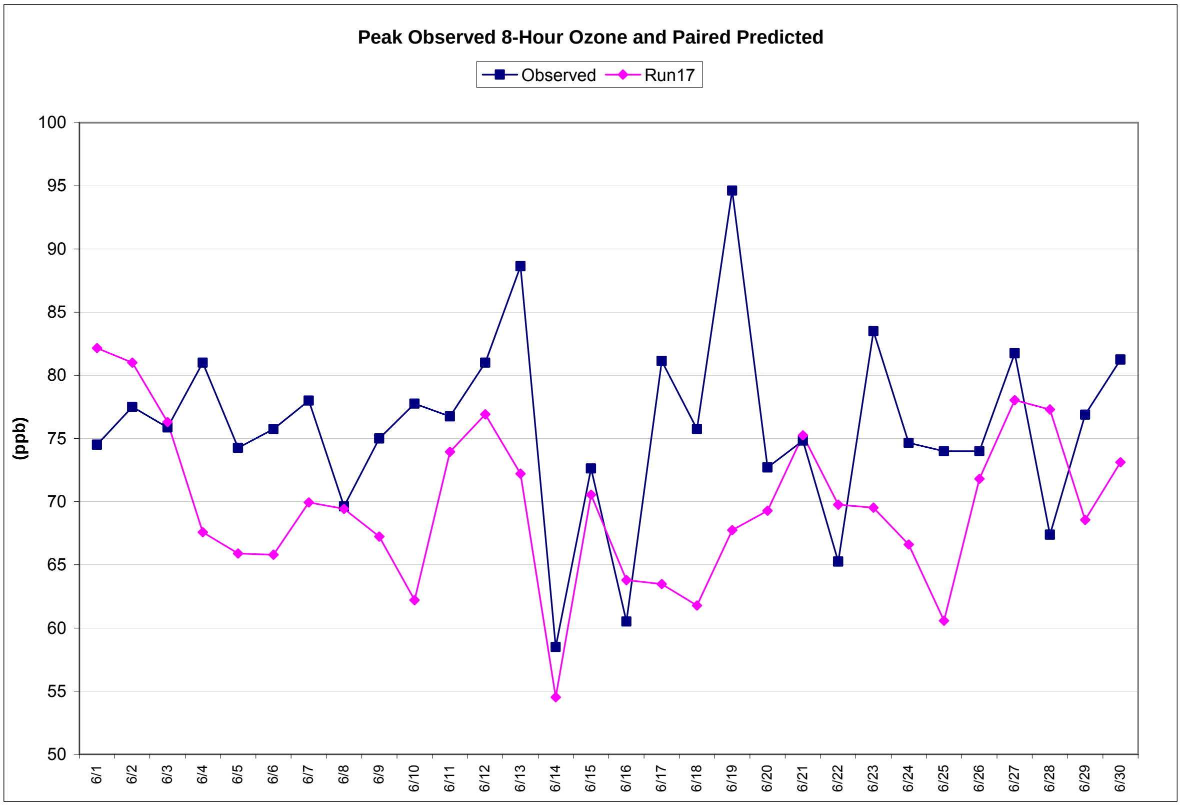


Figure 2-4b. Daily ozone model performance evaluation statistical performance measures in the Denver NAA and comparison with EPA performance goals for July 2006, the final CAMx Run17 2006 base case simulation and 8-hour ozone.

2.3.3 Daily Maximum 8-Hour Ozone Performance

The Unpaired Peak Accuracy performance metric compares the daily maximum observed ozone at any site in the Denver monitoring network with the model predicted maximum ozone anywhere within the Denver subregion (Figure 2-1). This is metric is somewhat biased because the monitoring network represents a limited spatial extent that may not record the actual daily maximum ozone concentration on that day, whereas the model has predictions throughout the region whose maximum may not occur at the locations of a monitor. In this case, a “perfect model” could exhibit an overprediction bias for this metric just because the modeled ozone peak occurs away from the monitoring sites. Thus, in this section we examine predicted and observed spatial paired daily maximum 8-hour ozone metrics, which is a particularly stringent test of model performance.

Figure 2-5 displays the highest observed daily maximum 8-hour ozone concentration at any monitoring in the Denver network along with the spatially paired predicted daily maximum 8-hour ozone concentration at the same monitor. The modeled daily maximum 8-hour ozone concentration at the site with the highest observed value tends to follow the observed day-to-day variations quite well, but it usually has an underprediction bias especially on the highest days. This is not surprising as small spatial displacement in the winds may slightly miss-locate an urban ozone plume so that it does not directly impact the ozone monitor. EPA accounts for such spatial displacements of the modeled peak from the observed peak in their attainment demonstration test by using the highest modeled 8-hour ozone near the ozone monitor, where near is defined as approximately within approximately 15 km. Thus, for making 8-hour ozone projections at a monitor EPA guidance recommends selecting the highest modeled daily maximum 8-hour ozone concentration from a 7 x 7 array of 4 km grid cells centered on the monitoring site (EPA, 2007).



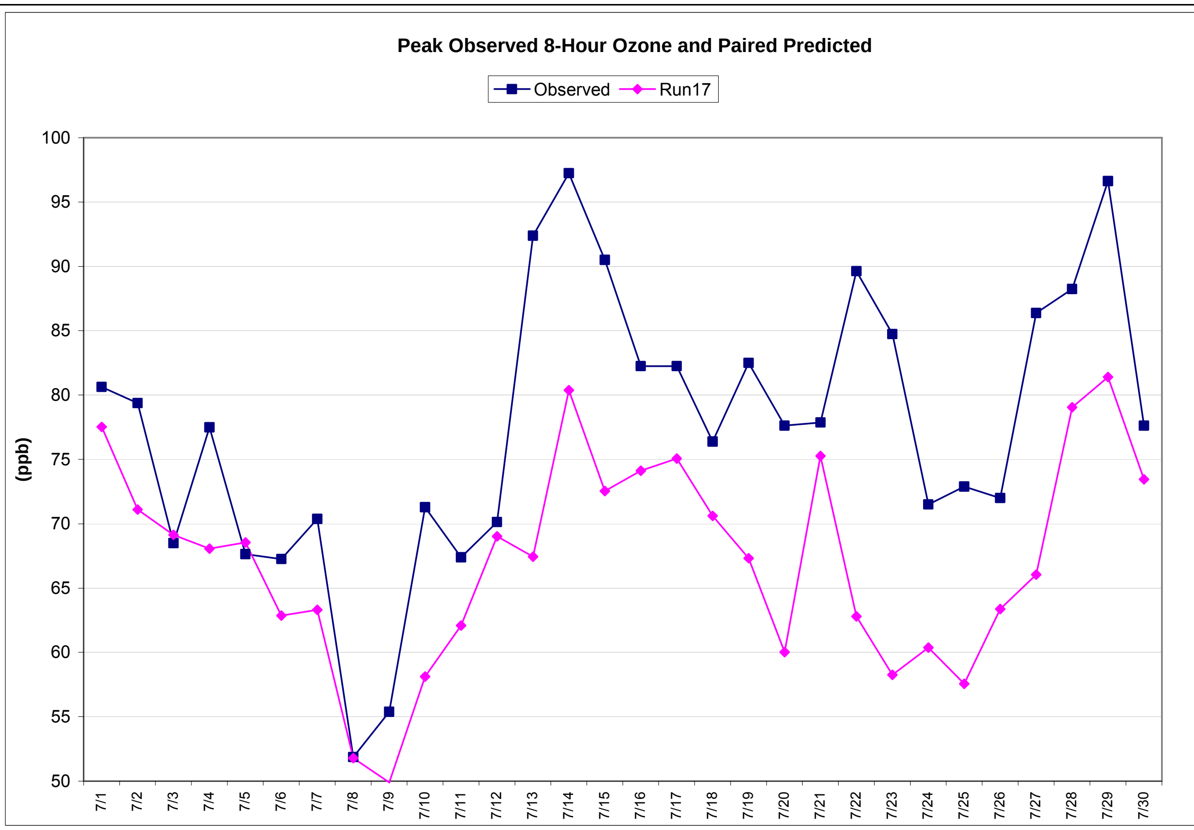


Figure 2-5. Compared of observed highest daily maximum 8-hour ozone concentration for each day during June (top) and July (bottom) 2006 with concurrent spatially paired prediction from the CAMx Run 17 2006 base case simulation.

As noted above, EPA's draft 8-hour ozone modeling guidance listed a performance goal for predicted daily maximum 8-hour ozone concentrations near a monitor of within ±20% for most of the monitor-days (EPA, 1999). By near the monitor we have presented three approaches (see Table 2-3) for selecting the modeled daily maximum 8-hour ozone concentration to pair with the observed value, the Maximum and Closest value within a 7 x 7 array of 4 km grid cells centered on the monitor and selection of the modeled value at the monitor location (Spatially Paired).

Figure 2-6 and Table 2-6 present the results of the comparisons of predicted and observed daily maximum 8-hour ozone concentrations and compares them with the ≤±20% performance goal. Using the closest modeled daily maximum 8-hour ozone concentration near the monitor to the observed value, 89% of the daily maximum 8-hour ozone concentrations prediction and observed monitor-days are within ±20% of each other. And when comparing predicted/observed daily maximum 8-hour ozone concentrations co-located at the monitor, 82% of the monitor-day pairs are within ±20% of each other. Thus, the CAMx Run 17 2006 base case simulation satisfies the performance goal from EPA's 1999 draft 8-hour ozone modeling guidance that most predicted daily maximum 8-hour ozone monitor-days be within ±20% of the observed value.

Table 2-6. Percent of the monitor-days that the model predicted daily maximum 8-hour ozone concentrations near the monitor is within ±20% of the observed value (total monitor-days = 1008).

Maximum Near the Monitor		
Percent Difference	# Days	% Days
<-20	9	1%
-20% to +20	769	76%
> +20	230	23%
Closest Near the Monitor		
Percent Difference	# days	%
<-20	23	2%
-20% to +20	902	89%
> +20	83	8%
Co-Located At the Monitor		
Percent Difference	# days	%
<-20	48	5%
-20% to +20	829	82%
> +20	131	13%

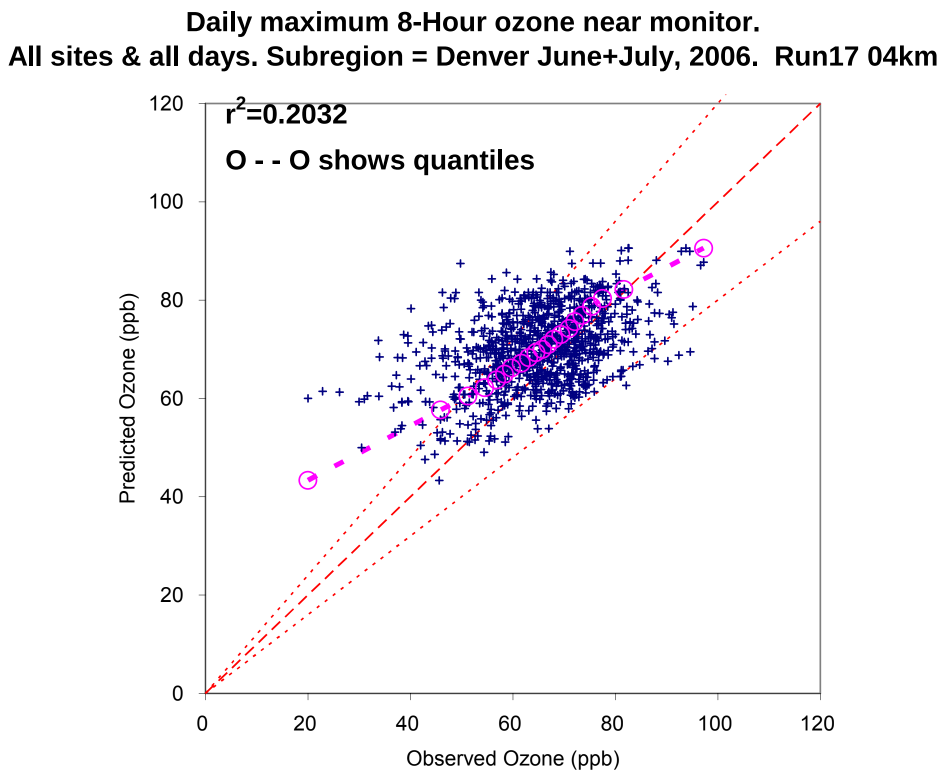


Figure 2-6a. Comparison of predicted and observed daily maximum 8-hour ozone concentrations for the June-July 2006 modeling period and the final CAMx Run 17 2006 base case simulation using the Maximum predicted value near the monitor.

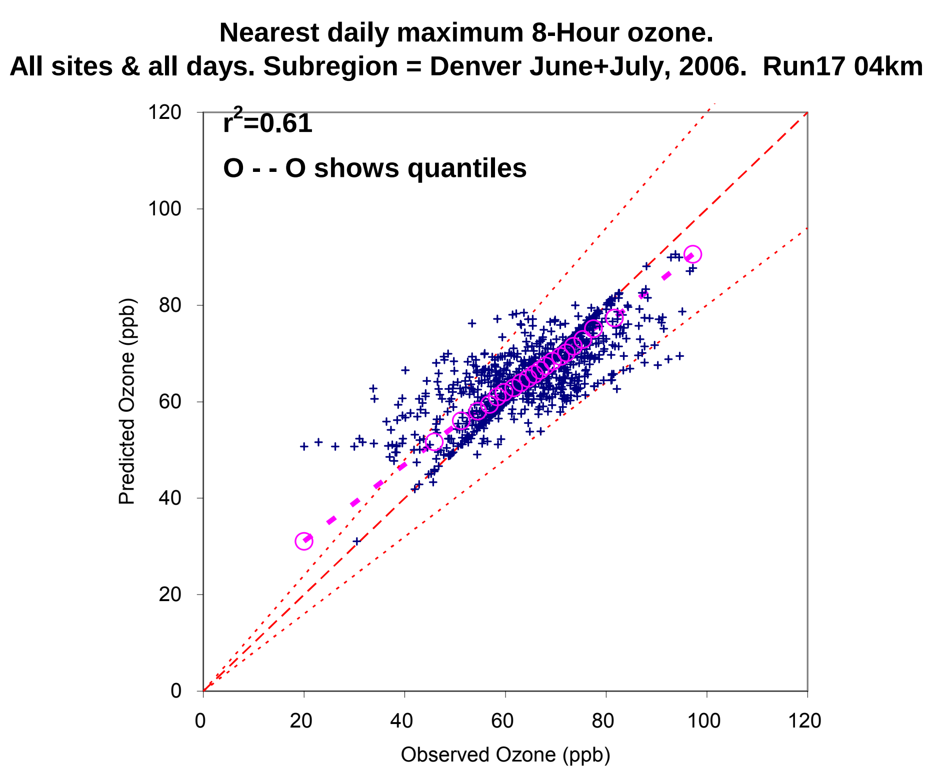


Figure 2-6b. Comparison of predicted and observed daily maximum 8-hour ozone concentrations for the June-July 2006 modeling period and the final CAMx Run 17 2006 base case simulation using the Closest predicted value near the monitor.

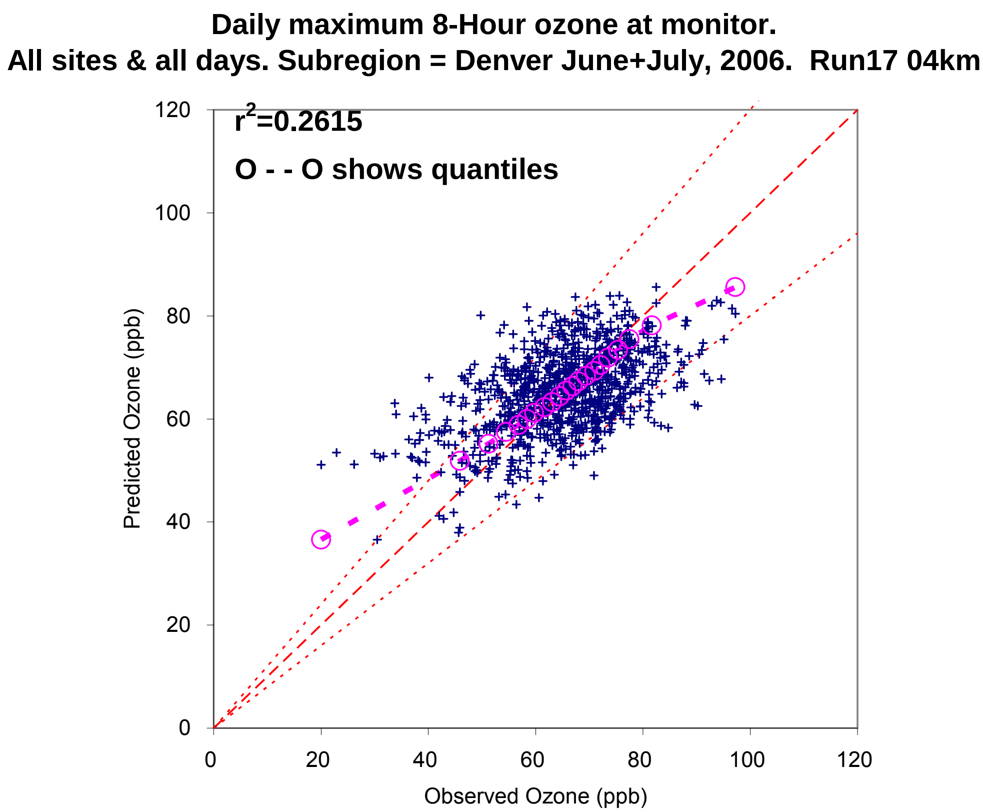


Figure 2-6c. Comparison of predicted and observed daily maximum 8-hour ozone concentrations for the June-July 2006 modeling period and the final CAMx Run 17 2006 base case simulation using the Co-Located predicted value near the monitor.

2.4 DETAILED PERFORMANCE FOR THREE 3-DAY EPISODES

In this section we perform a more detailed ozone model performance evaluation for three 3-day episode that occurred during the June-July 2006 modeling period. During these three 3-day episodes, 7 of the 9 8-hour ozone exceedance days from June-July 2006 modeling period occurred. This episodic ozone model performance evaluation makes use of performance statistics, spatial maps and time series plots that are provided for the entire June-July 2006 modeling period in Appendices B and C.

2.4.1 June 17-19, 2007

The first 3-day episode examined is the June 17-19, 2006 episode during which 8-hour ozone exceedances occurred at the RFNO (94 ppb), SOBC (87 ppb) and FTCW (87 ppb) monitoring sites on June 19. Elevated ozone also occurred at the Chatfield site (81 ppb) on June 17, and numerous monitors measured 8-hour ozone concentrations in excess of 70 ppb during this 3-day episode. Table 2-7 compares the ozone model performance statistical measures with EPA's goals (EPA, 1991) for monitoring sites in the DMA and vicinity and the three episode days. With the exception of 1-hour ozone normalized bias on June 17 (-17.2%) and unpaired peak accuracy on June 19 for 1-hour (-20.8%) and 8-hour (-23.8%) ozone, all of the ozone modeling performance statistics achieve EPA's goals. However, there is a consistent and pronounced underprediction bias in the ozone performance statistics.

Table 2-7. Final CAMx Run 17 2006 base case simulation daily 1-hour and 8-hour statistical performance measures for the June 17-19, 2006 episode and comparison with EPA performance goals.

Performance Statistic	EPA Goal	2006		
		June 17	June 18	June 19
1-Hour Ozone				
Unpaired Peak	≤±20%	-17.2	-2.2	-20.8
Normalized Bias	≤±15%	-17.2	-13.0	-11.9
Normalized Error	≤35%	17.3	13.0	15.9
8-Hour Ozone				
Unpaired Peak	≤±20%	-15.0	-8.9	-23.8
Normalized Bias	≤±15%	-6.1	-1.3	2.1
Normalized Error	≤35%	12.4	12.1	17.5

Figures 2-7 display the spatial distribution of the predicted and observed daily maximum 8-hour ozone concentrations on July 17-19, 2006 and the preliminary CAMx (Run1.1204) base case simulation. The spatial distribution of the modeled daily maximum 8-hour ozone concentrations on June 17th are extremely flat, ranging from 50 to 70 ppb (Figure 2-7a). This is compared to observed values that are also fairly flat, but about 10 ppb higher, ranging from 67 to 81 ppb. At the Chatfield and Highland monitors, where the highest observed values occur on this day (80-81 ppb), the model is predicting less than 70 ppb (60-70 ppb).

On June 18th the variations in spatial distribution of the modeled (50-70 ppb) and observed (63-76 ppb) daily maximum 8-hour ozone concentrations were both fairly flat, with the modeled values lower than observed (Figure 2-7b).

On the June 19th, the 8-hour ozone exceedance day for this 3-day episode, both the modeled and observed 8-hour ozone concentrations are higher. The model correctly simulates the observed slightly elevated daily maximum 8-hour ozone concentrations at the southern ozone monitors (74-76 ppb at CHAT and HIGH). However, the highest observed 8-hour ozone concentrations at RFNO (95 ppb) is underpredicted by the model by approximately 20 ppb, as is the ozone exceedance at FCTW (88 ppb).

Time series of predicted and observed hourly ozone concentrations for the June 17-19, 2006 period and several key monitoring sites are shown in Figure 2-8. The modeled diurnal variations of the hourly ozone concentrations at the ARVA and NREL sites northwest of Denver are much flatter than the observed values. There are nighttime ozone increases in both the modeled and observed ozone concentrations. At ARVA the model fails to capture the observed daytime peaks and nighttime lows, and at NREL the nighttime lows are captured, but the daytime peaks are underestimated. The underprediction of the daytime peaks is also apparent at the RFNO monitoring site, particular on the June 19th exceedance day. At RFNO, the modeled ozone increase begins to rise with the observed values at 9am, but flattens out at under 80 ppb at 11am as the observed values keep on rising to over 100 ppb. This may be due to too fast rise of the modeled mixing heights, a failure to capture a subsidence inversion and/or failure of the model to capture high ozone aloft.

At two sites south of Denver (CHAT and HIGH) the observed daytime peaks are underestimated on June 17-18, but reproduced quite well on June 19th. The nighttime lows are represented reasonably well at these two sites. Similar results are seen at the two Fort Collins sites north of

Denver with the modeled daytime peaks underestimated by the model. The model does identify June 19th as the worst ozone day, but ozone formation at the Fort Collins sites is too slow and peaks15-20 ppb below the observed ozone peaks.

Figure 2-9 displays the predicted and observed hourly time series plots for NOx (top), CO (middle) and ozone (bottom) for two sites in downtown Denver, WELB and CAMP. At WELB the model is estimating higher daytime NOx than observed. At CAMP, the model matches the diurnal variations of the observed NOx concentrations reasonably well, suggesting that the mobile source NOx emissions in downtown Denver are reasonably well characterized.

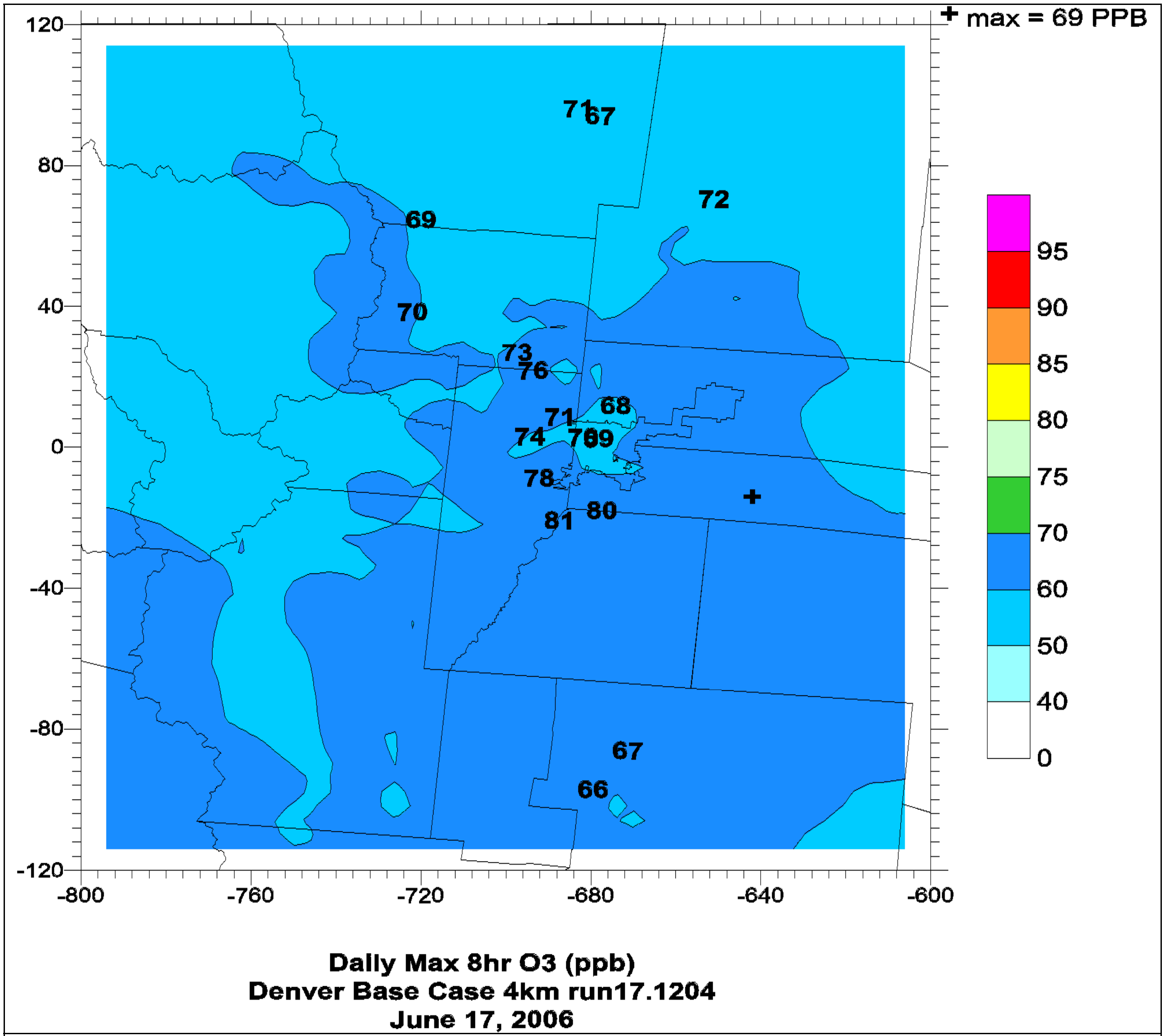


Figure 2-7a. Spatial distribution of the predicted and observed daily maximum 8-hour ozone concentrations (ppb) in the Denver area on July 17, 2006 for the final CAMx Run 17 2006 base case simulation.

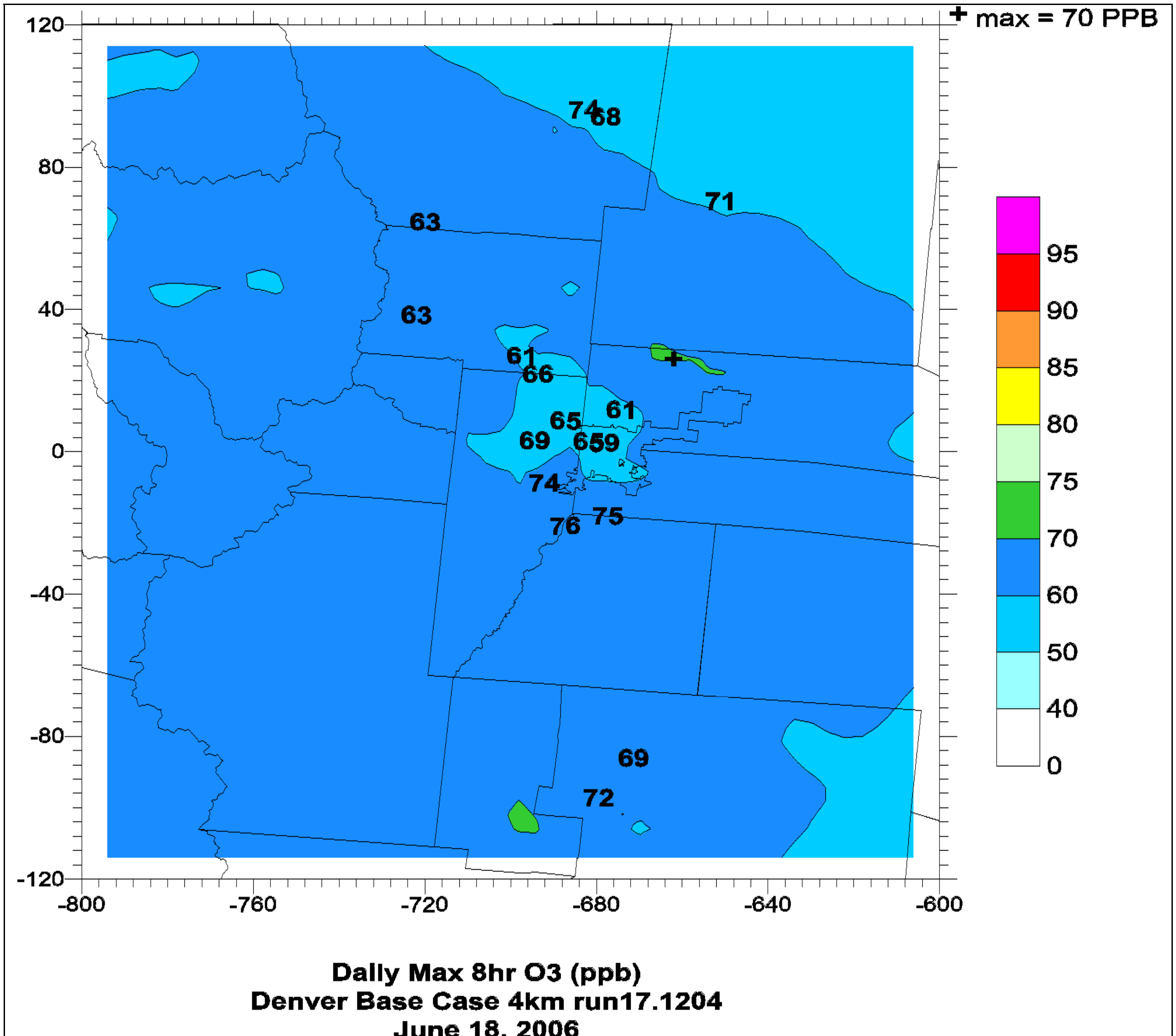


Figure 2-7b. Spatial distribution of the predicted and observed daily maximum 8-hour ozone concentrations (ppb) in the Denver area on July 18, 2006 for the final CAMx Run 17 2006 base case simulation.

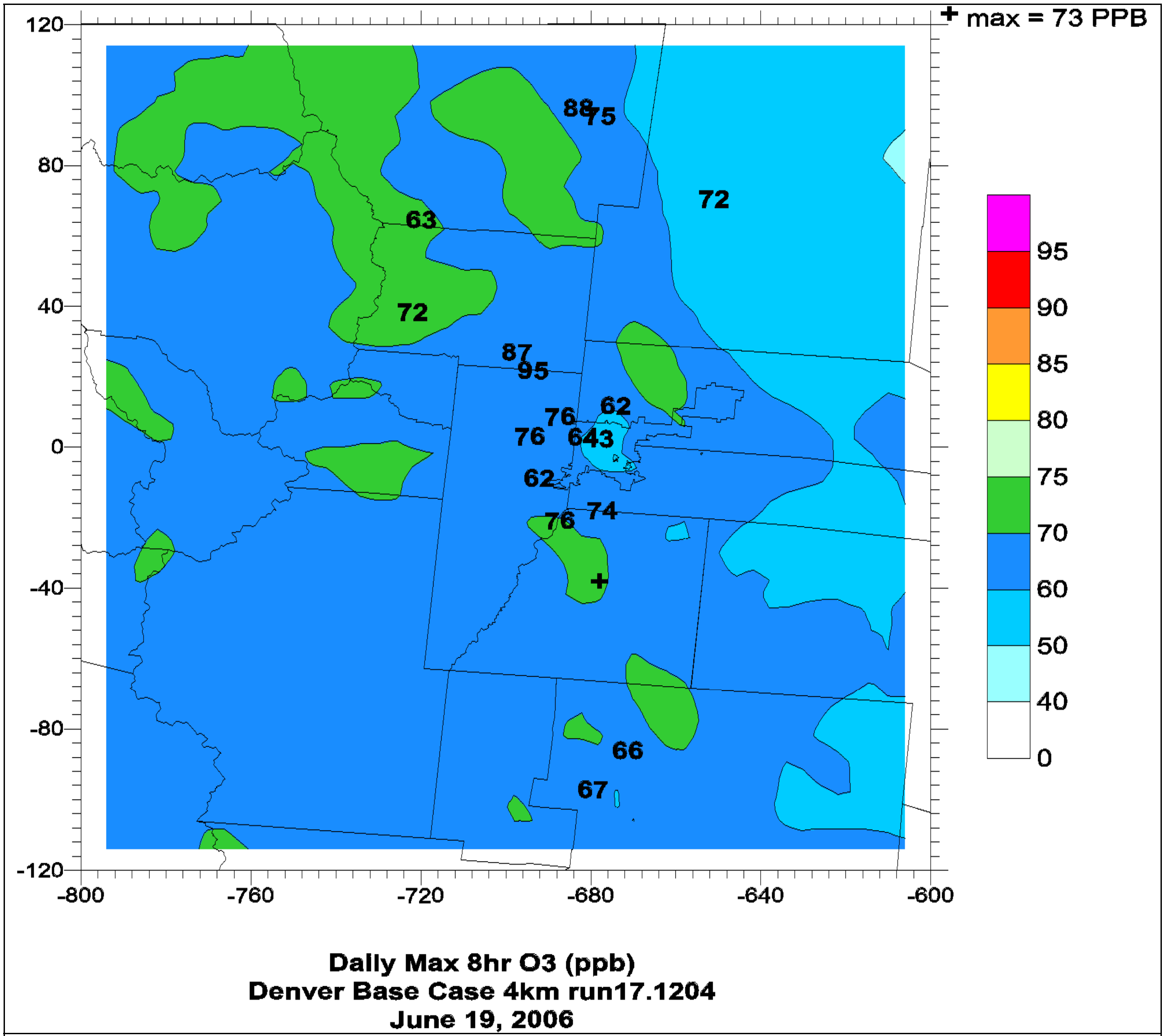
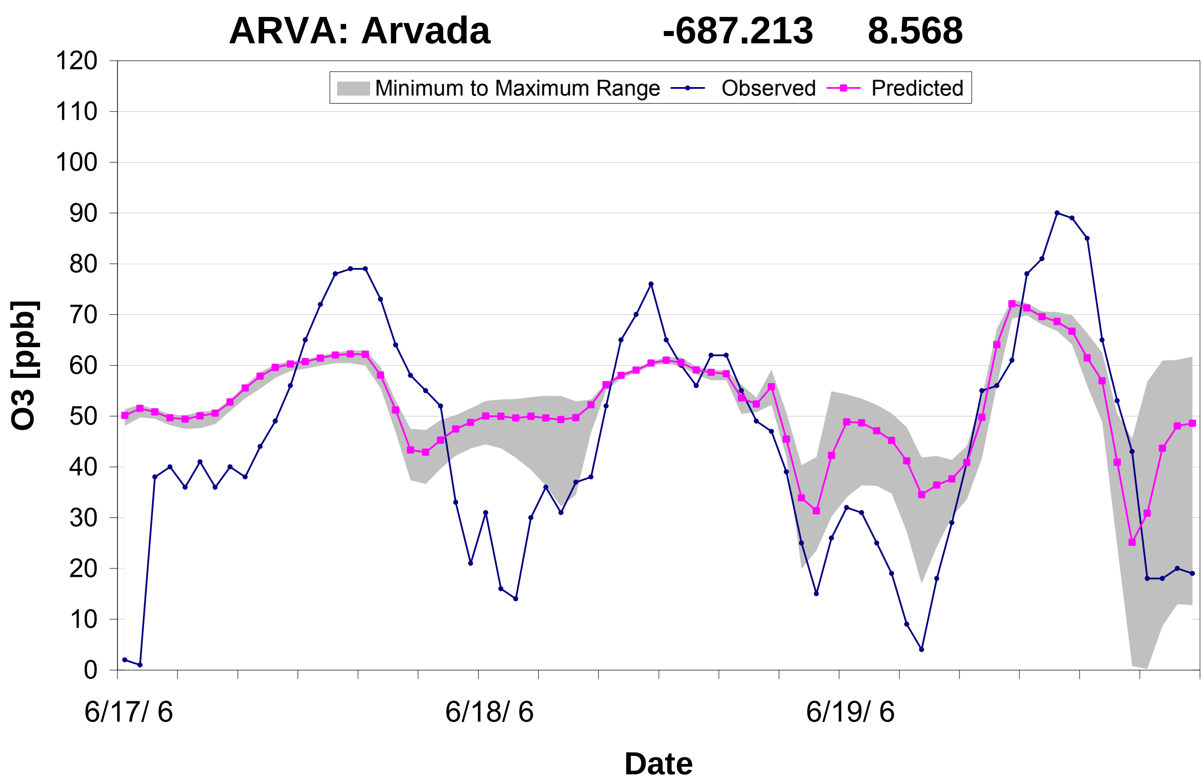
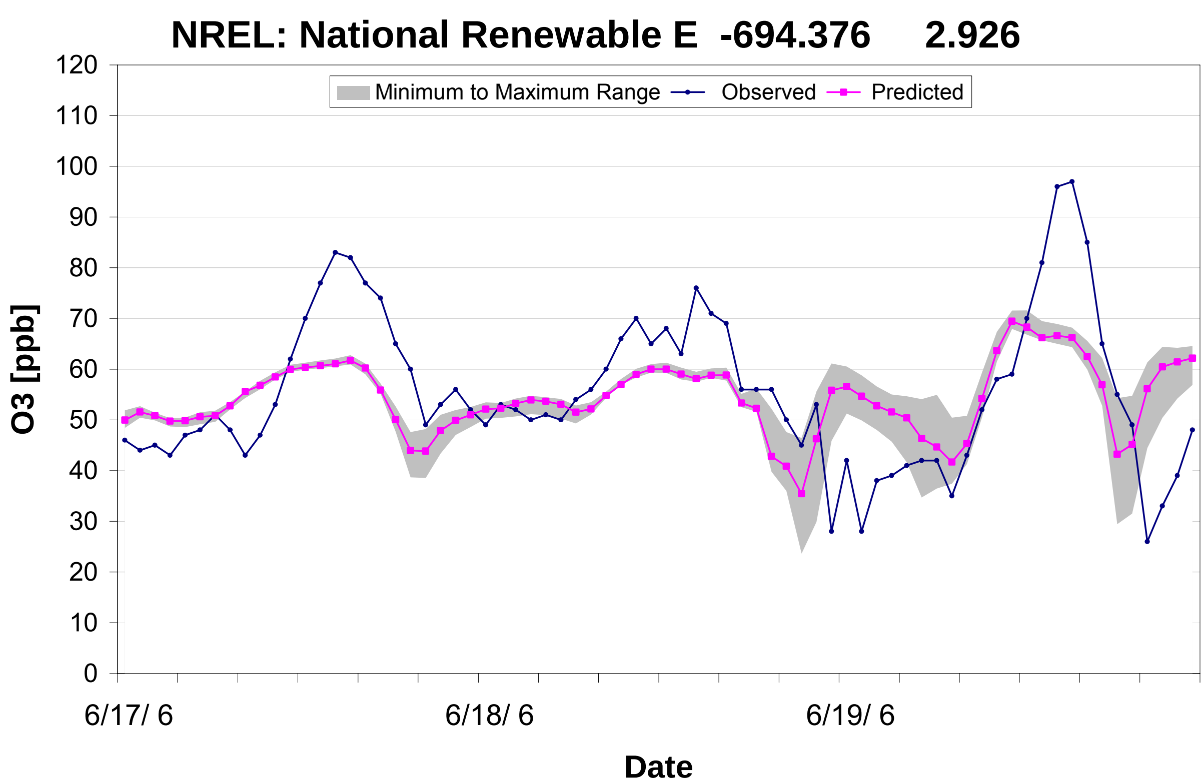
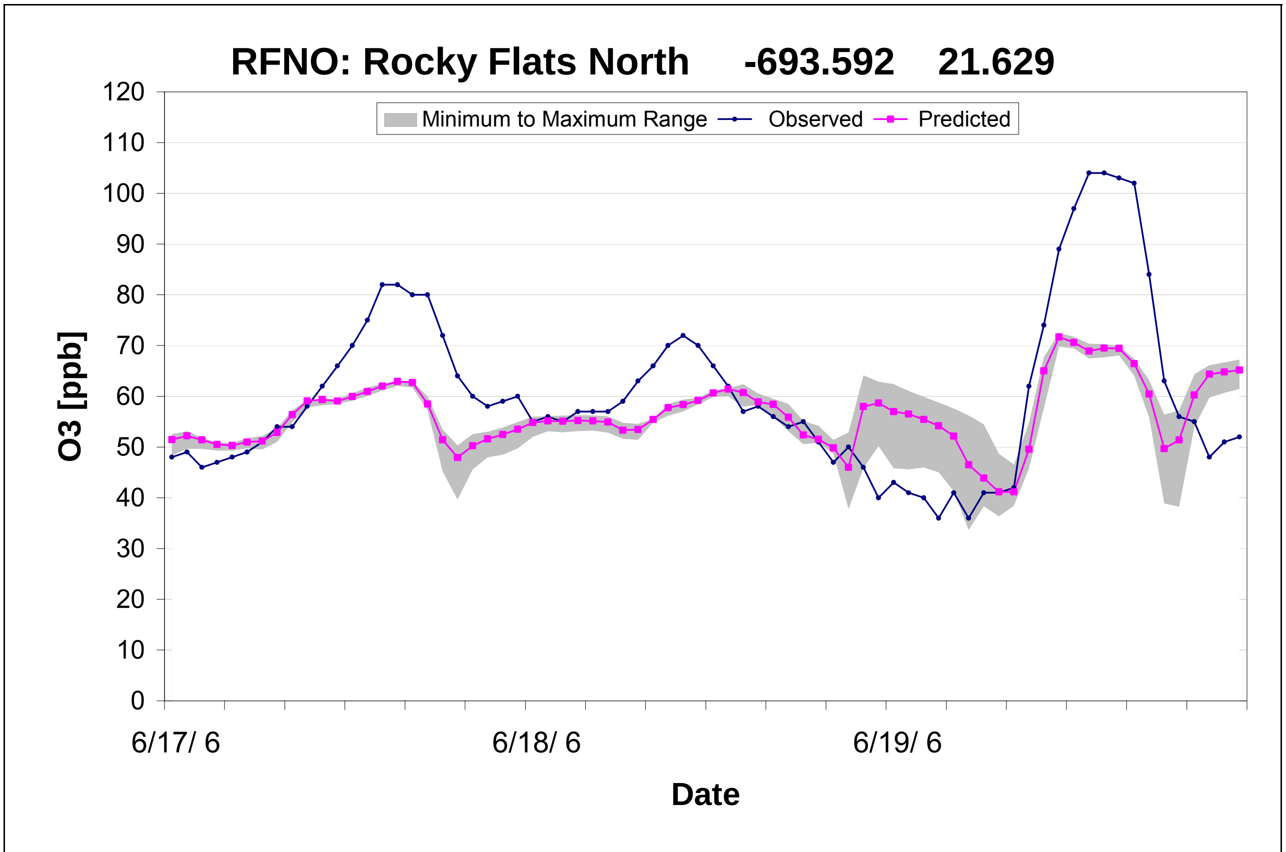
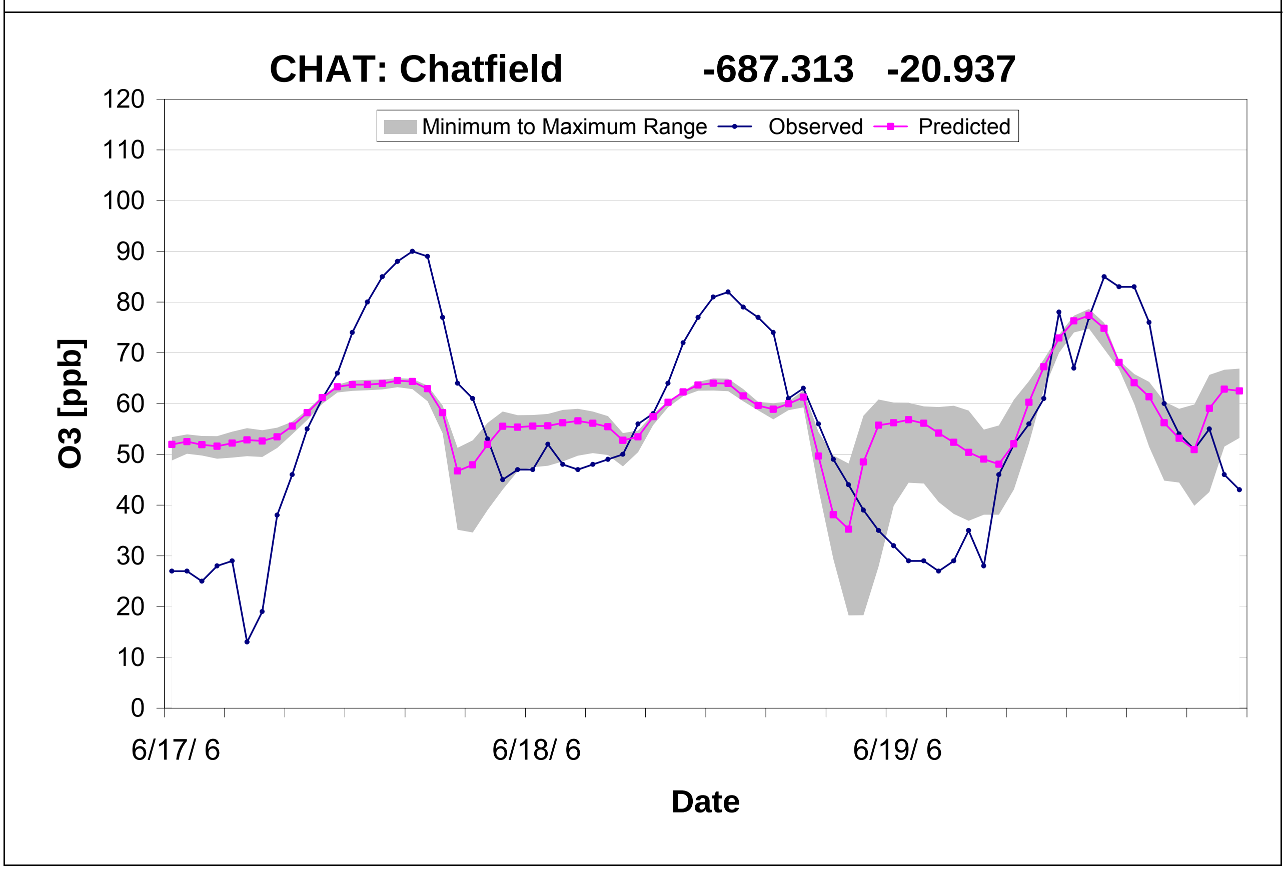


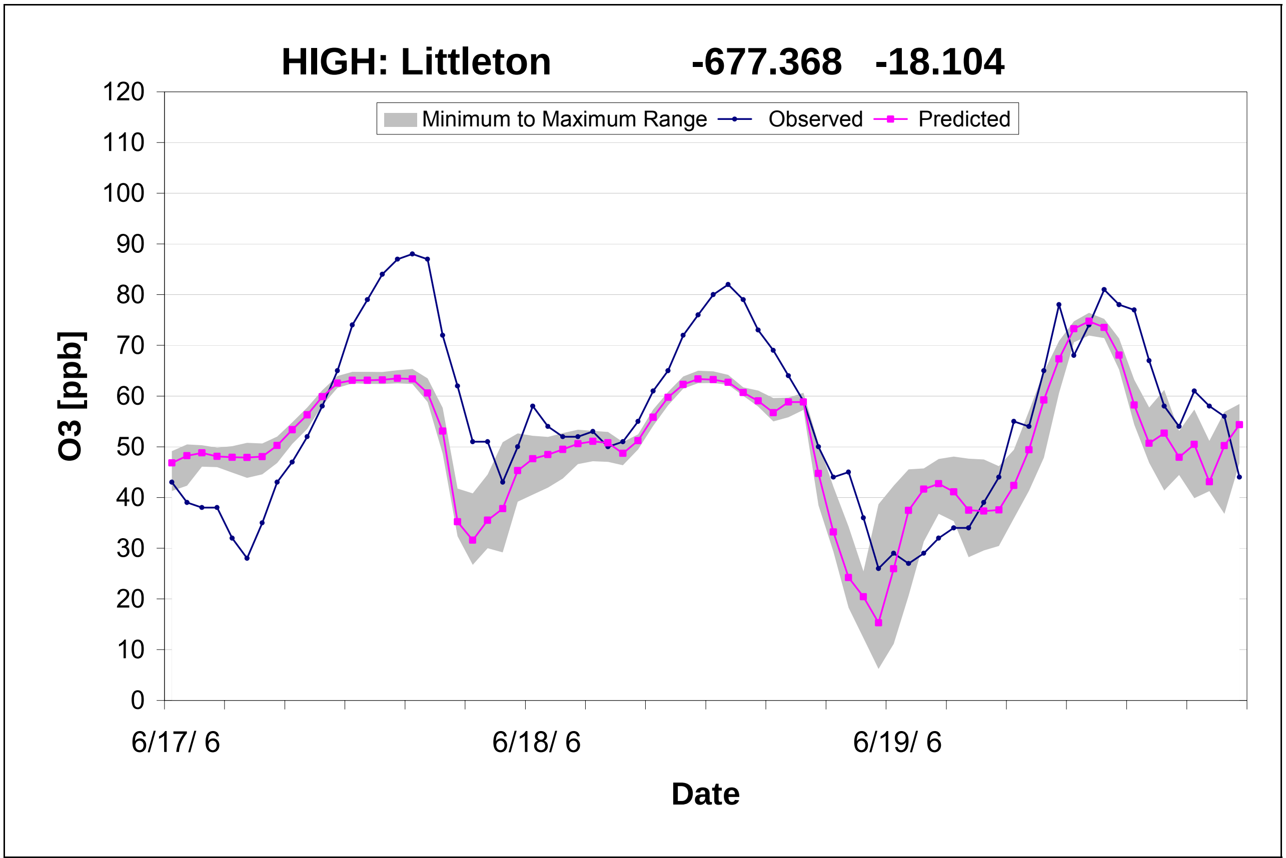
Figure 2-7c. Spatial distribution of the predicted and observed daily maximum 8-hour ozone concentrations (ppb) in the Denver area on July 19, 2006 for the final CAMx Run 17 2006 base case simulation.

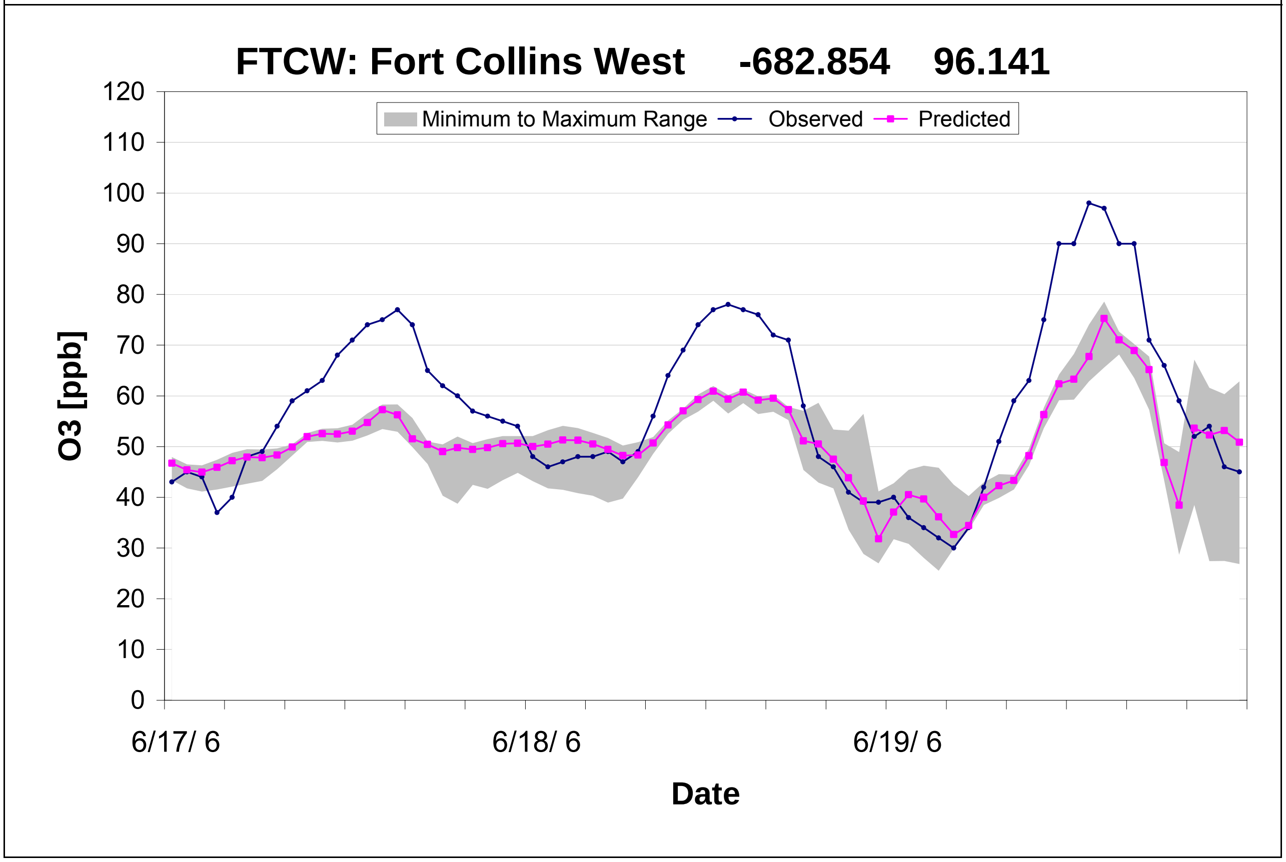

ARVA: Arvada -687.213 8.568
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
120
110
100
90
80
70
60
50
40
30
20
10
0
6/17/ 6
6/18/ 6
6/19/ 6
Date


NREL: National Renewable E -694.376 2.926
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
120
110
100
90
80
70
60
50
40
30
20
10
0
6/17/ 6
6/18/ 6
6/19/ 6
Date


RFNO: Rocky Flats North -693.592 21.629
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
120
110
100
90
80
70
60
50
40
30
20
10
0
6/17/ 6
6/18/ 6
6/19/ 6
Date


CHAT: Chatfield -687.313 -20.937
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
120
110
100
90
80
70
60
50
40
30
20
10
0
6/17/ 6
6/18/ 6
6/19/ 6
Date


HIGH: Littleton -677.368 -18.104
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
120
110
100
90
80
70
60
50
40
30
20
10
0
6/17/ 6
6/18/ 6
6/19/ 6
Date


FTCW: Fort Collins West -682.854 96.141
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
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110
100
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80
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60
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40
30
20
10
0
6/17/ 6
6/18/ 6
6/19/ 6
Date

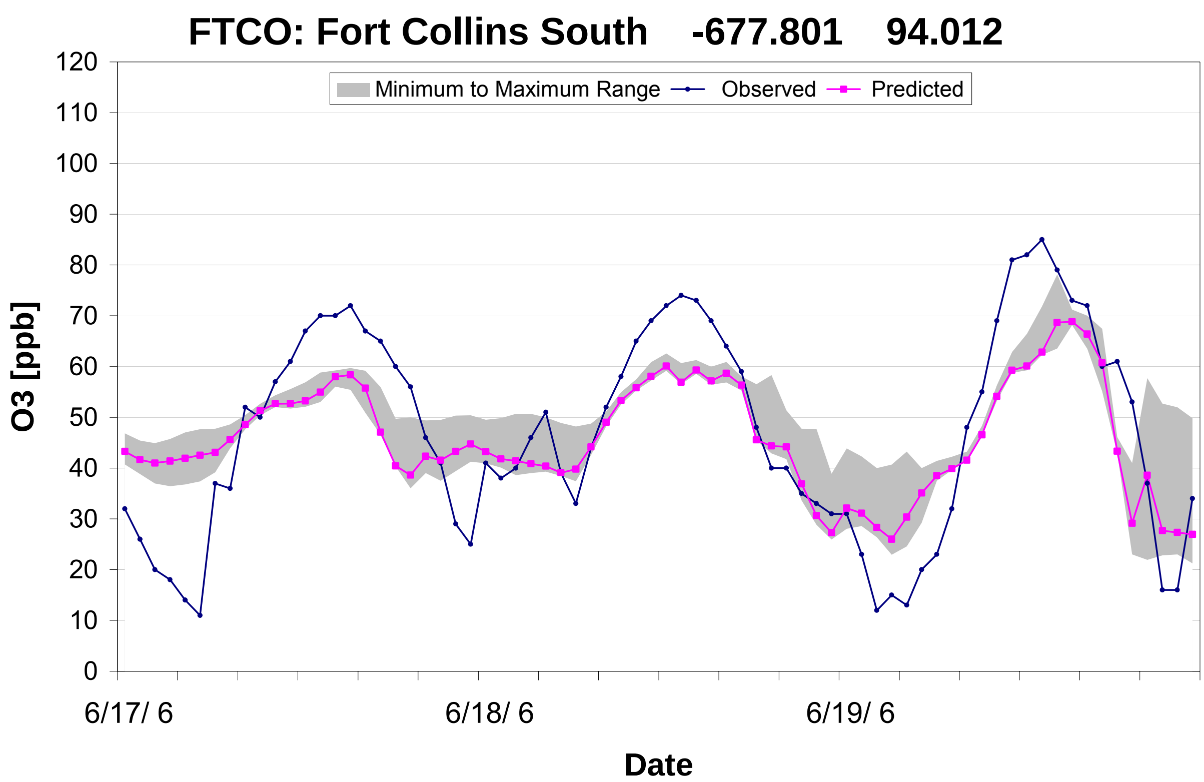


Figure 2-8. Time series of predicted and observed hourly ozone concentrations (ppb) during June 17-19, 2006 for the final CAMx Run 17 2006 base case simulation.

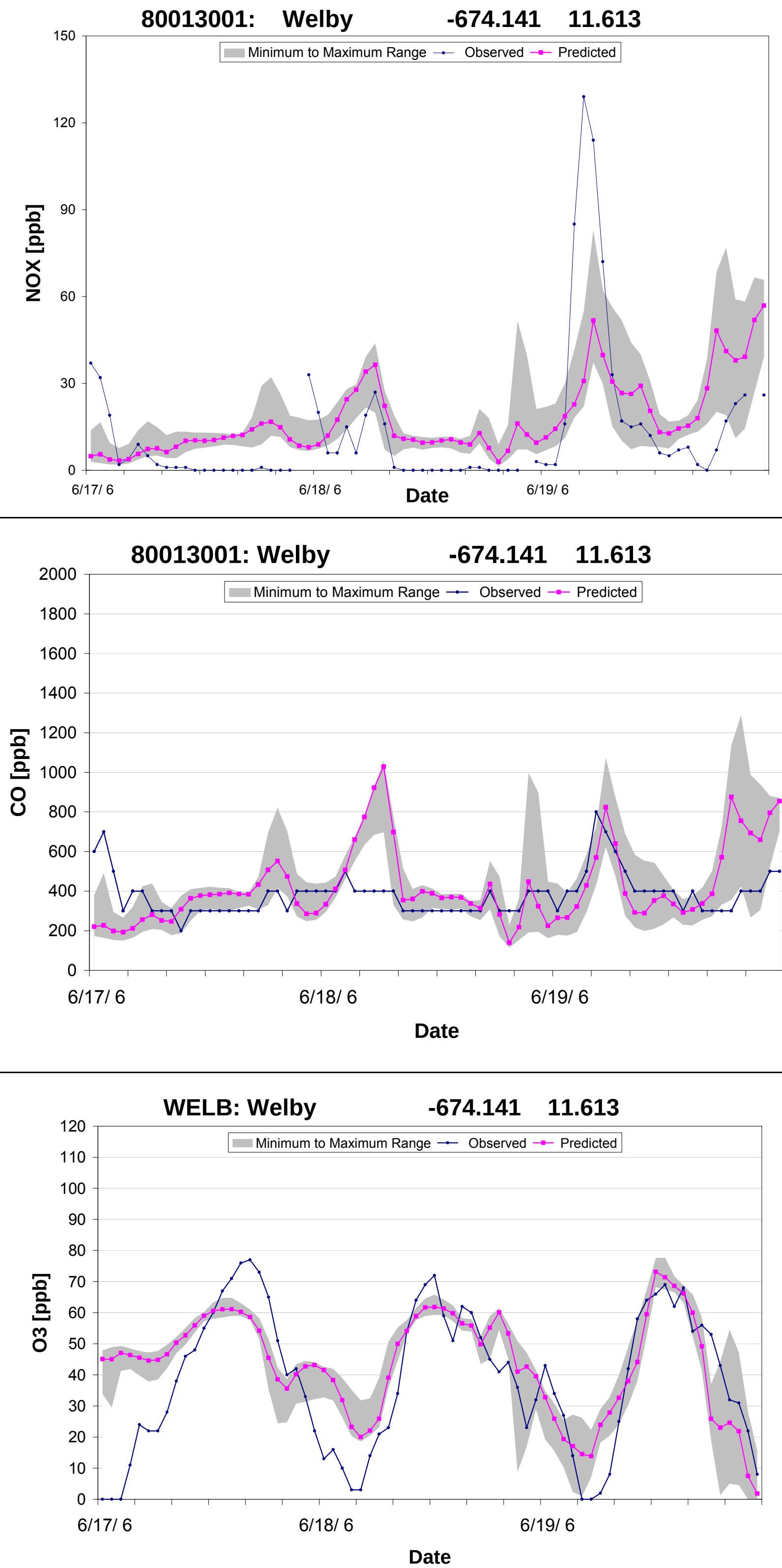


Figure 2-9a. Comparison of hourly NOx (top), CO (middle) and ozone (bottom) predicted and observed time series at the Welby monitoring site for June 17-19, 2006 and the final CAMx Run17 2006 base case simulation.

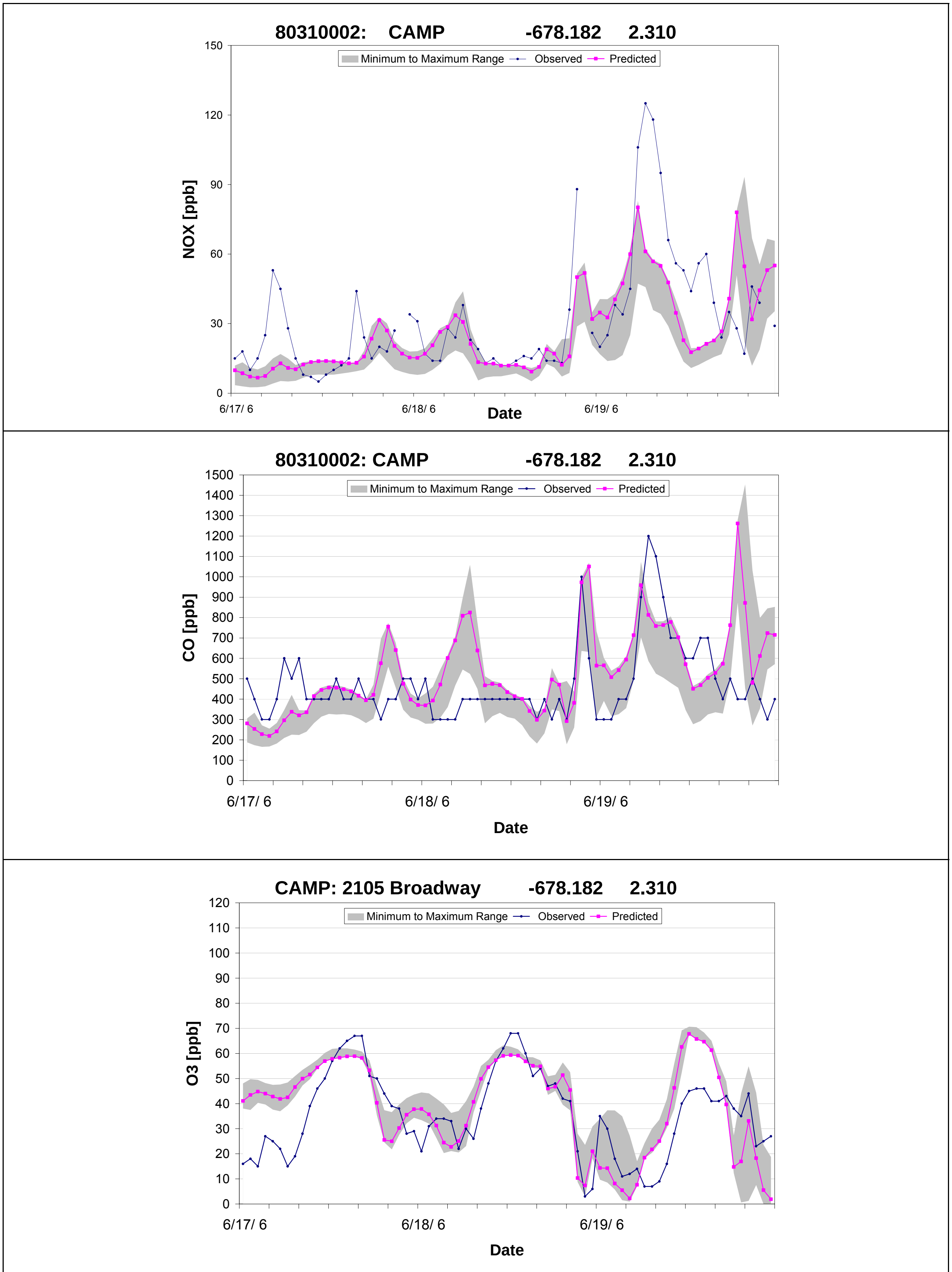


Figure 2-9b. Comparison of hourly NOx (top) and ozone (bottom) predicted and observed time series at the CAMP monitoring site for June 17-19, 2006 and the preliminary CAMx Run17 2006 base case simulation.

2.4.2 July 13-15, 2006

The July 13-15, 2006 episode was a very severe 3-day ozone episode in the DMA with 11 instances of monitors exceeding the 85 ppb 8-hour ozone NAAQS and with two exceedance days each at the SOBC, RFNO and FCTW monitoring sites. Table 2-8 summarizes the 1-hour and 8-hour ozone performance statistics for this 3-day episode. Although there is a large ozone underprediction bias on July 13th, so that the EPA normalized bias goal is not achieved, performance on July 14-15 is better achieving EPA's performance goals for all metrics.

Table 2-8. Final CAMx Run 17 2006 base case simulation daily 1-hour and 8-hour statistical performance measures for the July 13-15, 2006 episode and comparison with EPA performance goals.

Performance Statistic	EPA Goal	2006		
		July 13	July 14	July 15
1-Hour Ozone				
Unpaired Peak	≤±20%	-18.6	-0.3	-7.6
Normalized Bias	≤±15%	-181	-12.7	-5.3
Normalized Error	≤35%	18.1	13.4	9.8
8-Hour Ozone				
Unpaired Peak	≤±20%	-18.5	-9.5	-6.5
Normalized Bias	≤±15%	-6.1	-6.4	7.7
Normalized Error	≤35%	14.8	13.3	12.7

The poor performance on July 13th is also reflected in the comparisons of the spatial distribution of the observed and predicted daily maximum 8-hour ozone concentrations in Figure 2-10a. The high observed ozone at the monitoring sites south of Denver (86-92 ppb) is underpredicted by the model by approximately 20 ppb.

Better performance is seen on July 14, 2006 (Figure 2-10b). The model correctly places a large expanse of elevated ozone concentrations stretching from northwest Denver to Fort Collins that also impacts the Niwot Ridge and RMNP sites where ozone exceedances are observed (91 ppb). The modeled ozone peak (88 ppb) is located very close to the monitored ozone peak (97 ppb) at FTCW monitoring site. If the modeled ozone was about 10 ppb higher and extended a little further west, model performance would be excellent on this day.

On July 15th the modeled elevated ozone cloud is located to the northeast of Denver, when it should be located to the northwest of the city. This is clearly a case of spatial displacement due to errors in the wind fields (Figure 2-10c).

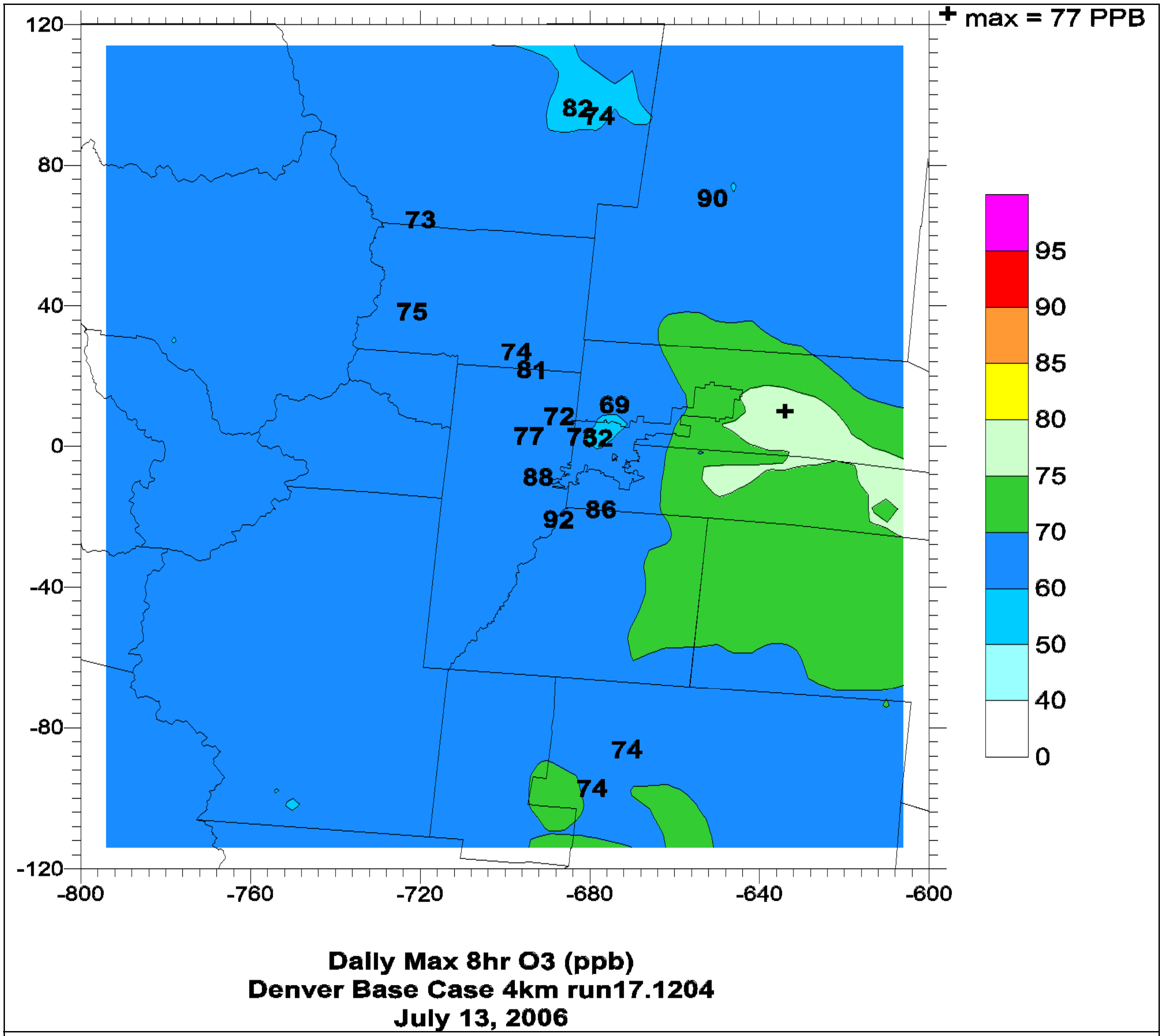


Figure 2-10a. Spatial distribution of the predicted and observed daily maximum 8-hour ozone concentrations (ppb) in the Denver area on July 13, 2006 for the final CAMx Run 17 2006 base case simulation.

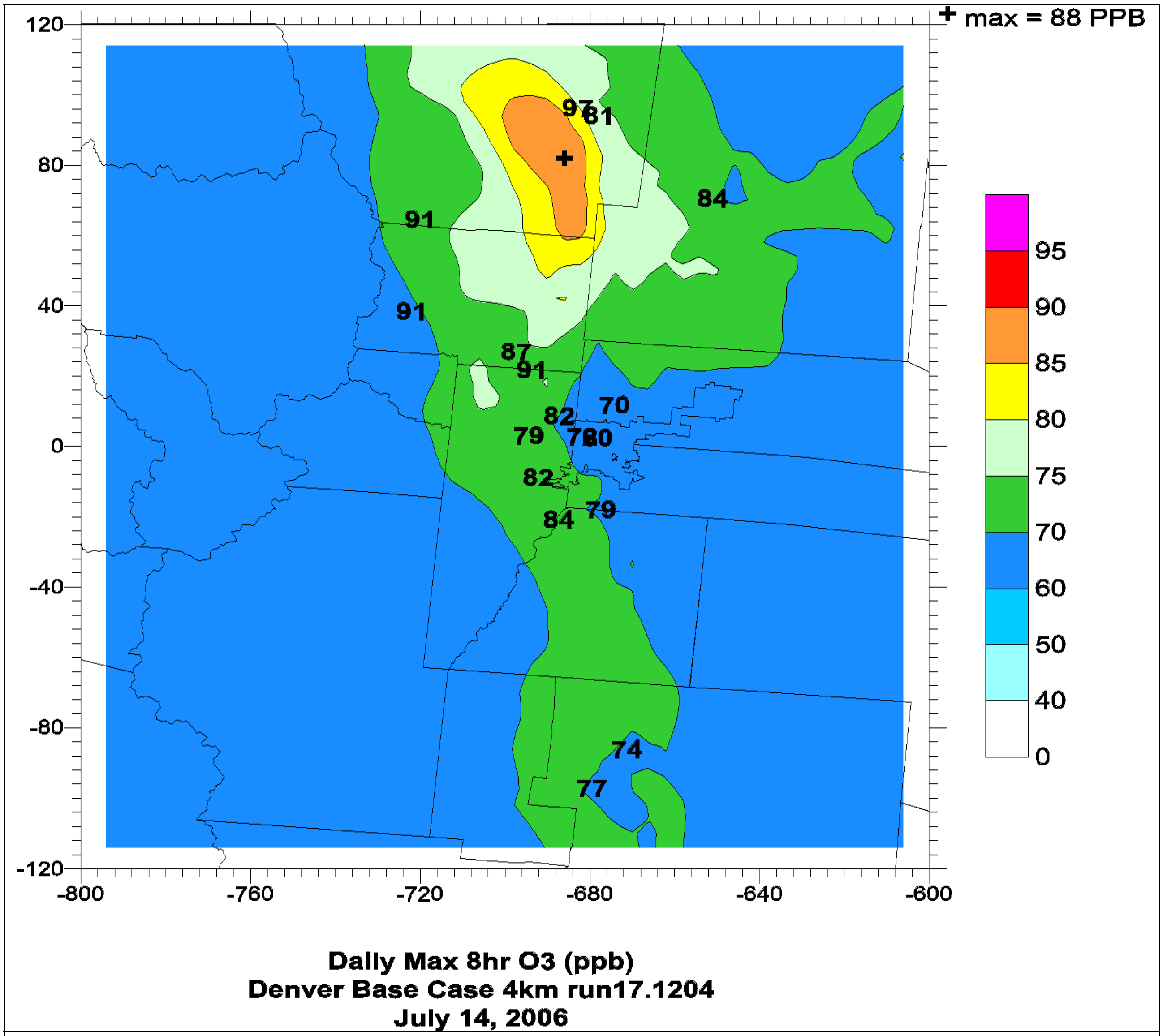


Figure 2-10b. Spatial distribution of the predicted and observed daily maximum 8-hour ozone concentrations (ppb) in the Denver area on July 14, 2006 for the final CAMx Run 17 2006 base case simulation.

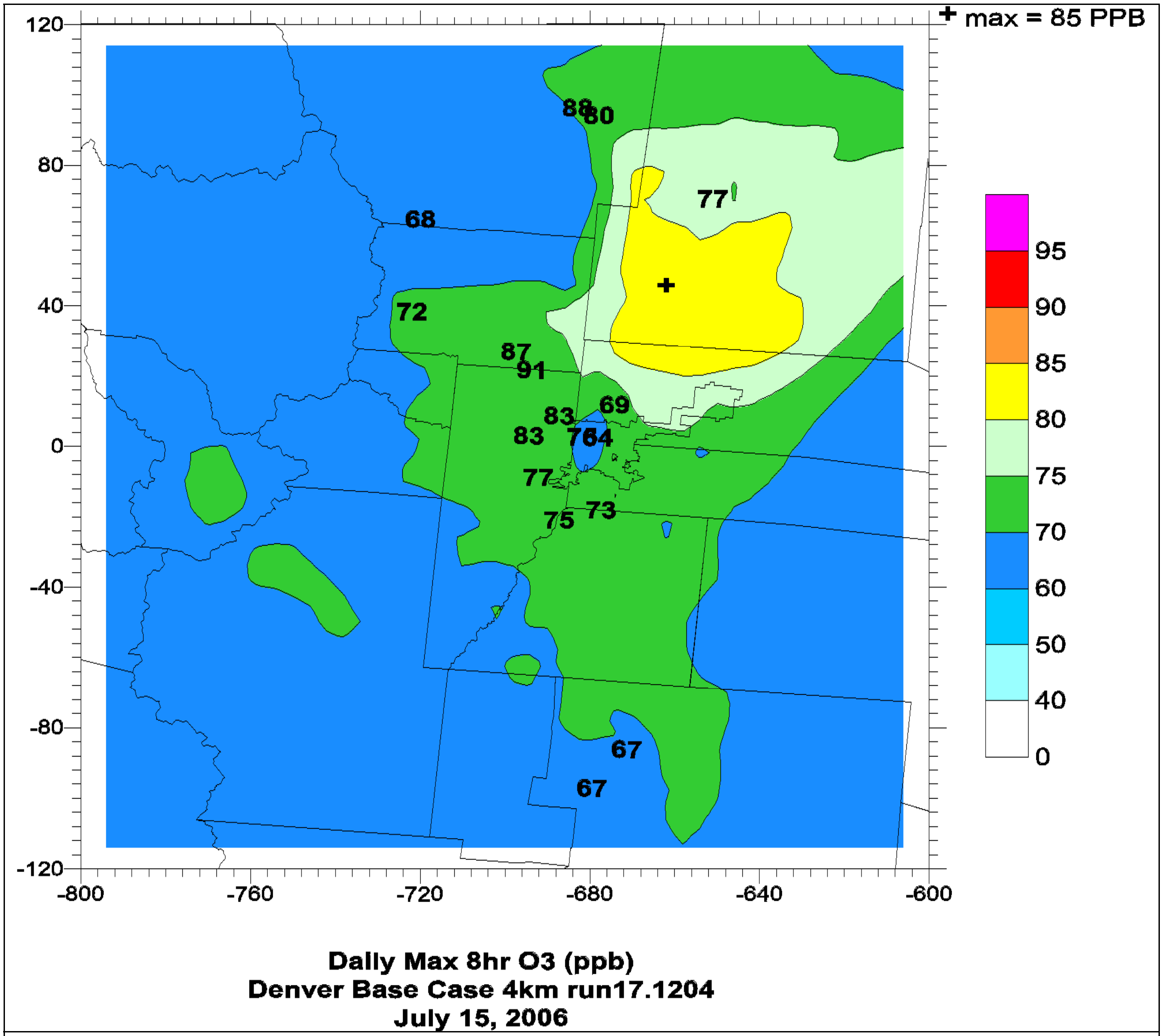


Figure 2-10c. Spatial distribution of the predicted and observed daily maximum 8-hour ozone concentrations (ppb) in the Denver area on July 15, 2006 for the final CAMx Run 17 2006 base case simulation.

The time series of predicted and observed hourly ozone concentrations for the July 13-15, 2006 3-day episode are shown in Figure 2-11. The model does a better job of reproducing the observed diurnal variation of the observed hourly concentrations at the ARVA and NREL sites just northwest of Denver on July 13-15 than the June 17-19 episode, but still shaves the observed daytime ozone peaks. The 8-hour ozone exceedances at the RFNO monitor on July 14-15 are underestimated by over 20 ppb.

The modeled ozone at RMNP is nearly constant 60 ppb except for a 20 ppb increase on July 14 to 80 ppb. The observed values are more variable (typically 50 ppb to 70 ppb) and also exhibit an increase on July 14th that is twice as high (40 ppb) as the modeled increase (20 ppb). As noted in the spatial comparisons in Figure 2-10b), the modeled elevated ozone cloud is displaced slightly eastward. This is a fairly common attribute of the MM5 winds inability to fully simulate the upslope flows during the day.

Ozone model performance at the monitoring sites south of Denver (WELC, CHAT and HIGH) is quite good on July 14-15, with the observed daytime ozone underestimated on July 13.

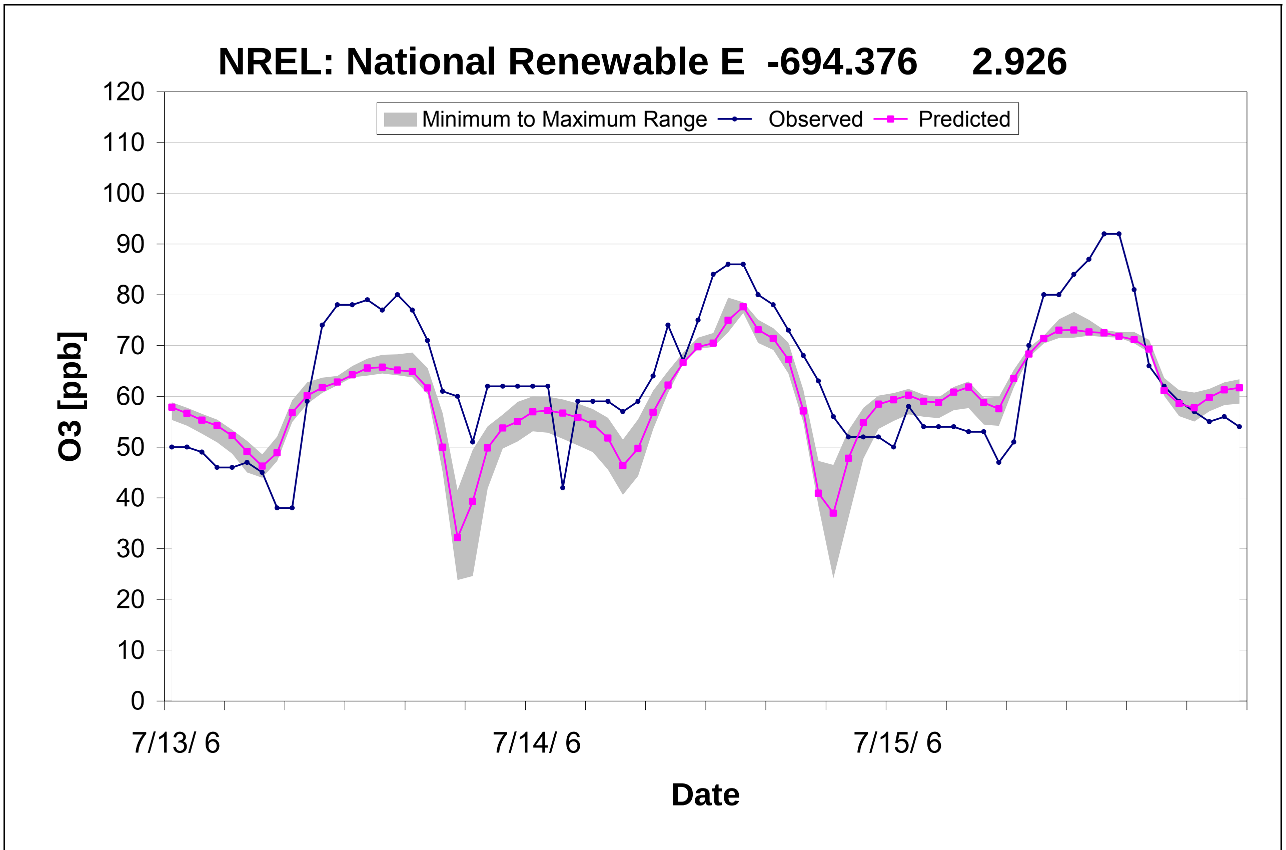
At the monitoring sites north of Denver (FTCO, FTCW and WCTO), daytime ozone is underestimated on July13th at all three monitors with better performance seen on July 14-15, albeit with a daytime underestimation bias.

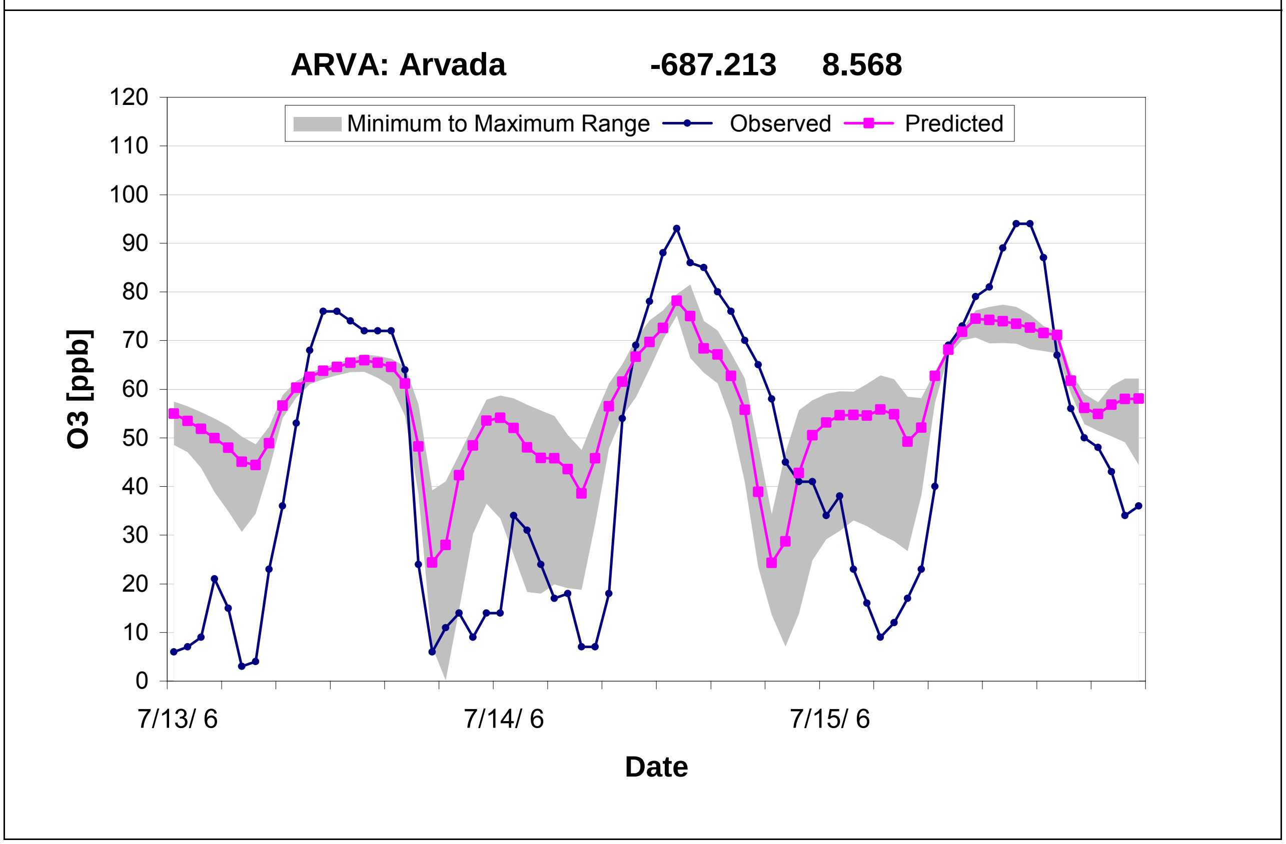
Figure 2-12 compares the predicted and observed hourly NOx, CO and ozone concentrations at the WELB and CAMP central Denver sites. At these sites the NOx, CO and ozone concentrations are reproduced quite well, with daytime modeled NOx values higher than observed at WELB, but matched quite well at CAMP. As NOx and CO at these two sites will be dominated by on-road mobile source emissions, these results suggest that the on-road mobile source NOx and CO emissions are reasonably well characterized.

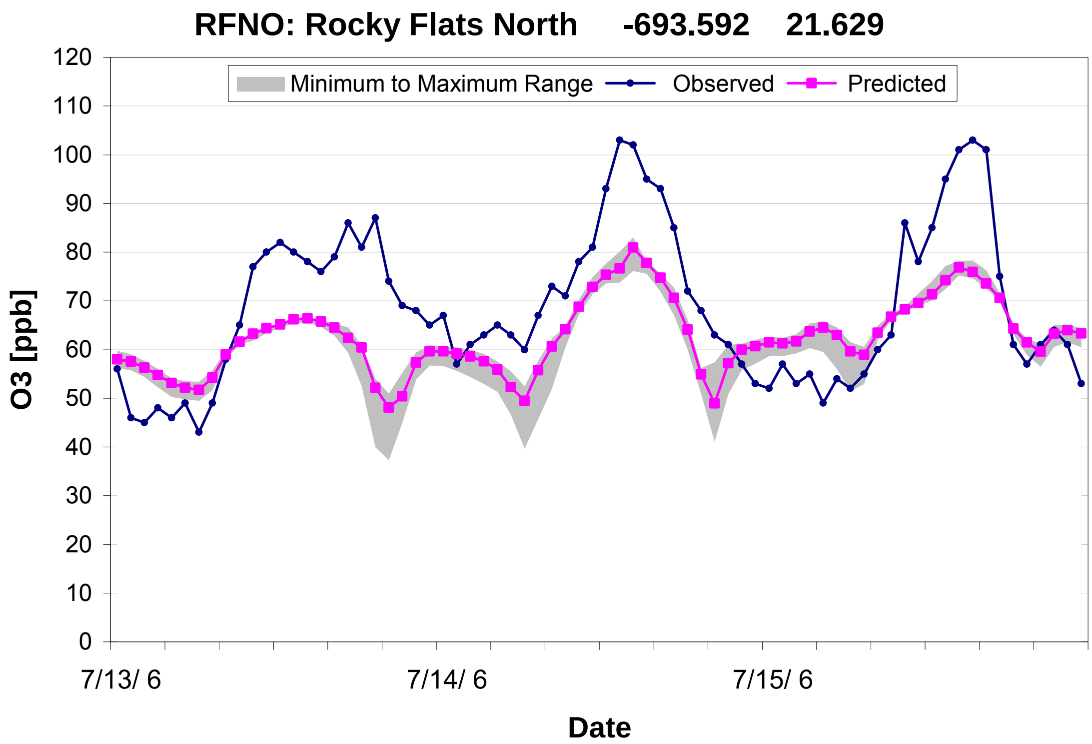
ALPINE GEOPHYSICS

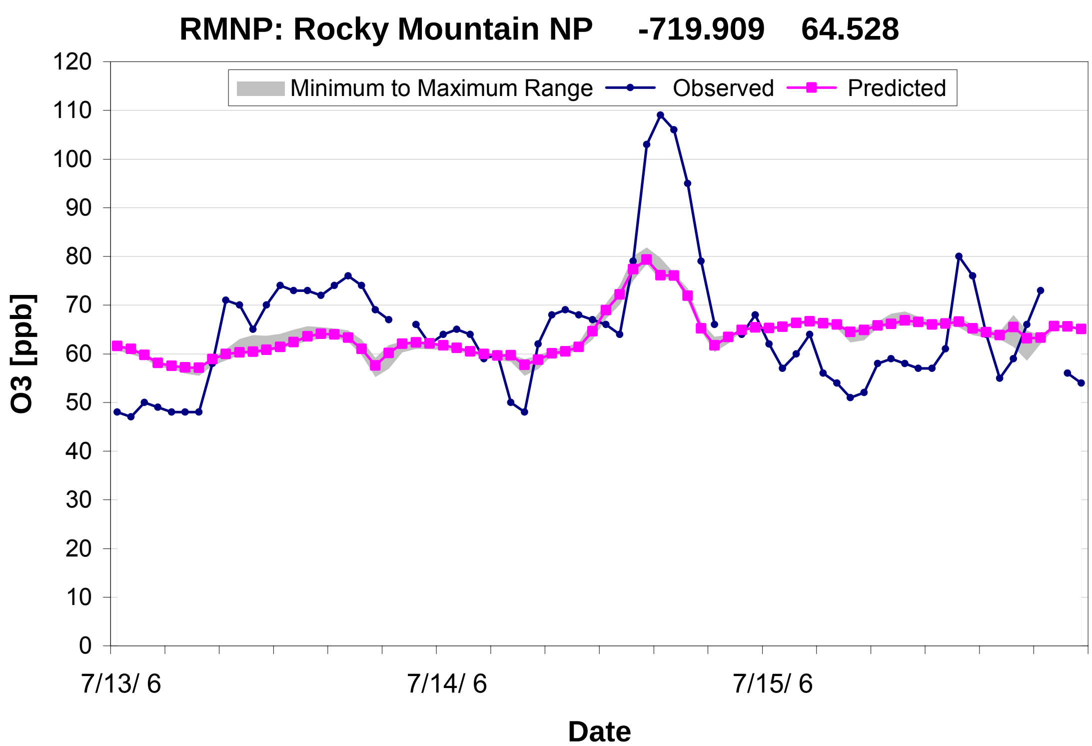
REGIONAL AIR QUALITY COUNCIL

ENVIRON






RFNO: Rocky Flats North -693.592 21.629
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
0
10
20
30
40
50
60
70
80
90
100
110
120
7/13/ 6
7/14/ 6
7/15/ 6
Date


RMNP: Rocky Mountain NP -719.909 64.528
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
0
10
20
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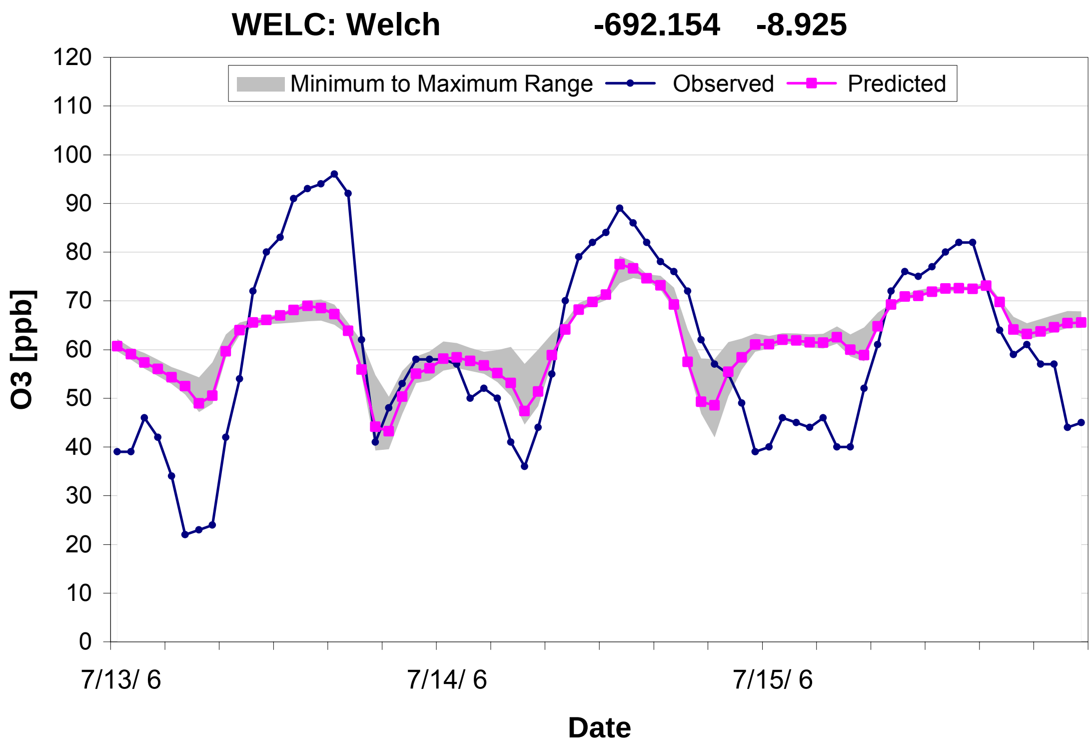
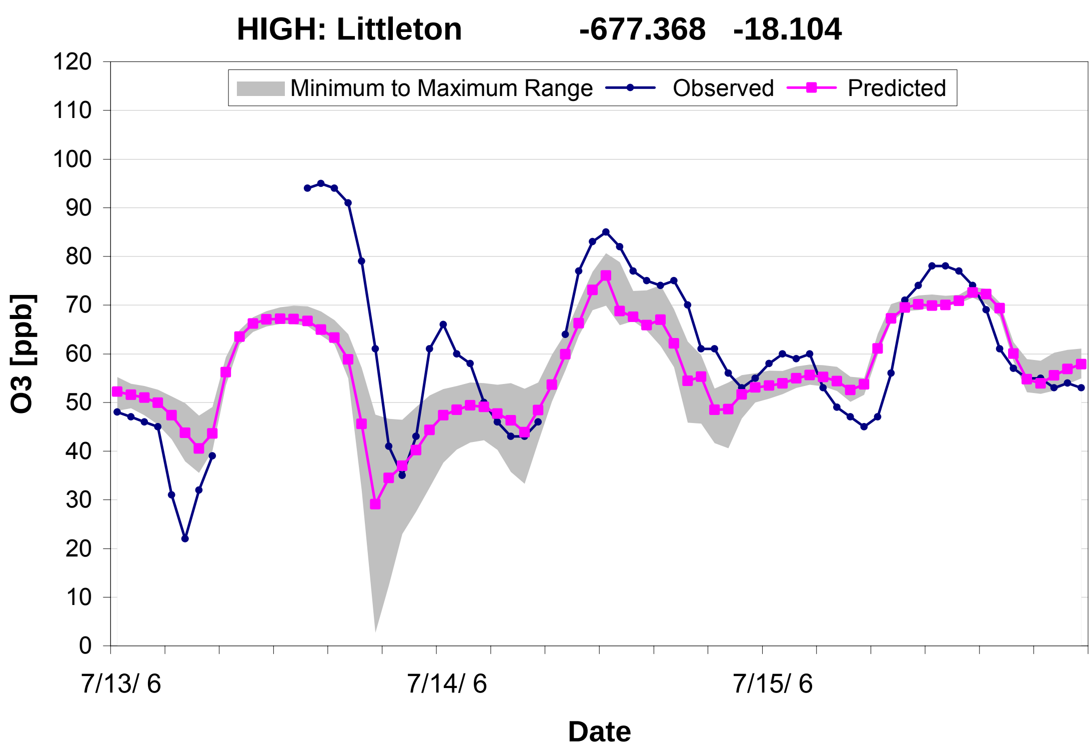
70
80
90
100
110
120
7/13/ 6
7/14/ 6
7/15/ 6
Date


WELC: Welch -692.154 -8.925
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
120
110
100
90
80
70
60
50
40
30
20
10
0
7/13/ 6
7/14/ 6
7/15/ 6
Date


HIGH: Littleton -677.368 -18.104
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
120
110
100
90
80
70
60
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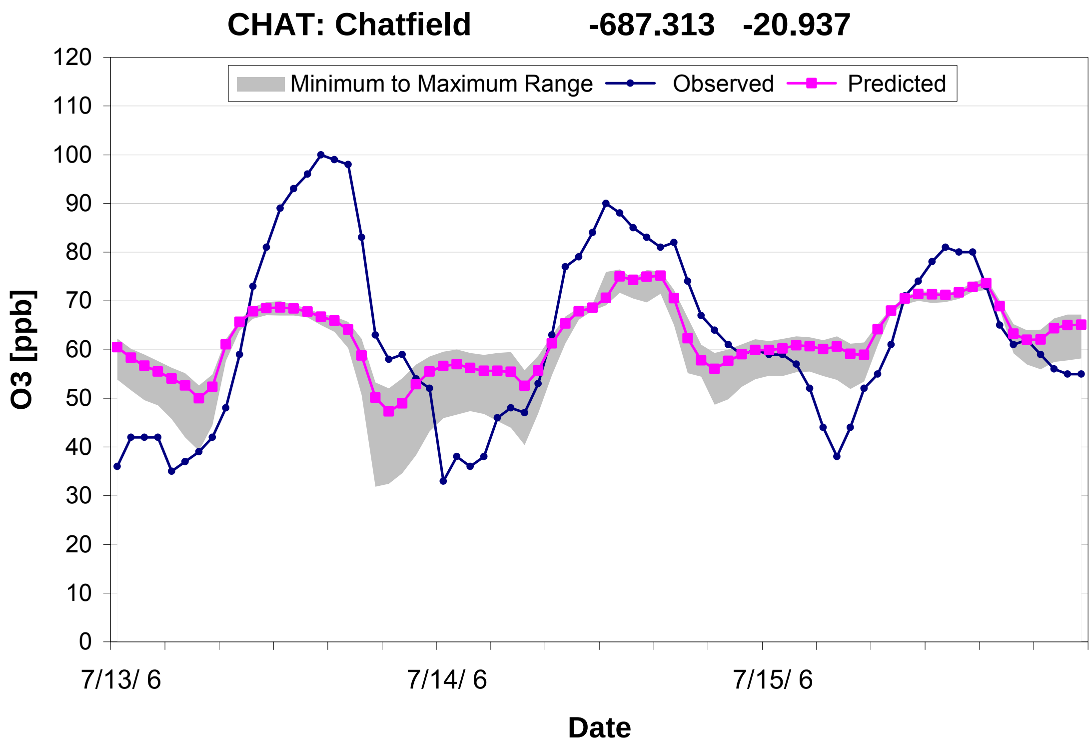
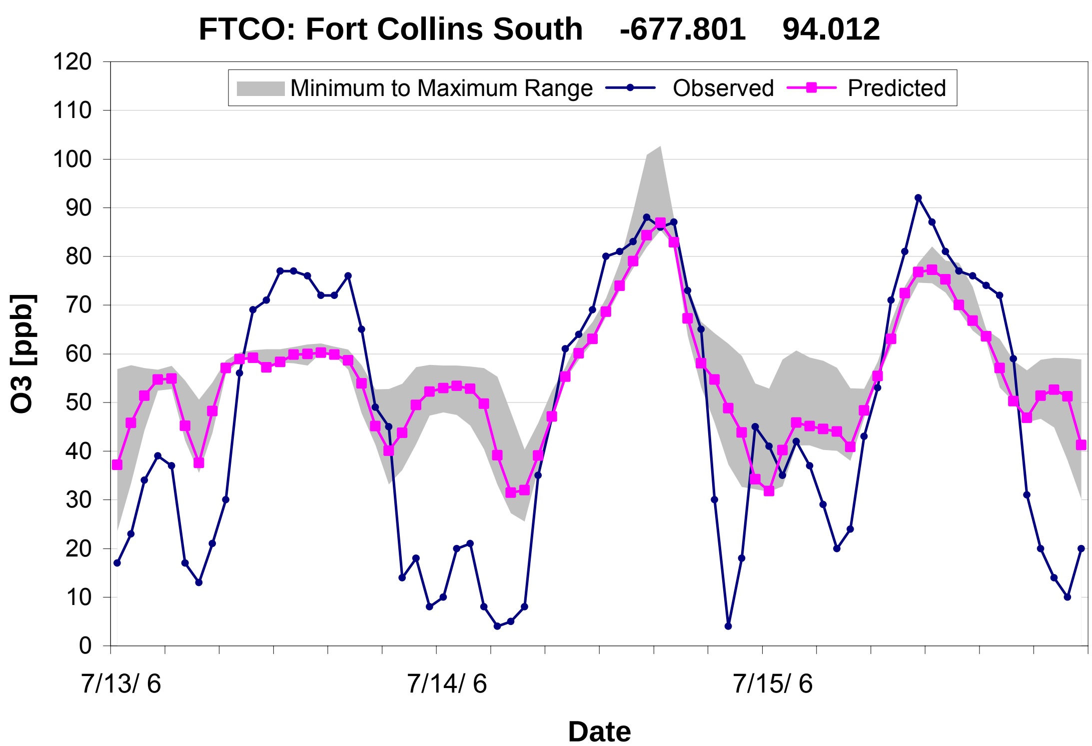
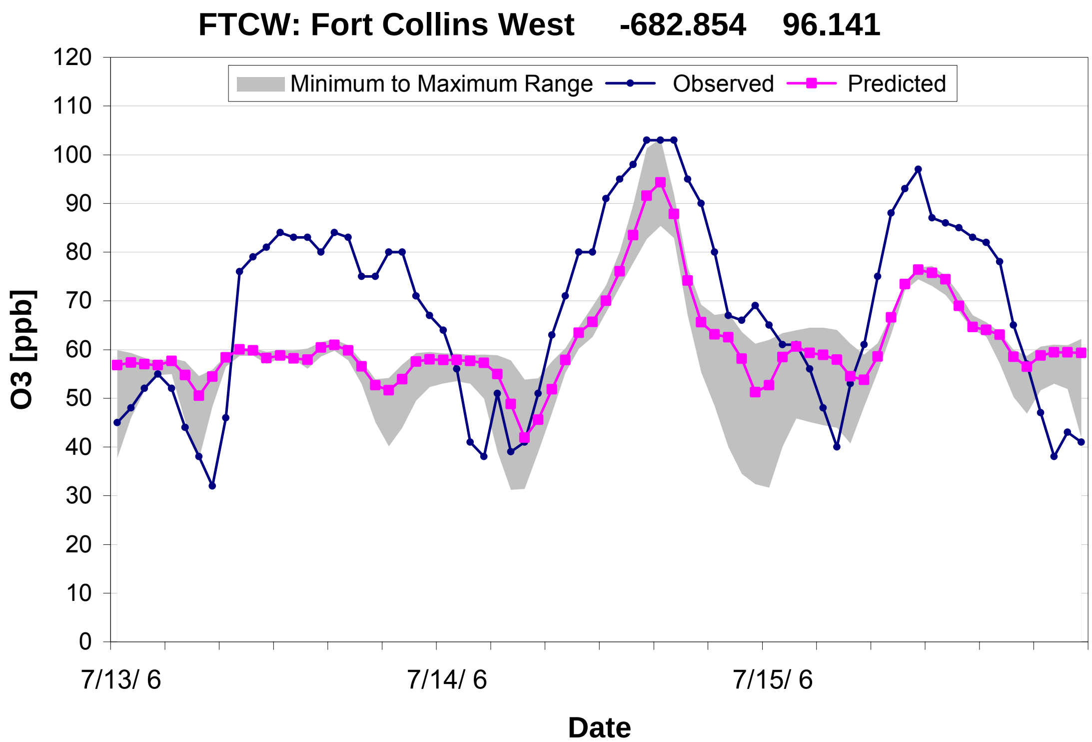
40
30
20
10
0
7/13/ 6
7/14/ 6
7/15/ 6
Date



CHAT: Chatfield -687.313 -20.937
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
0
10
20
30
40
50
60
70
80
90
100
110
120
7/13/ 6
7/14/ 6
7/15/ 6
Date



FTCO: Fort Collins South -677.801 94.012
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
0
10
20
30
40
50
60
70
80
90
100
110
120
7/13/ 6
7/14/ 6
7/15/ 6
Date



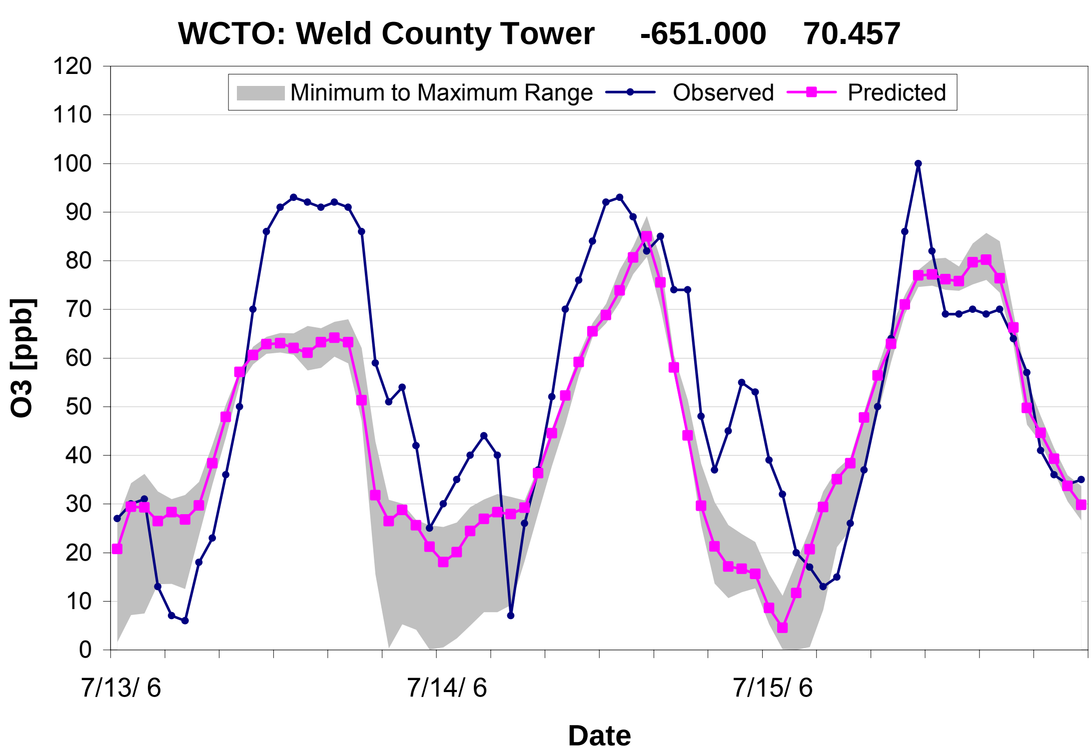
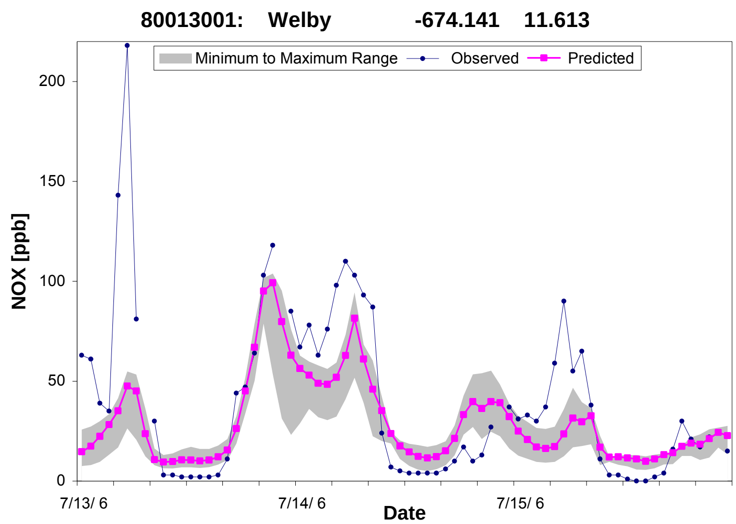
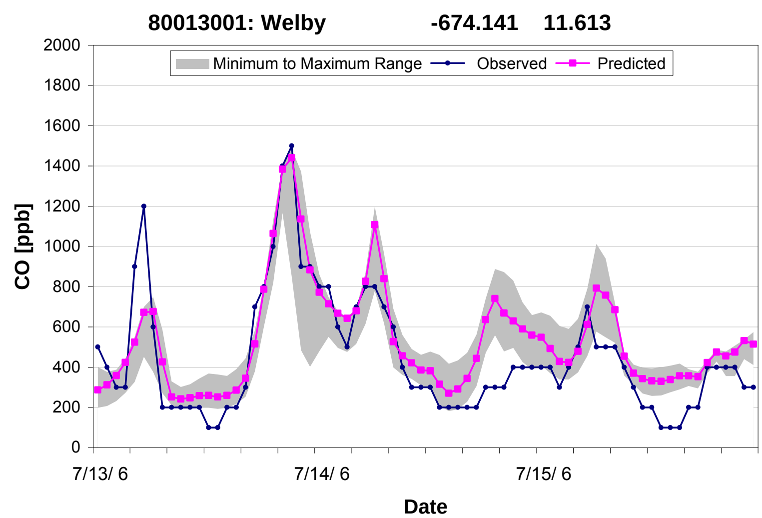


Figure 2-11. Hourly time series of predicted and observed hourly ozone concentrations for the July 13-15, 2006 period and the final CAMx Run17 2006 base case simulation.





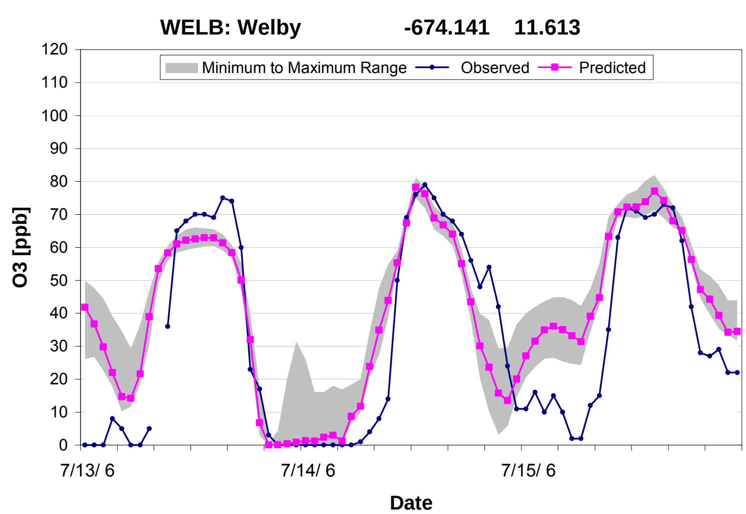
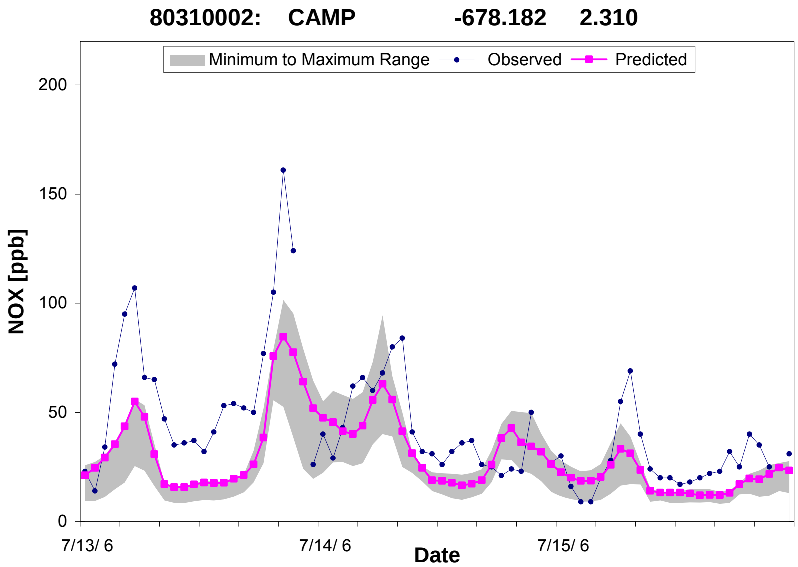
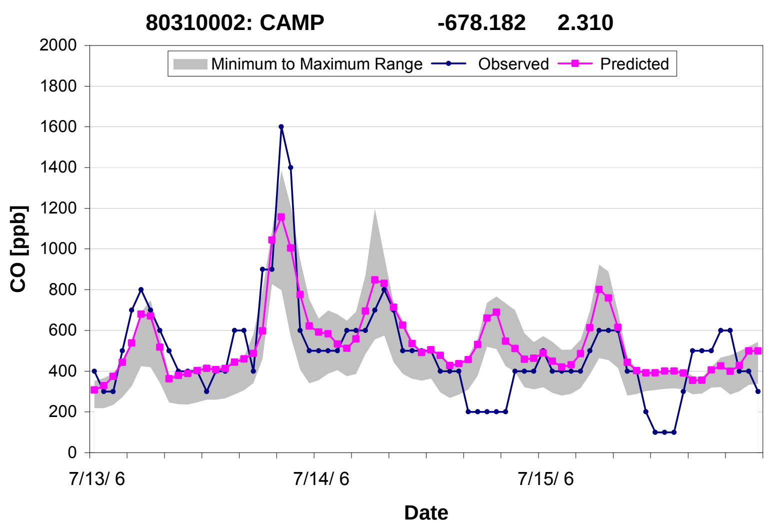


Figure 2-12a. Comparison of hourly NOx (top) and ozone (bottom) predicted and observed time series at the Welby monitoring site for July 13-15, 2006 and the final CAMx Run17 2006 base case simulation base case simulation.





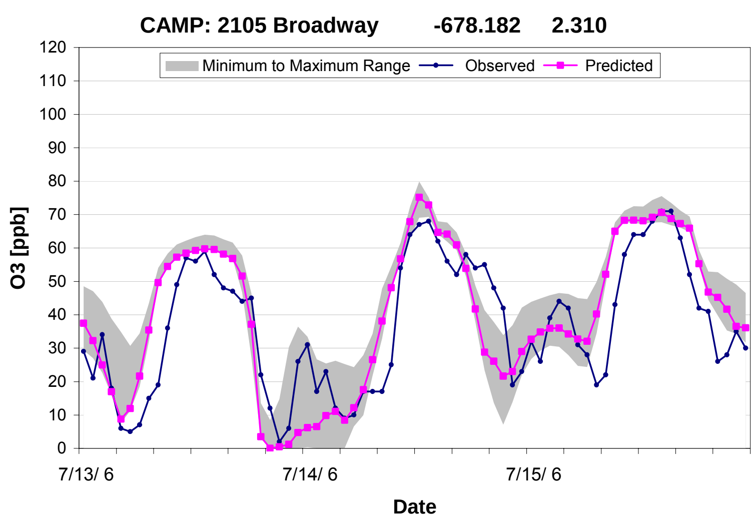


Figure 2-12b. Comparison of hourly NOx (top) and ozone (bottom) predicted and observed time series at the CAMP monitoring site for July 13-15, 2006 and the final CAMx Run17 2006 base case simulation base case simulation.

2.4.3 July 27-29, 2006

The July 27-29, 2006 episode was the most severe 3-day ozone episode that occurred during 2006. 8-hour ozone exceedances occurred on all three days and there were a total of 10 monitor-days of exceedances in the Denver area, including 2 days at the key RFNO monitoring site.

Table 2-9 displays the 1-hour and 8-hour performance statistics for July 27-29, 2006 all of which achieve EPA's performance goals, although with an underprediction bias of the 1-hour ozone statistics.

Table 2-9. Final CAMx Run 17 2006 base case simulation daily 1-hour and 8-hour statistical performance measures for the July 27-29, 2006 episode and comparison with EPA performance goals.

Performance Statistic	EPA Goal	2006		
		July 27	July 28	July 29
1-Hour Ozone				
Unpaired Peak	≤±20%	-11.8	7.8	-1.2
Normalized Bias	≤±15%	-9.6	-9.7	-9.1
Normalized Error	≤35%	13.1	14.8	12.4
8-Hour Ozone				
Unpaired Peak	≤±20%	-10.3	-6.2	-6.3
Normalized Bias	≤±15%	1.0	-1.8	3.2
Normalized Error	≤35%	13.6	12.3	14.2

The comparison of the predicted and observed spatial distributions of daily maximum 8-hour ozone concentrations on July 27th confirm the model underprediction bias on this day (Figure 2-13a). The model predicts elevated ozone mainly to the north and northwest of downtown, whereas the peak observed values are south of Denver. Although the modeled 8-hour ozone peak (78 ppb) is in the direction of an observed 82 ppb ozone peak in Weld County. Clearly the model is failing to capture what caused the observed high ozone south of Denver on this day.

Better ozone performance is seen on July 28th (Figure 2-13b). The model correctly locates the elevated ozone cloud northwest of Denver, although ozone formation appears to be slower in then model than observed so the peak ozone occurs farther downwind. The model elevated ozone cloud also appears to be slight displaced westward only glancing the FTCW monitor where high ozone was recorded (87 ppb).

July 29, 2006 was the most adverse ozone day during 2006 in the DMA. High ozone values were recorded at numerous monitors with exceedances even recorded at the Carriage monitor close to downtown. On other days we noted the too slow ozone formation in the model that caused the modeled ozone to occur too far downwind and away from Denver, such is not the case on this day. The highest modeled ozone in excess of 85 ppb is estimated south of downtown Denver where observed values of 83-97 are recorded. Elevated predicted ozone is estimates at RFNO (~80 ppb) where an exceedance is observed (97 ppb). And high modeled values are estimated to stretch to the FCTW monitor (~75 ppb), where another ozone exceedance is observed (95 ppb).

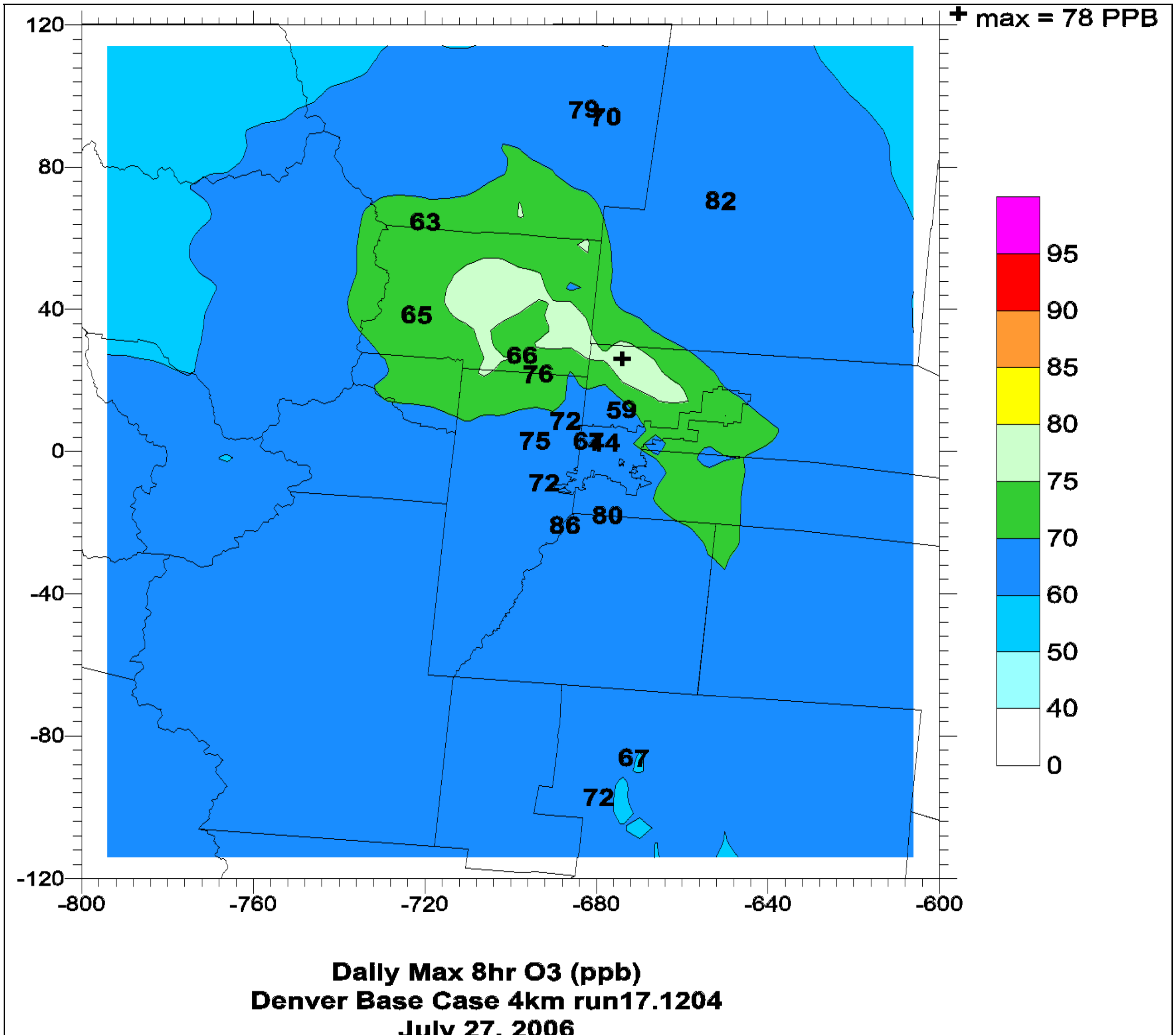


Figure 2-13a. Spatial distribution of the predicted and observed daily maximum 8-hour ozone concentrations (ppb) in the Denver area on July 27, 2006 for the final CAMx Run 17 2006 base case simulation.

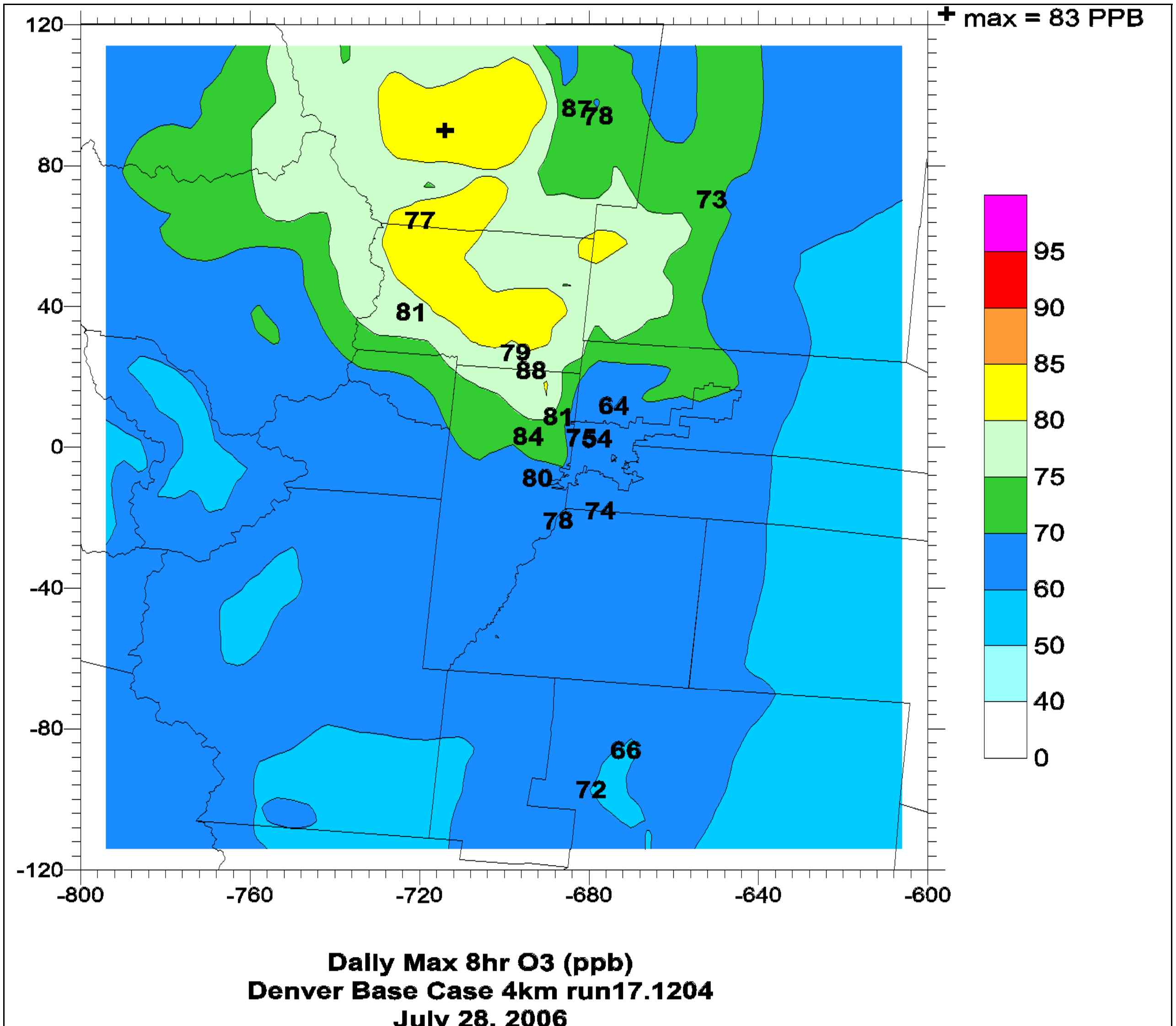


Figure 2-13b. Spatial distribution of the predicted and observed daily maximum 8-hour ozone concentrations (ppb) in the Denver area on July 28, 2006 for the final CAMx Run 17 2006 base case simulation.

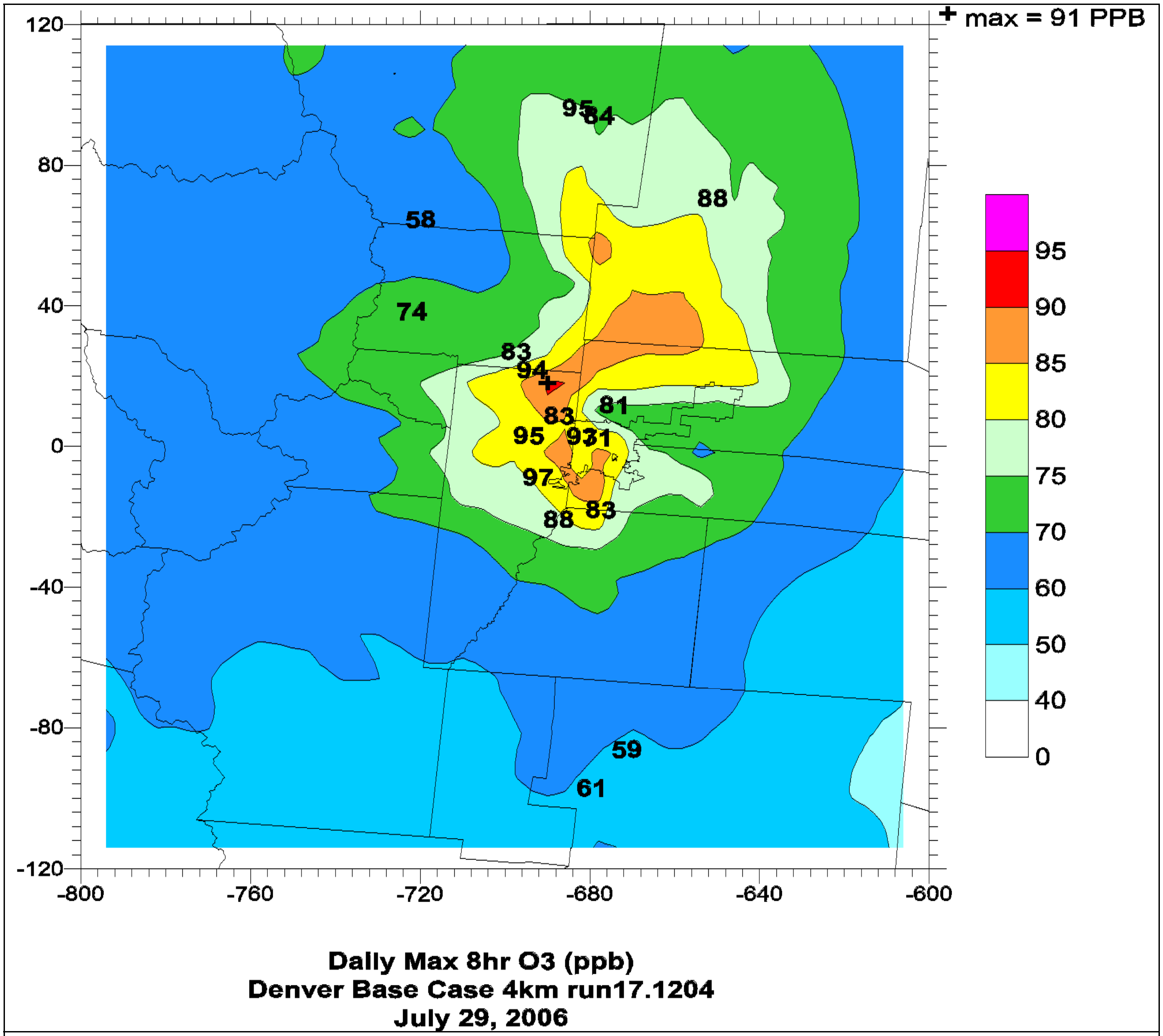


Figure 2-13c. Spatial distribution of the predicted and observed daily maximum 8-hour ozone concentrations (ppb) in the Denver area on July 29, 2006 for the final CAMx Run 17 2006 base case simulation.

Figure 2-14 displays the time series of predicted and observed hourly ozone concentrations at key sites for the July 27-29, 2006 episode. For sites to the northeast of Denver (Figure 2-14a), the ozone model performance is quite good. The model follows the observed ozone variations at the NREL and ARVA well, although the hourly ozone peaks on July 29th are underestimated a little. The observed hourly ozone at RFNO is tracked well on July 27-29, 2006, again the hourly ozone peak on July 29th is underpredicted slightly. Further northeast from Denver at the SOBC, the ozone model performance is also quite good.

At the CARR site just west of downtown Denver and WELC site to the southwest of downtown Denver, ozone model performance is also good, albeit the peaks on July 29th are underestimated (Figure 2-14b). South of Denver at the CHAT and HIGH monitoring sites the observed ozone on July 27th is underestimated, but model performance for July 28 and 29 is quite good.

At sites north of Denver (Figure 2-14c), ozone model performance is not as good as seen for the other sites with the daytime ozone peaks too low. As seen on some of the other days, the model reproduces the observed rate of ozone formation in the morning but then stalls out around noon while the observed values continue to rise.

Figure 2-15 compares the predicted and observed hourly NOx, CO and ozone time series at the CAMP and WELB sites in Denver. The model reproduces the observed NOx and CO concentrations reasonable well, but with an overprediction bias during the day at WELB. The ozone is also reproduced well at these two sites. The model fuels to reproduce the very high observed morning NOx spike on July 28th at both sites and overpredicts the CO spikes on July 29th at WELB but less so at CAMP, whether this is an emissions or mixing issue can not be discerned.

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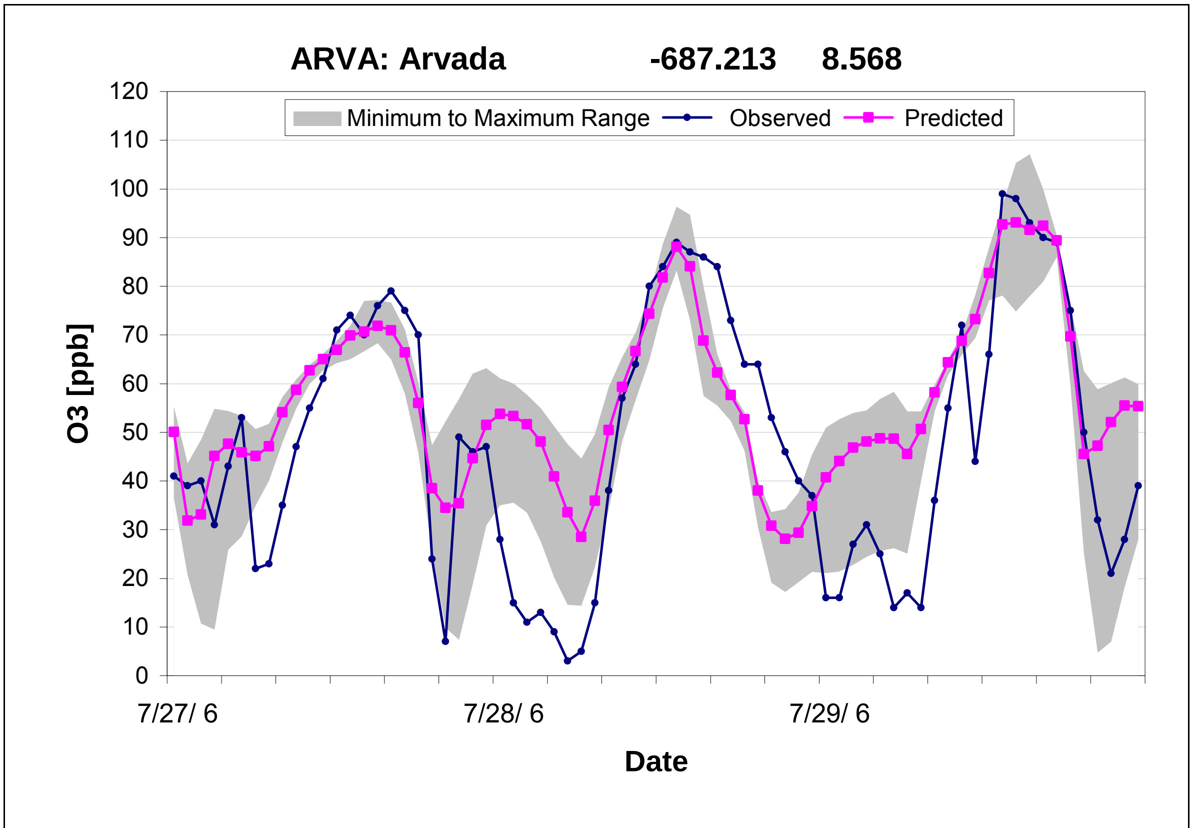
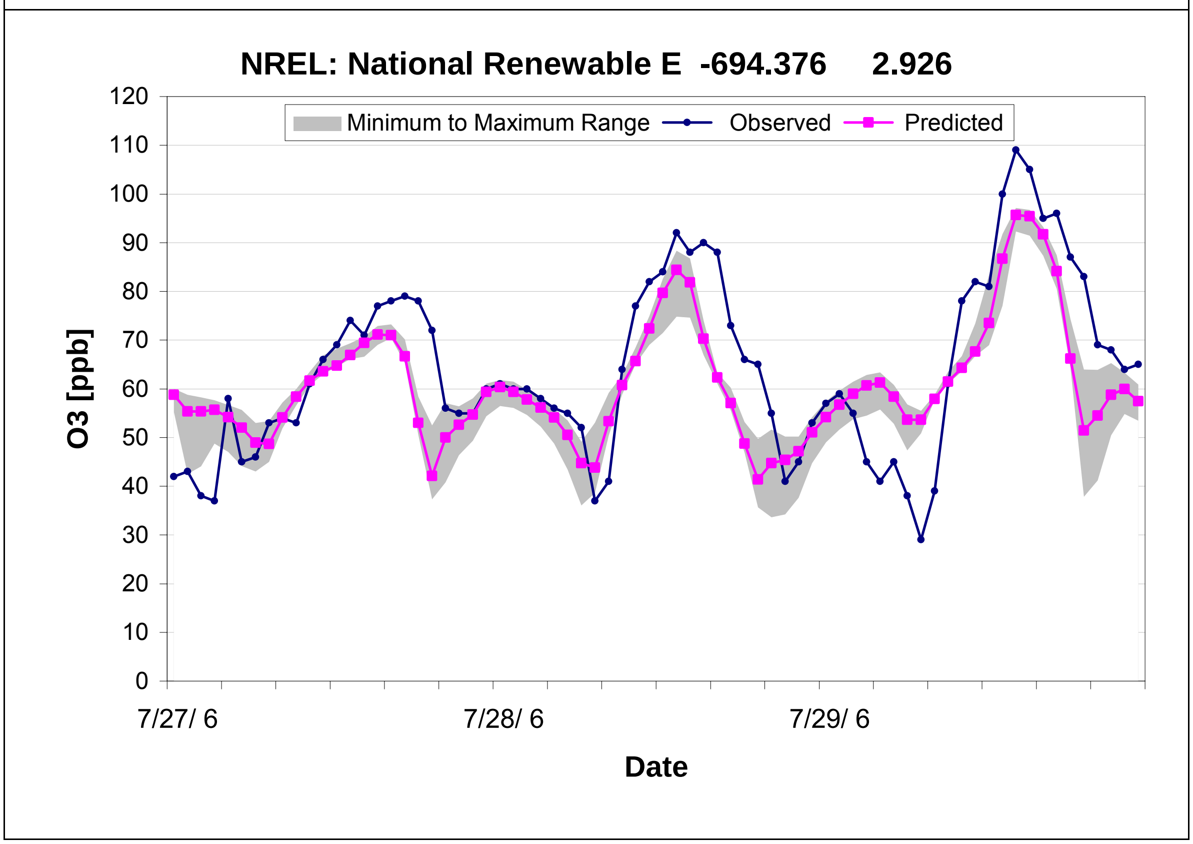
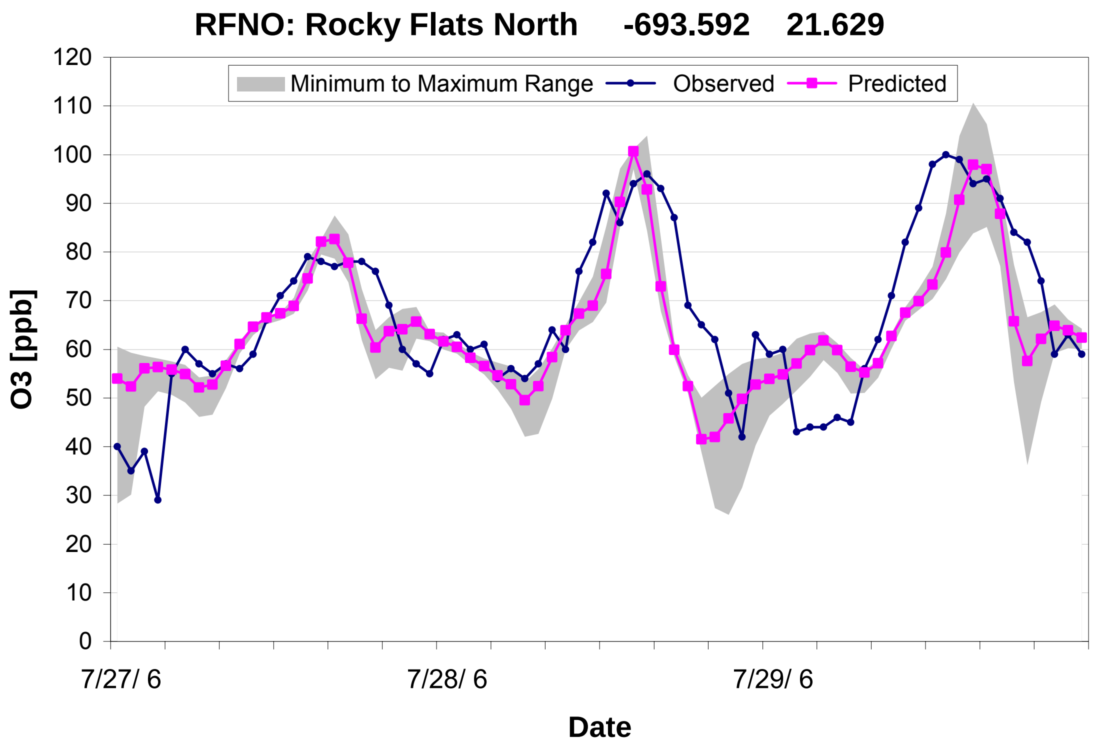

ARVA: Arvada -687.213 8.568
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
0
10
20
30
40
50
60
70
80
90
100
110
120
7/27/ 6
7/28/ 6
7/29/ 6
Date


NREL: National Renewable E -694.376 2.926
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
0
10
20
30
40
50
60
70
80
90
100
110
120
7/27/ 6
7/28/ 6
7/29/ 6
Date



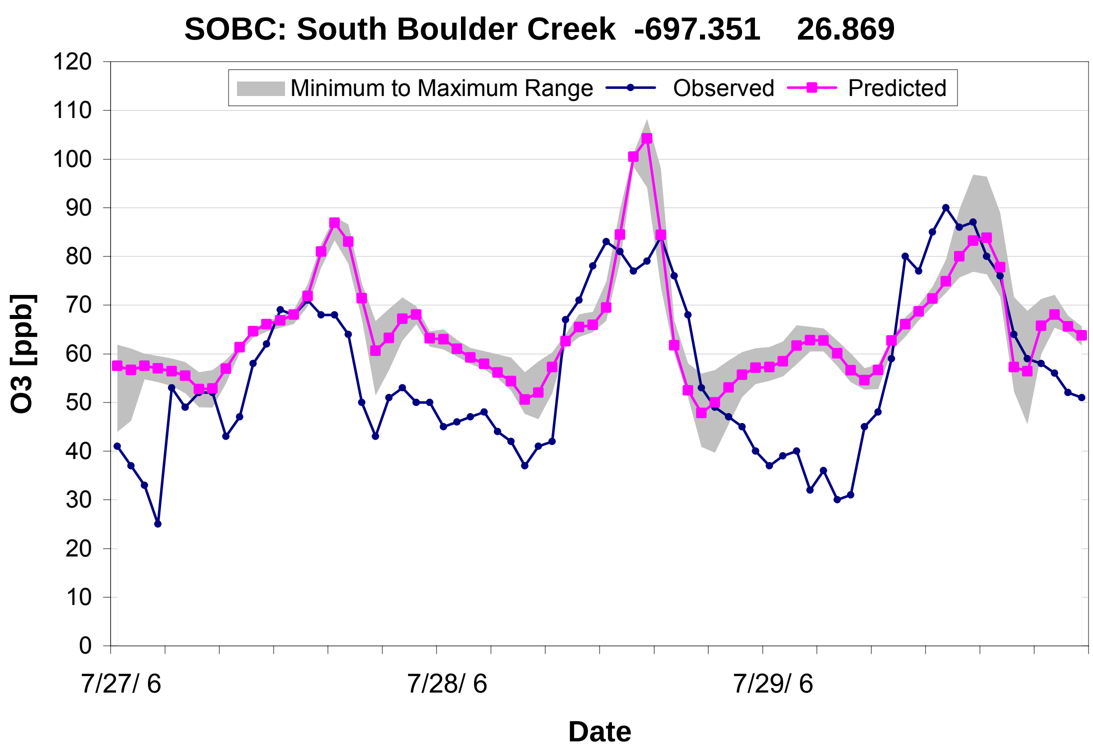
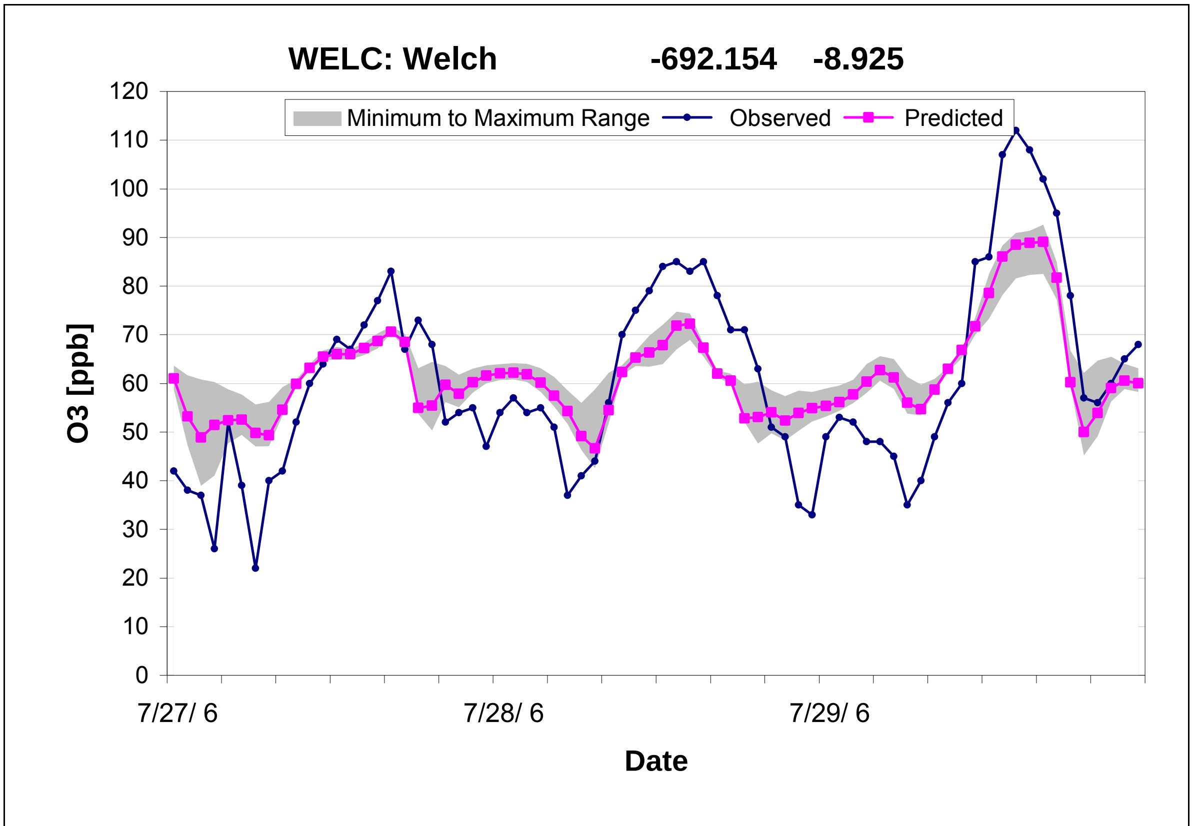
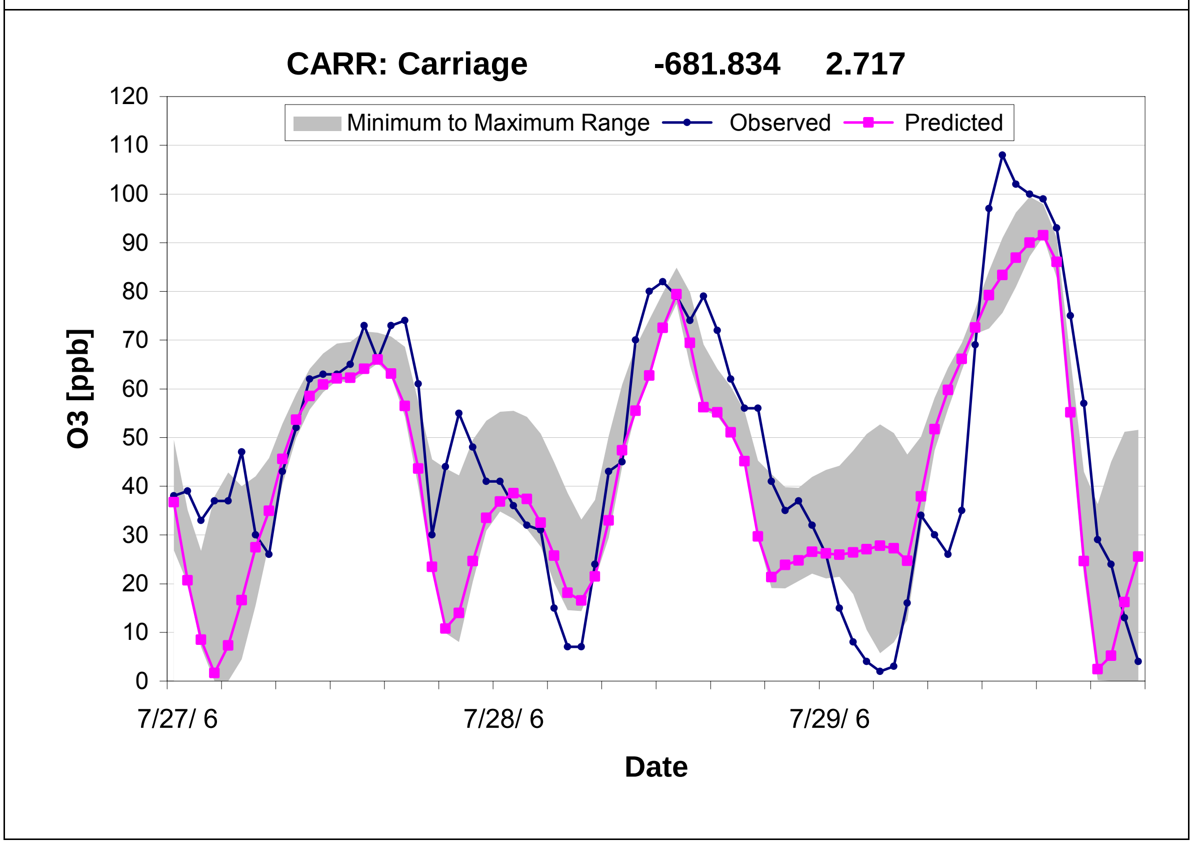
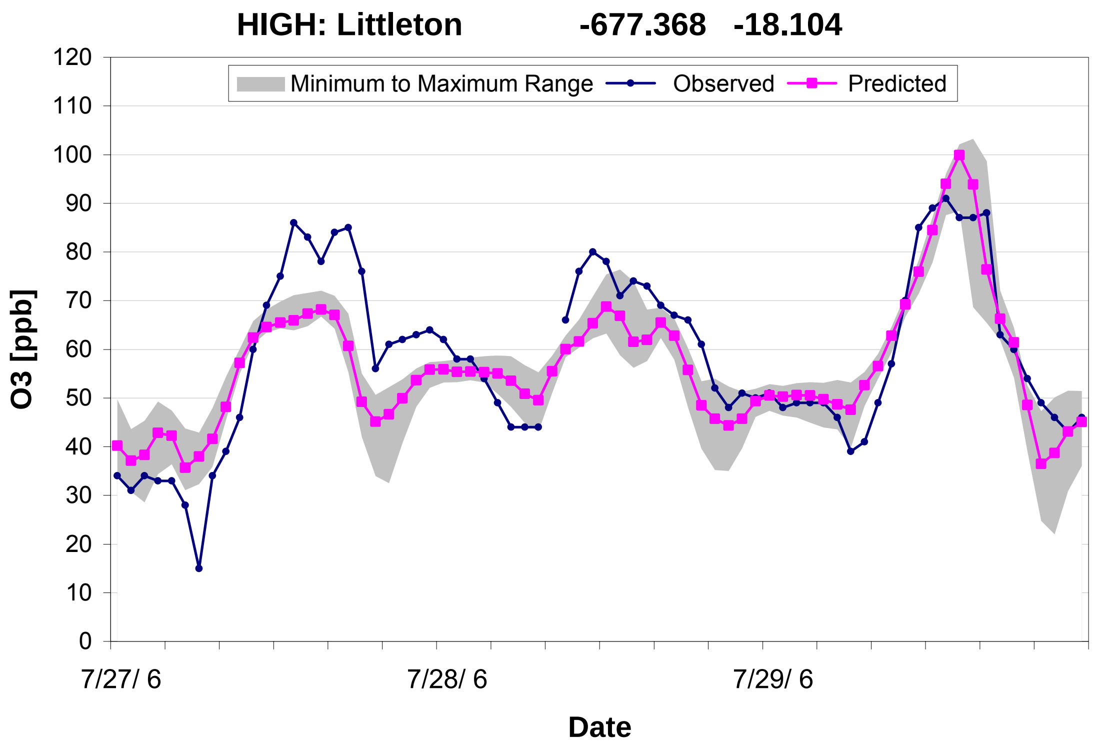


Figure 2-14a. Time series of predicted and observed hourly ozone concentrations (ppb) for the July 27-29, 2006 period, monitoring sites to the Northwest of downtown Denver and the final CAMx Run17 2006 base case simulation.


WELC: Welch -692.154 -8.925
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
120
110
100
90
80
70
60
50
40
30
20
10
0
7/27/ 6
7/28/ 6
7/29/ 6
Date


CARR: Carriage -681.834 2.717
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
120
110
100
90
80
70
60
50
40
30
20
10
0
7/27/ 6
7/28/ 6
7/29/ 6
Date



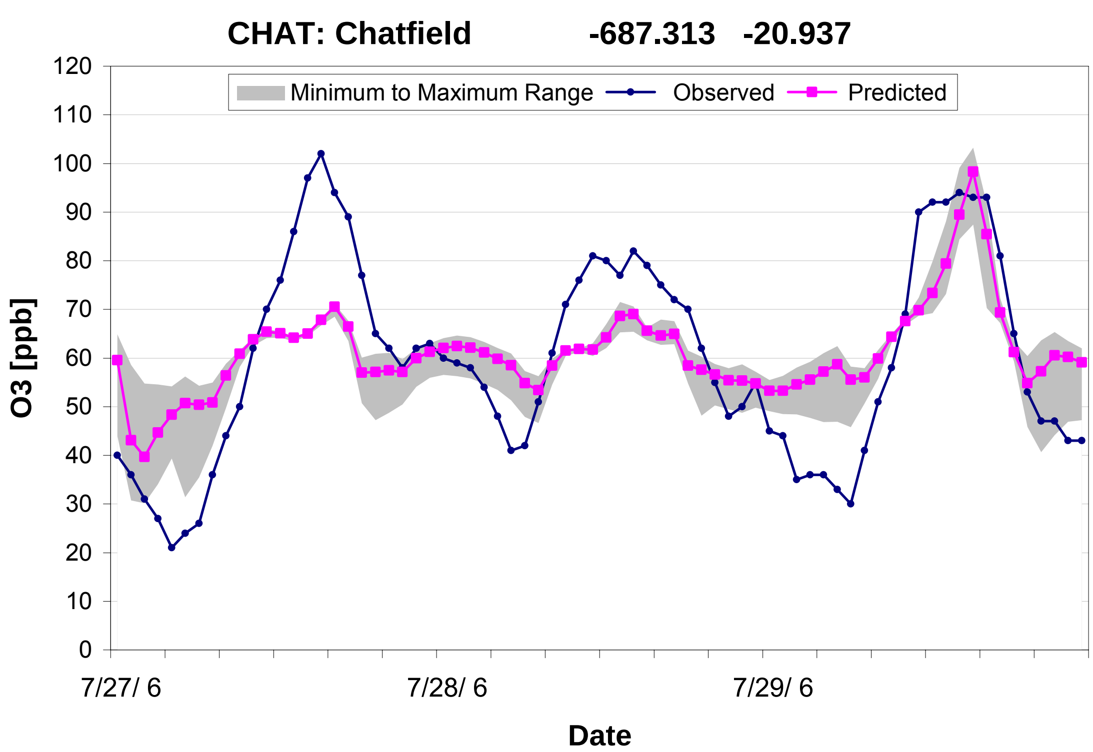
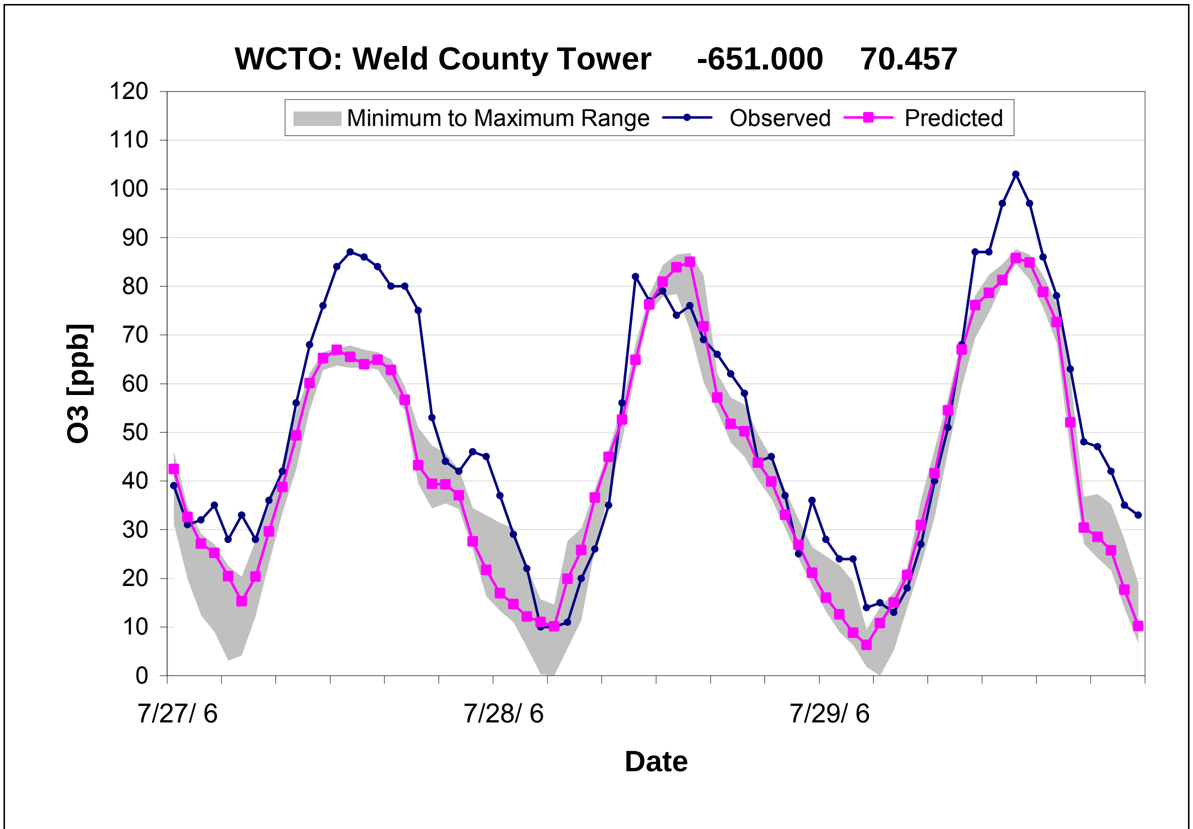
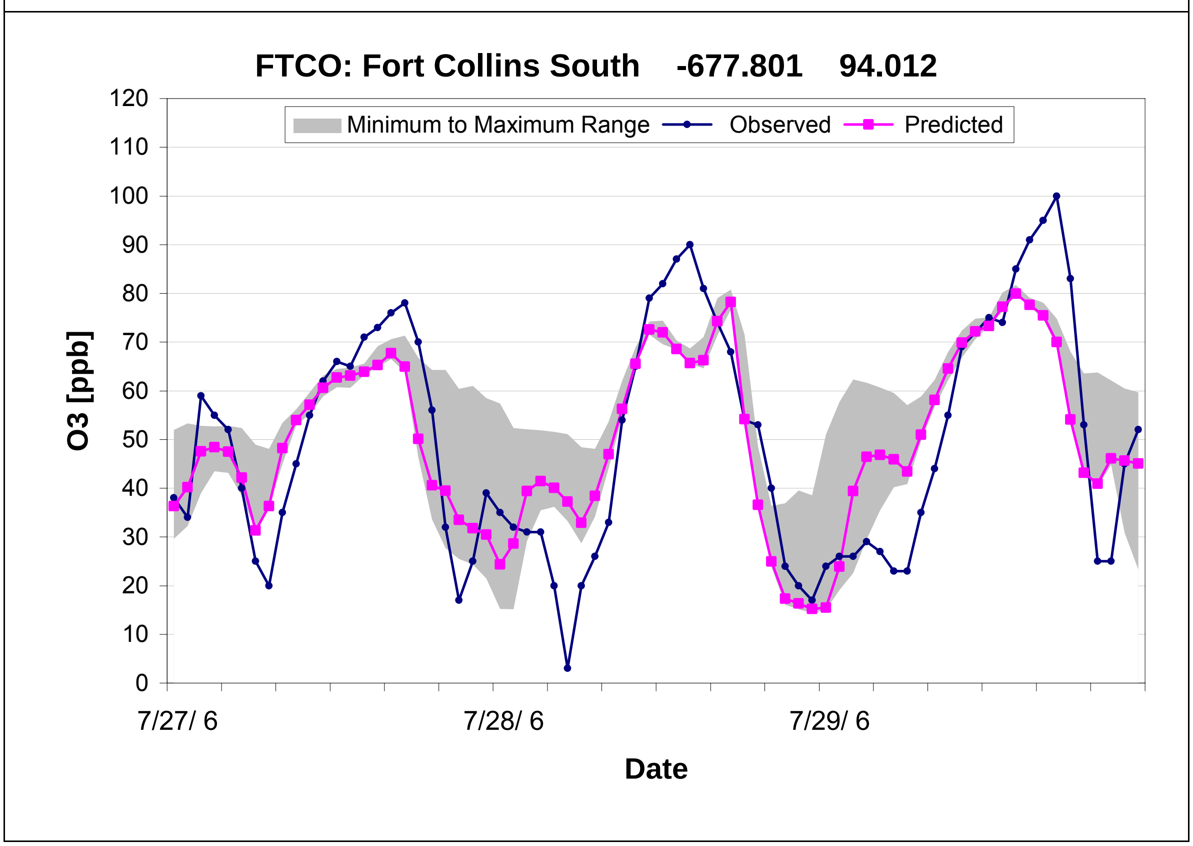


Figure 2-14b. Time series of predicted and observed hourly ozone concentrations (ppb) for the July 27-29, 2006 period, monitoring sites mostly south of downtown Denver and the final CAMx Run17 2006 base case simulation.


WCTO: Weld County Tower -651.000 70.457
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
0
10
20
30
40
50
60
70
80
90
100
110
120
7/27/ 6
7/28/ 6
7/29/ 6
Date


FTCO: Fort Collins South -677.801 94.012
Minimum to Maximum Range
Observed
Predicted
O3 [ppb]
0
10
20
30
40
50
60
70
80
90
100
110
120
7/27/ 6
7/28/ 6
7/29/ 6
Date

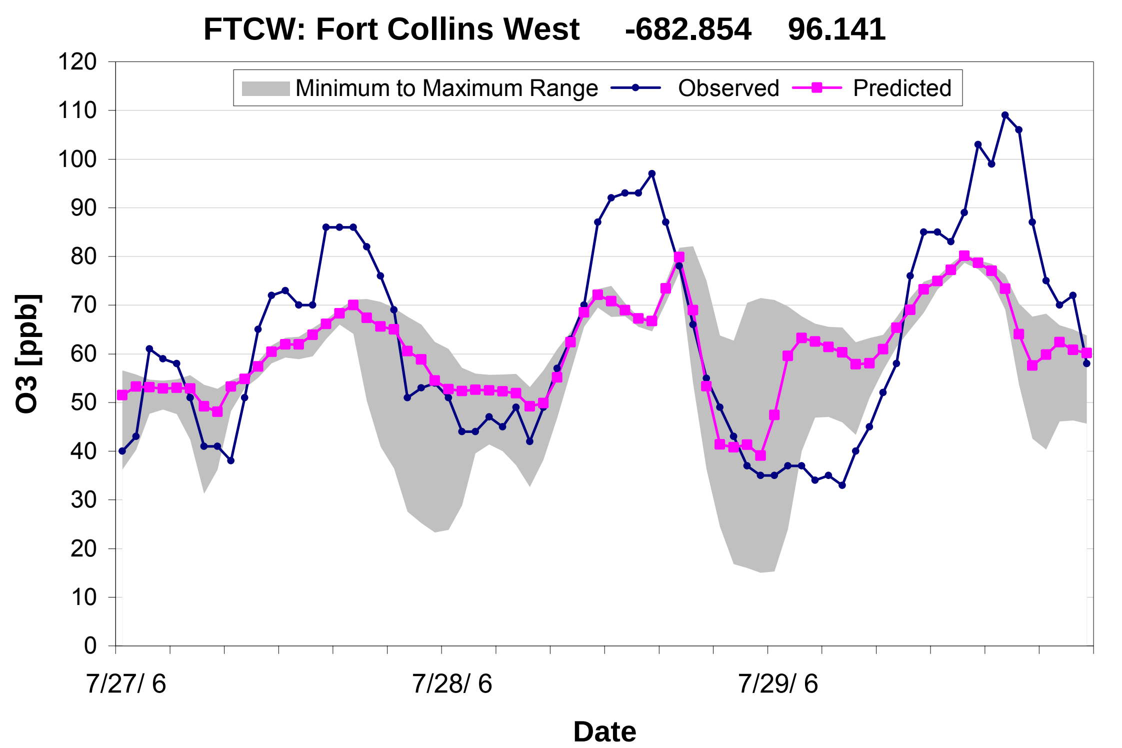


Figure 2-14c. Time series of predicted and observed hourly ozone concentrations (ppb) for the July 27-29, 2006 period, monitoring sites to the North of downtown Denver and the final CAMx Run17 2006 base case simulation.

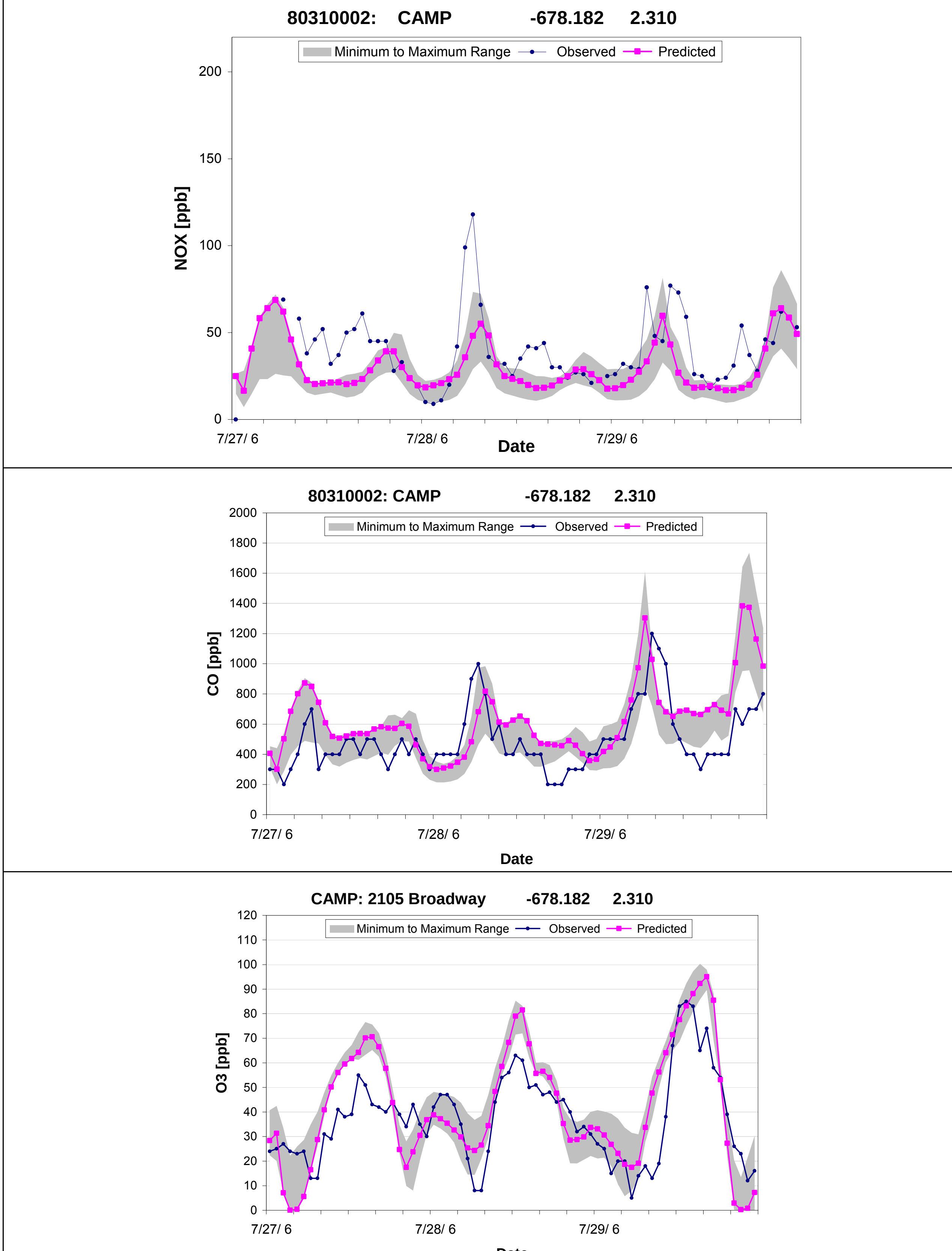
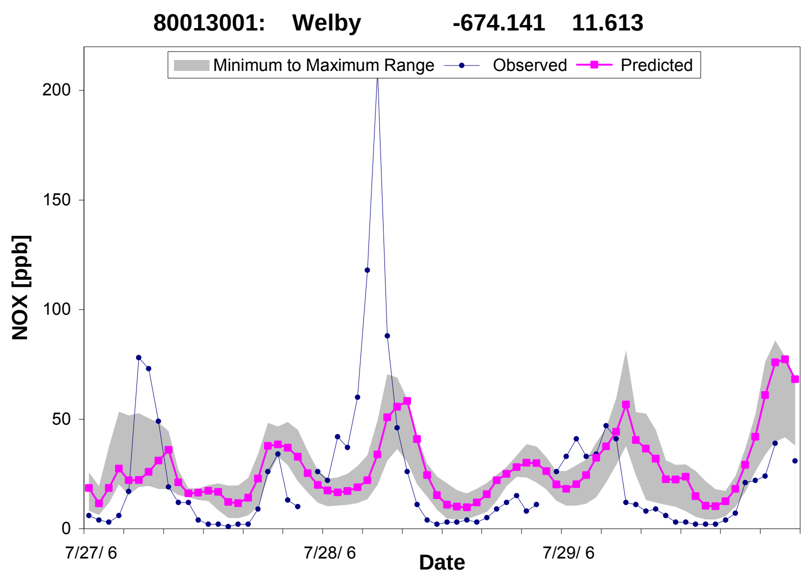
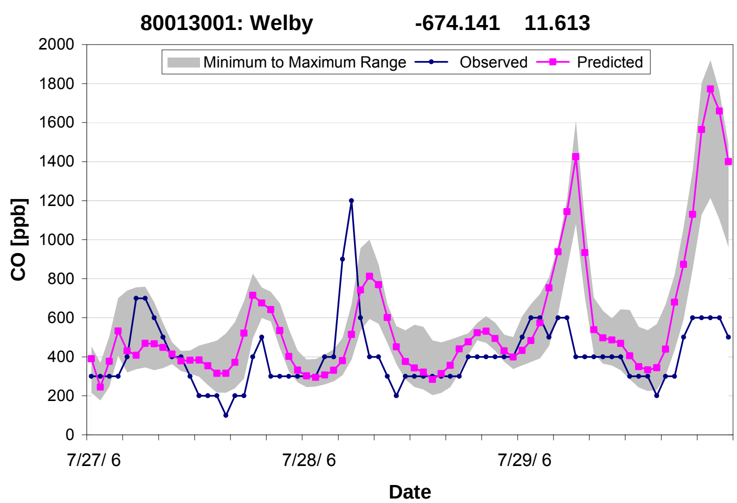


Figure 2-15a. Comparison of hourly NOx (top) and ozone (bottom) predicted and observed time series at the CAMP monitoring site for July 27-29, 2006 and the final CAMx Run17 2006 base case simulation.





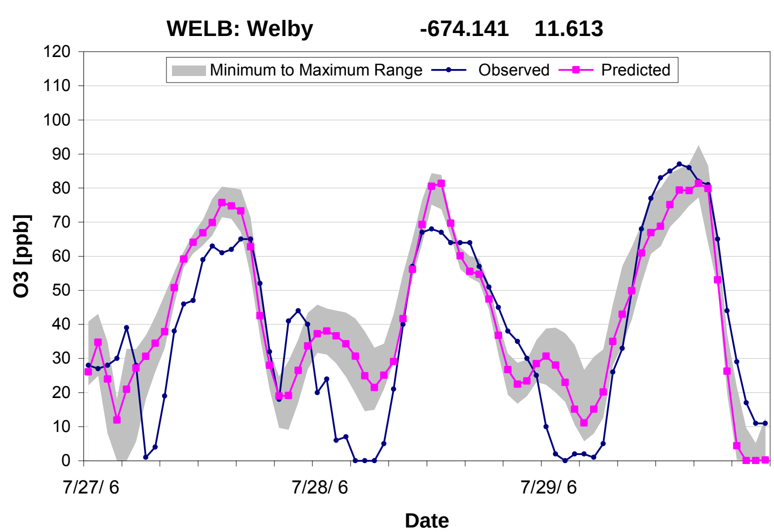


Figure 2-15b. Comparison of hourly NOx (top) and ozone (bottom) predicted and observed time series at the Welby monitoring site for July 27-29, 2006 and the final CAMx Run17 2006 base case simulation.

2.5 OZONE OPERATIONAL MODEL PERFORMANCE EVALUATION CONCLUSIONS

The ozone operational model performance evaluation of the CAMx Run 17 2006 base case simulation of the June-July 2006 period has found some days when the model reproduces the observed ozone quite well, where as others where the model does not simulate the ozone well. A vast majority of the modeling days achieve EPA's ozone model performance goals, lending some confidence that the model is performing well enough for use in making future year ozone projections. However, we should be taken that such ozone projections are not relying solely on poorly performing model days.

3.0 DIAGNOSTIC MODEL PERFORMANCE EVALUATION

3.1 INTRODUCTION

In the previous section we performed an operational model performance evaluation of the final CAMx Run 17 2006 base case simulation that addressed how well the model reproduces the surface hourly and 8-hour ozone concentrations in the Denver Metropolitan Area (DMA) (i.e., does the model get the right answer). In this section we perform a diagnostic model performance evaluation that compares the model predictions against ozone precursors, ozone aloft, key indicator species and tries to address the issue of whether the model is getting the right answer for the right reason. We also present in this section an evaluation of the base case simulation for particulate matter (PM) species. However, because the focus of the Denver June-July 2006 modeling was on ozone, very little effort was devoted to developing the PM precursor emissions inventory and no effort was made to optimize the model configuration for PM performance.

3.2 OZONE PRECURSOR MODEL PERFORMANCE

The performance for ozone precursors is examine using the routine hourly NOx and CO monitoring network in the DMA and using special study Volatile Organic Compound (VOC) grab sampling at several sites conducted by the CDPHE/APCD that occurred during portions of the June-July 2006 episode.

3.2.1 Routine Performance for Hourly NOx and CO Concentrations

Figure 3-1 displays the same daily model performance statistics for hourly NOx concentrations in the DMA as used for ozone. NOx is collected at two sites in the DMA (CAMP and WELB) and is a primary emitted pollutant. We would not expect the model to produce model performance for NOx anywhere near as good for ozone as NOx is highly influenced by subgrid-scale emissions variations that can not be captured by the model. Although the ozone model performance goals are provided in Figure 3-1, they are not expected to be achieved for NOx model performance. For example, the CAMP monitor is located at the intersection of several major downtown streets that is affected by local mobile sources, whereas the model is predicting a 4 km by 4 km average concentration. Given this, it is not surprising that the model usually underestimates the maximum hourly NOx concentrations at the monitor (top panel in Figure 3-1). Over all hours the model is exhibiting an overprediction bias in hourly NOx concentrations that is mainly due to an underprediction of the daytime low NOx concentrations at Welby shown in the previous Chapter. Because the normalized bias performance metric normalizes the difference in the predicted and observed hourly NOx concentrations by the observation, as the observed NOx concentration approaches zero it tends to blow up and become very large.

Figure 3-2 displays model performance statistics for hourly CO concentrations that are collected at 13 sites in the DMA. Again because CO is a primary emitted species that is emitted mainly by mobile sources, it can exhibit large spatially variations within short distances that is not captured by a photochemical grid model using a 4 km grid resolution. Even with these caveats, the model appears to estimate reasonable levels of CO concentrations that are similar to the observed values on average.

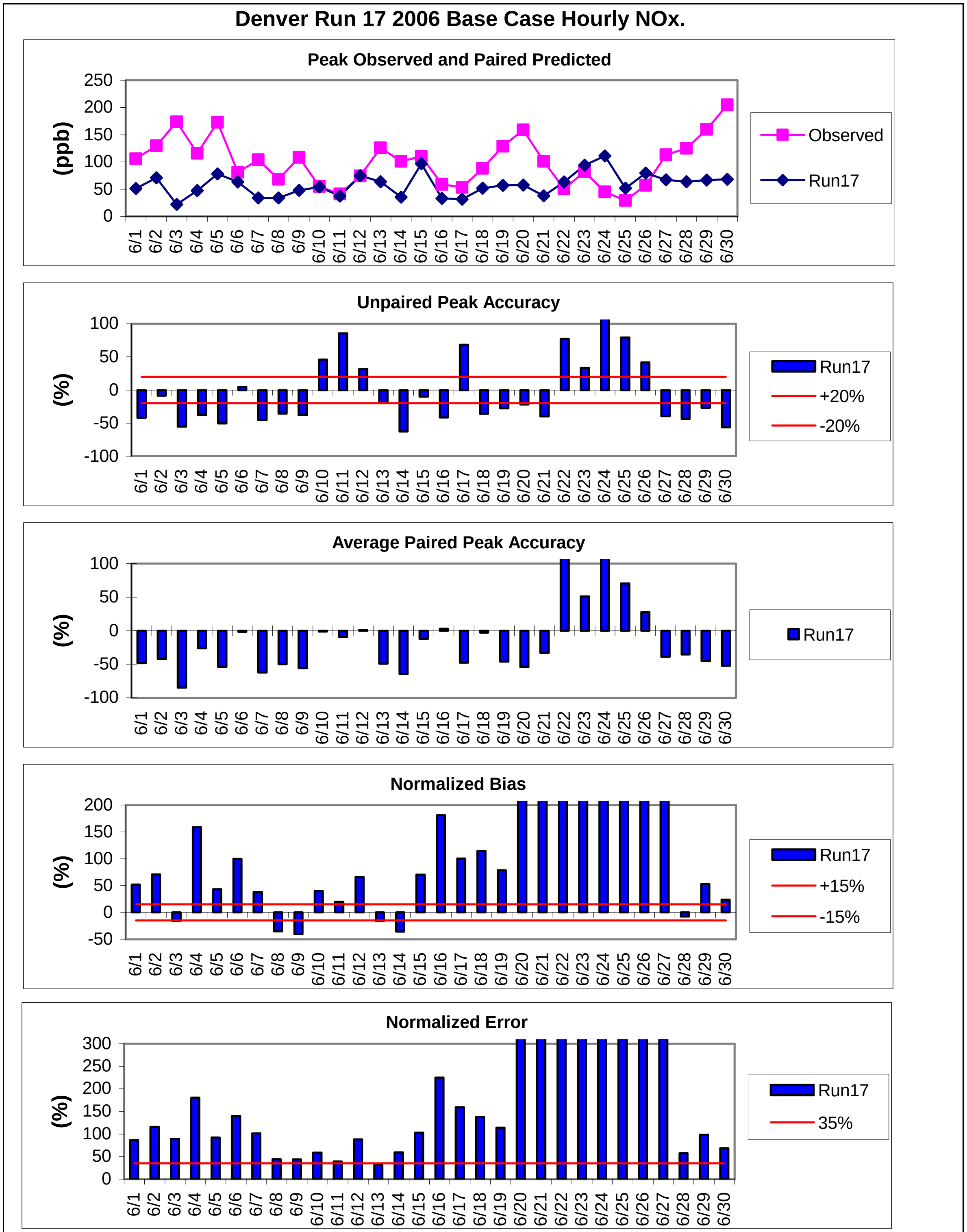


Figure 3-1a. Daily model performance statistics for June 2006, hourly NOx concentrations in the DMA (CAMP and WELB) and the final CAMX Run 17 2006 base case simulation.

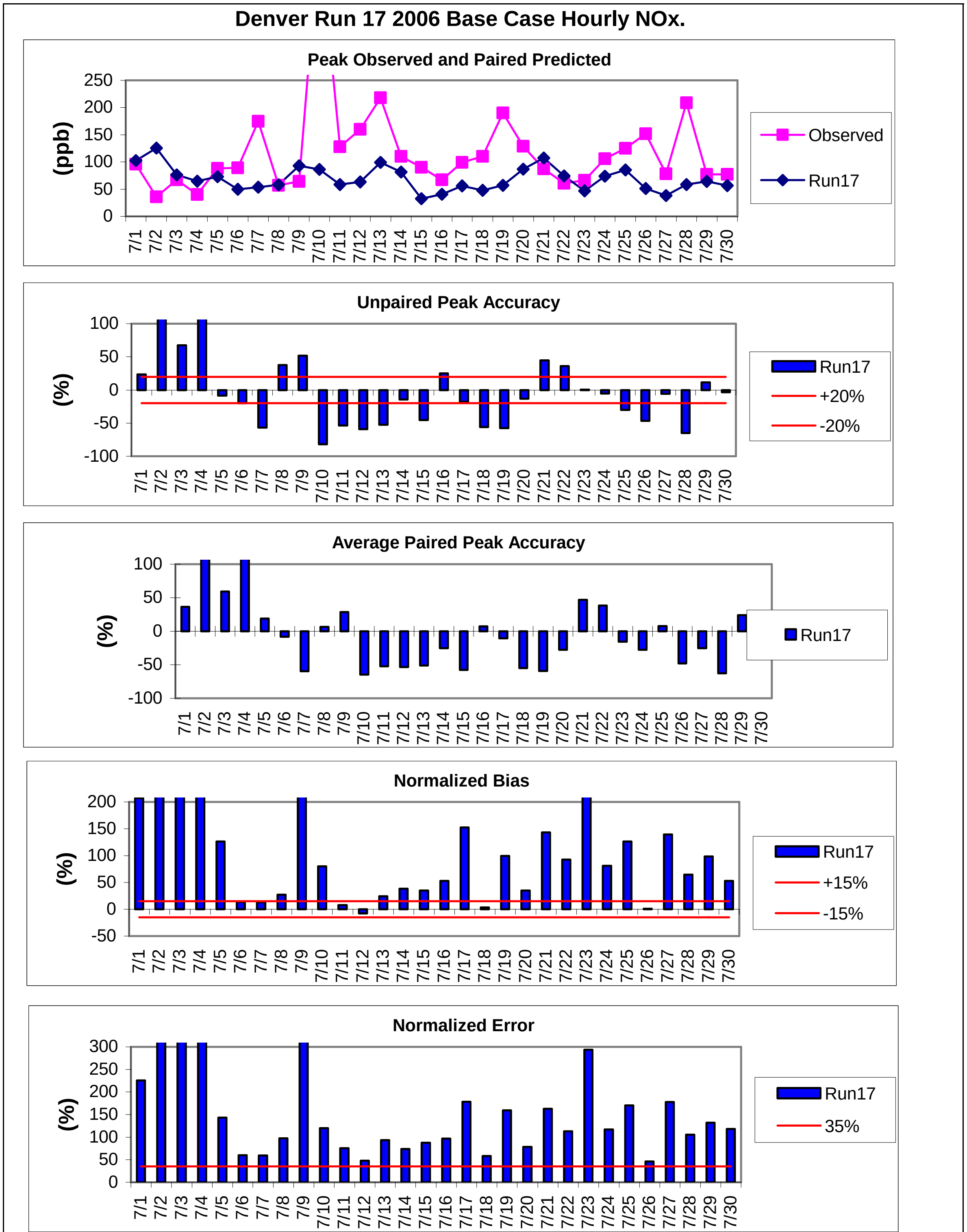


Figure 3-1b. Daily model performance statistics for July 2006, hourly NOx concentrations in the DMA (CAMP and WELB) and the final CAMX Run 17 2006 base case simulation.

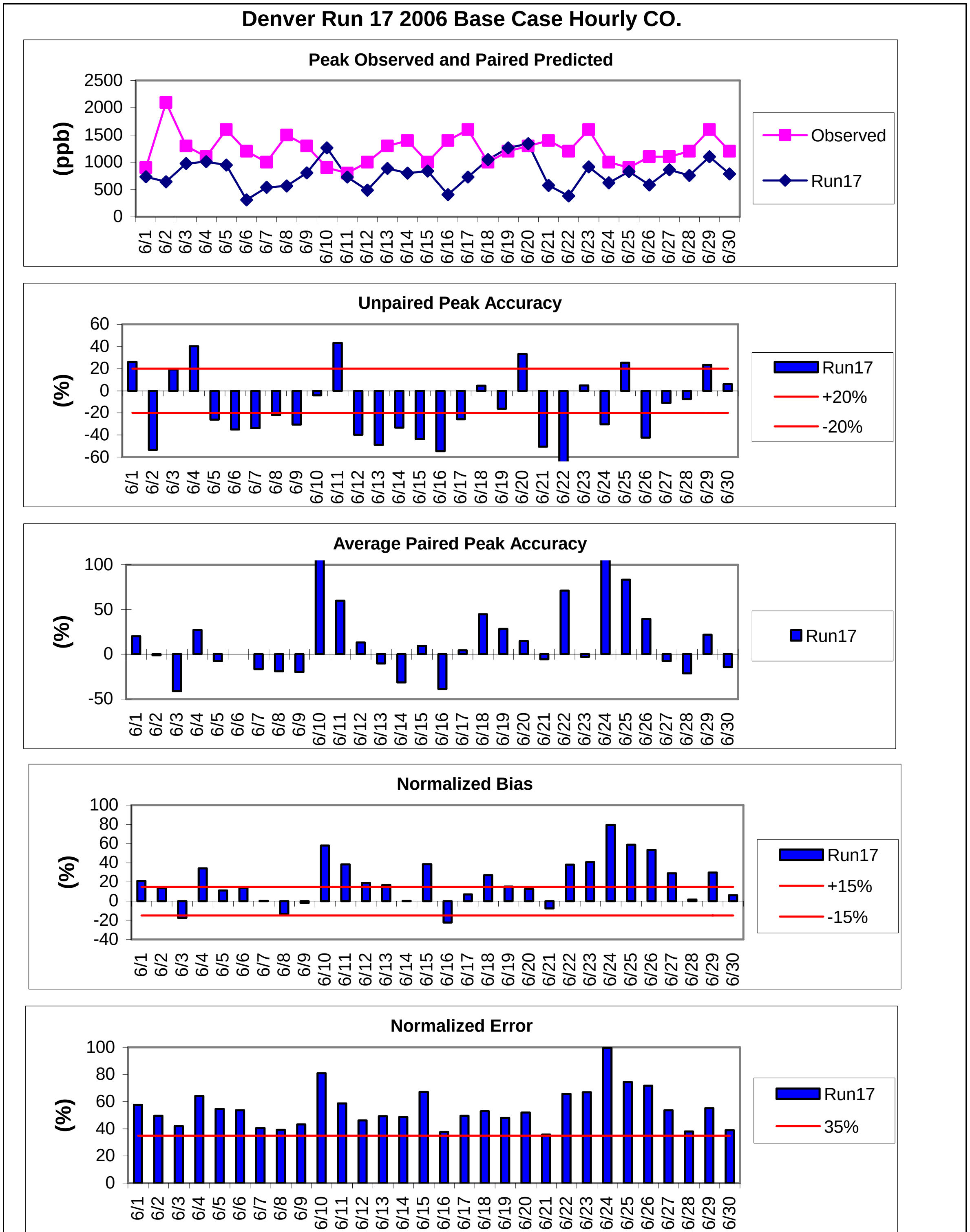


Figure 3-2a. Daily model performance statistics for June 2006, hourly CO concentrations in the DMA (13 sites) and the final CAMX Run 17 2006 base case simulation.

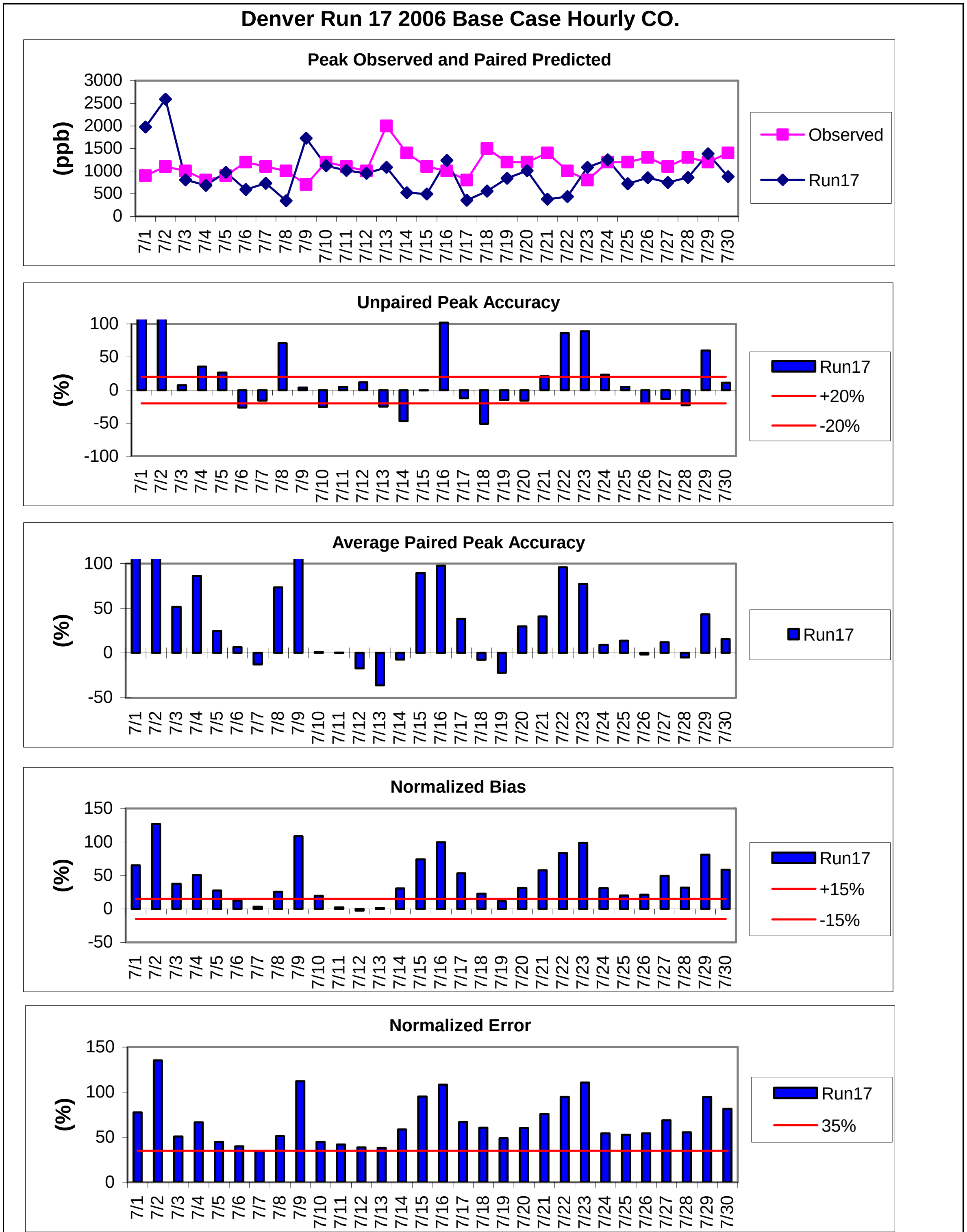


Figure 3-2b. Daily model performance statistics for July 2006, hourly CO concentrations in the DMA (13 sites) and the final CAMX Run 17 2006 base case simulation.

3.2.2 VOC and Key Indicator Model Performance

During the summer of 2006, the CDPHE/APCD collected 3-hour grab canister samples at several sites in the DMA as shown in Figure 3-3 and Table 3-1. Morning VOC samples were collected at the CAMP and Welby sites in the metropolitan Denver as well as Fort Lupton and Platteville up in Weld County. Afternoon VOC samples were collected at the Rocky Flats North and Fort Collins West high ozone (downwind) monitors. The VOC samples at the two Denver sites (CAMP and WELB) will provide an evaluation of the model's on-road mobile source emissions inventory, whereas the morning samples at the two Weld County sites will provide an evaluation of the oil and gas VOC emissions inventory that dominates the VOC inventory in Weld County.

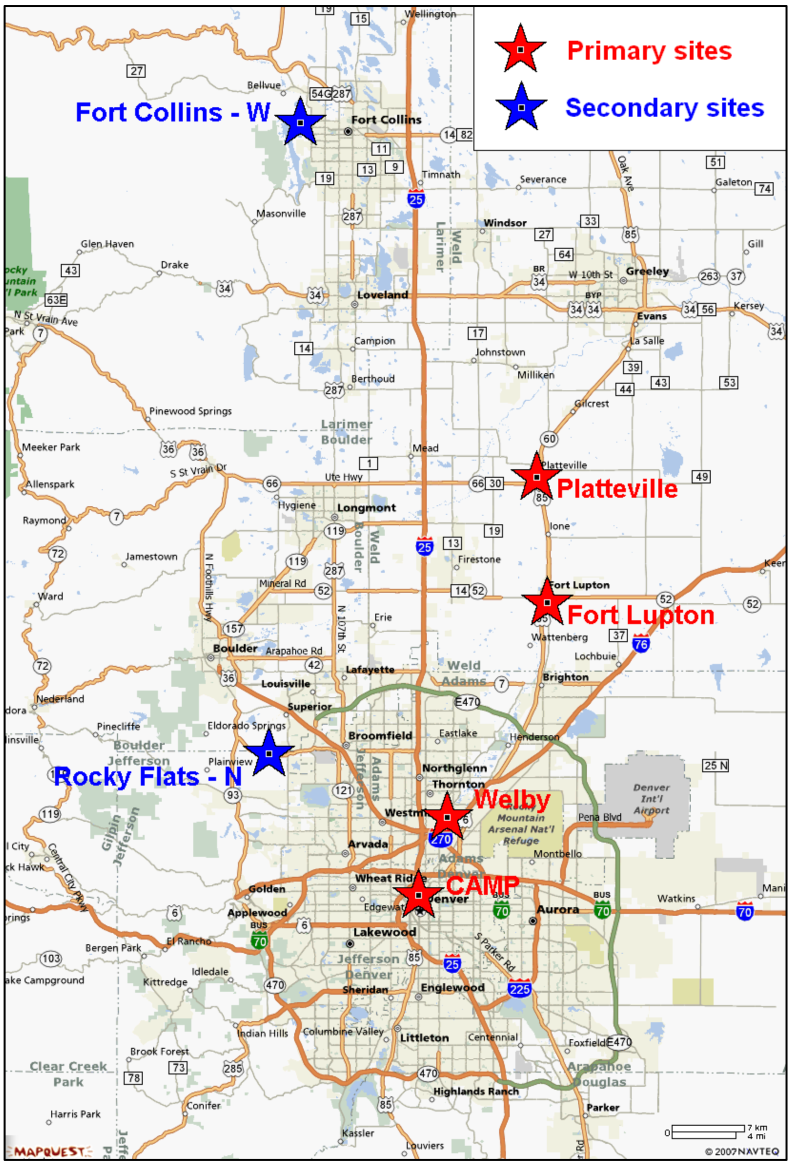


Figure 3-3. Locations of monitoring sites where VOC samples were collected during the summer of 2006.

Table 3-1a. Locations of monitoring sites where VOC samples were collected during the summer of 2006.

2006 Ozone Precursor Monitoring Sites					
AQS #	**Site Name**	**Address**	**Latitude**	**Longitude**	**Elevation**
08-001-3001	Welby	3174 E. 78th Ave., Denver, 80229	39 50 21	104 56 56	1550 m
08-031-0002	CAMP	2105 Broadway, Denver, 80205	39 45 04	104 59 14	1591 m
08-123-0008	Platteville	1004 Main St., Platteville, 80651	40 12 40	104 49 25	1476 m
08-123-0011	Fort Lupton	Kahil St. & Fulton Ave., Fort Lupton, 80621	40 04 28	104 48 53	1498 m
08-059-0006	Rocky Flats - N	16600 W. Highway 128, Broomfield, 80021	39 54 46	105 11 18	1796 m
08-069-0011	Fort Collins - West	3416 W. LaPorte Ave., Fort Collins, 80525	40 35 32	105 08 27	1575 m

Table 3-1b. Sampling schedule and times for summer of 2006 VOC sampling study in the DMA.

2006 Ozone Precursor Monitoring Sites			
AQS #	**Site Name**	**Sample Period**	**Time Period**
08-001-3001	Welby	16 June – 31 July 2006, every 3rd day	A.M. --- 06:00 – 09:00 (MDT)
08-031-0002	CAMP	16 June – 31 July 2006, every 3rd day	A.M. --- 06:00 – 09:00 (MDT)
08-123-0008	Platteville	16 June – 31 July 2006, every 3rd day	A.M. --- 06:00 – 09:00 (MDT)
08-123-0011	Fort Lupton	16 June – 31 July 2006, every 3rd day	A.M. --- 06:00 – 09:00 (MDT)
08-059-0006	Rocky Flats - N	28 June – 13 July 2006, on-call basis	P.M. --- 13:00 – 16:00 (MDT)
08-069-0011	Fort Collins - West	19 July – 28 July 2006, on-call basis	P.M. --- 13:00 – 16:00 (MDT)

These VOC canister samples were speciated to obtain individual VOC species concentrations along with total nonmethane hydrocarbon (TNMHC) concentrations that were compared against the model results to determine how well the model predicted total VOC concentrations, concentrations of individual VOC species as well as predicting the key VOC/NOx indicator species ratios. However, before the measured VOC concentrations could be compared against the modeled values the following activities had to be performed:

- Time shift of the measured data to the MST time zone being used in the modeling;
- Adjustment of the VOC species to account for concentrations below the minimum detection level (MDL) whereby a fairly standard practice of setting VOC species concentrations that are below diction to half of the MDL; and
- Speciated the VOC speciation samples to the CB05 VOC species used in the modeling.

The speciation of the VOC samples into the CB05 species was performed by the research group at Colorado University under the direction of Dr. Jana Milford whose assistance was greatly appreciated.

The conversions of the measured VOC species concentrations to the CB05 species was necessary in order to obtain an “apples-to-apples” comparison of VOC species and total VOC between the model predictions and observations. The raw VOC measurements can not be directly compared with the modeled VOC concentrations. There are portions of several VOC species that are considered nonreactive (NR) in the CB05 VOC classification system so are dropped in the model VOC species. In addition, the VOC sampling did not speciate their samples for methanol (MeOH) and ethanol (EtOH) that are two species in the CB05 chemical mechanism so those two species were dropped from the comparison. In addition, ethane (ETHA) is an explicit species in CB05 but is considered nonreactive by EPA's reactivity classification scheme so is not included in the definition of "total VOC" used in this evaluation. However, the model performance for ethane is evaluated separately. Thus, the total VOC comparisons presented below will not include all VOC compounds, but they will include consistent compounds between the observations and model predictions so are an appropriate comparison from a model performance evaluation perspective. However, when looking at the VOC/NOx ratios and trying to interpret results in terms of whether ozone formation is more VOC-limited or NOx-limited the user should be aware that not all VOC compounds are present in the "total VOC" concentrations used in the model performance evaluation.

3.2.2.1 VOC Performance in Denver Urban Area

VOC samples were collected at the CAMP and Welby monitoring sites that are located within the heart of the DMA. VOC, NOx and CO concentrations at these two urban sites will be dominated by on-road mobile sources. Consequently, the model performance at these two sites will help assess the accuracy of the on-road mobile source emissions inventory. As noted above, there are a lot of local- and microscale effects (e.g., streets) that result in high spatial variability in the observed VOC, NOx and CO concentrations that can not be captured by the model predictions that are averaged across a 4 km by 4 km grid cell with a layer 1 top of approximately 36 m AGL. Thus, in evaluating model performance for ozone precursors at these sites, more emphasis is placed on the performance for VOC/NOx and CO/NOx ratios then for VOC, NOx and CO concentrations. Since VOC, NOx and CO are all dominated by on-road mobile sources at these two sites, the subgrid-scale effects on the three pollutants should be very similar. Given that there is more confidence in the on-road mobile source NOx emissions than the VOC and CO emissions, then an evaluation of the model at these sites for VOC/NOx and CO/NOx ratios provides a good indication of the accuracy of the on-road mobile source VOC and CO emissions. The performance for VOC/NOx ratios will also provide an indication of whether the model is predicting the correct chemical regimes and will predict ozone responses to changes in VOC and NOx emissions in the correct fashion (i.e., getting the right answer for the right reason).

Figure 3-4a compares the predicted and observed morning 3-hour average VOC, NOx and CO concentrations at the CAMP monitor. Although there are a few outliers, in general the observed VOC concentrations are approximately 200 ppbC that is approximately a factor of two higher than the modeled values (~100 ppbC). Similarly, the observed NOx concentrations are approximately 100 ppb that are approximately a factor of 2 higher than predicted (~50 ppb). With one exception, the observed VOC and NOx concentrations are always the same or higher than the predicted values. The exception is on July 4, 2006 when the observed value is 10 ppb that is twice as low is the next lowest NOx observation and an order of magnitude lower than the average observed NOx concentrations at this site. July 4 has very unusual and atypical traffic patterns and it is not surprising that it is an outlier compared to the other days. On-road mobile source emissions representative of a Sunday were used for July 4, but that likely did not fully capture the unusual and atypical traffic patterns for this holiday day.

Of the 15 days with morning samples at the CAMP monitor, there is excellent agreement with the predicted and observed VOC/NOx ratios for 11 of the 15 days (73% of the days; Figure 3-4b, top). On the four days when there is not excellent agreement with the predicted and observed VOC/NOx ratios at the CAMP monitor, one is the July 4th outlier day discussed previously. On July 22, 2006 (a Saturday) the model predicts a 2.5 VOC/NOx ratio when an 8.3 ratio was observed. Whereas on June 25 (a Sunday) and July 22 (a Thursday) VOC/NOx ratios of 5.9 and 5.1 were observed with modeled values of 3.8 and 3.2, respectively.

The model is generally overpredicting the observed morning CO/NOx ratio at the CAMP monitor (Figure 3-4b, middle). With a few exceptions, this overprediction is not large, but is systematic and may indicate an overrestimation of the on-road mobile source CO emissions.

With the exception of July 19, 2006, observed morning ethane (ETHA) concentrations at the CAMP monitoring are underpredicted by a large amount at the CAMP monitor with average observed values near 25 ppbC and average modeled values an order magnitude lower (~2.5 ppbC). This is undoubtedly partly due to EPA's classification of ethane as a nonreactive VOC species so it is not included in a standard VOC emissions inventory. Although ethane was included in the WRAP Phase III oil and gas emissions inventory for the Denver-Julesburg Basin, it is likely missing for some sources in the DMA so it is not surprising that it is underestimated by the model. Since ethane has very low reactivity this should not adversely affect ozone formation, model performance or response to controls, but it certainly affects ethane model performance.

The comparison of VOC, NOx and CO concentrations and VOC/NOx and CO/NOx ratios at the Welby monitor are shown in Figure 3-5. As noted in Chapter 2, there appear to be more issues with subgrid-scale variability at the Welby monitor then at CAMP. There is also more missing data at Welby so there are less VOC/NOx and CO/NOx ratio comparisons. Results at Welby are similar to CAMP with the model underestimating VOC and NOx concentrations, but generally predicting the same magnitude of CO concentrations as observed (Figure 3-5a). Although there is good agreement with the modeled and observed VOC/NOx ratios on some days (June 19 and July 7, 10 and 16) the model underpredicts the observed VOC/NOx ratio on June 16 and 22 and July 1 and 4.

Table 3-2 summarizes the predicted and observed morning VOC/NOx ratio comparisons at the CAMP monitoring site in downtown Denver that also includes the day of week. As noted above, for most days these comparisons are very good, which is likely due to the extra effort invested in the Denver modeling of on-road mobile sources using the CONCEPT emissions model. Both the observed and predicted VOC/NOx ratios are higher on the weekend days, with Sunday being higher than Saturday, and lower on weekdays. The model underestimates the observed VOC/NOx ratio on Sunday June 25 by -25%, but agrees quite well on Sunday July 16. Similar results are seen for the two Saturday comparisons with good agreement on July 1 (+13%) and an underprediction bias on July 22 (-38%). Thus, the model appears to be capturing much of the weekend effect on mobile sources, but may not be capturing the full effect on all days. However, with just four days of weekend comparisons it is hard to draw firm conclusions.

Table 3-2. Comparison of predicted and observed morning CB05-VOC/NOx ratios at the downtown Denver CAMP monitoring site.

		VOC/NOx Ratios		
Date	**Day of Week**	**Observed**	**Predicted**	**Percent Difference**
June 16	Fri	3.31	2.56	-22%
June 19	Mon	1.58	2.18	+38%
June 22	Thurs	8.30	2.52	-70%
June 25	Sun	5.85	3.81	-35%
June 28	Wed	2.27	2.01	+13%
July 1	Sat	3.04	3.42	+13%
July 4	Holiday	17.74	2.18	-88%
July 7	Fri	2.57	2.21	+36%
July 10	Mon	2.07	2.82	+36%
July 13	Thurs	2.42	2.39	-1%
July 16	Sun	3.68	3.81	+3%
July 19	Wed	1.64	2.39	+46%
July 22	Sat	5.13	3.17	-38%
July 25	Tue	2.60	2.20	-15%
July 28	Fri	2.00	2.50	+25%

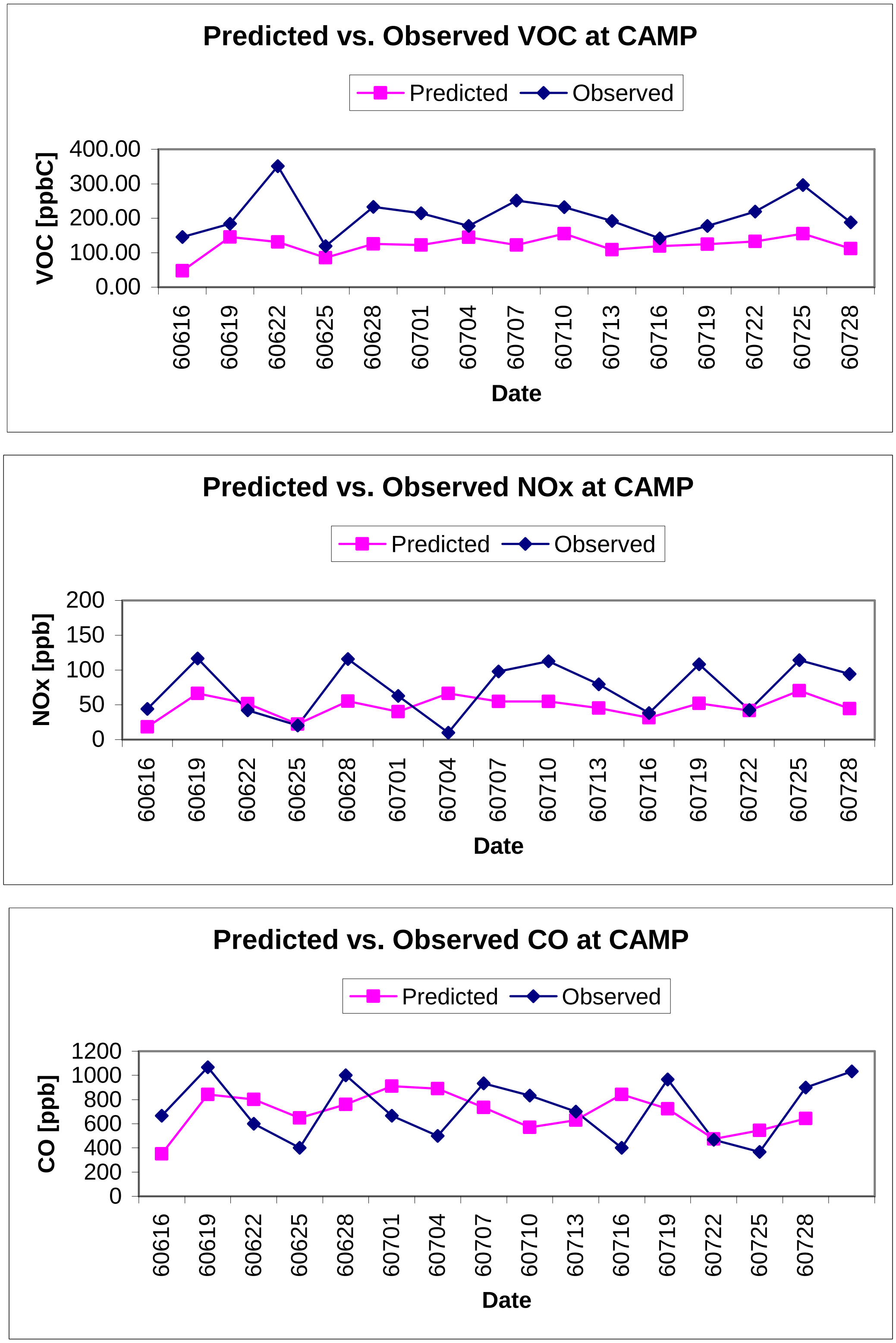
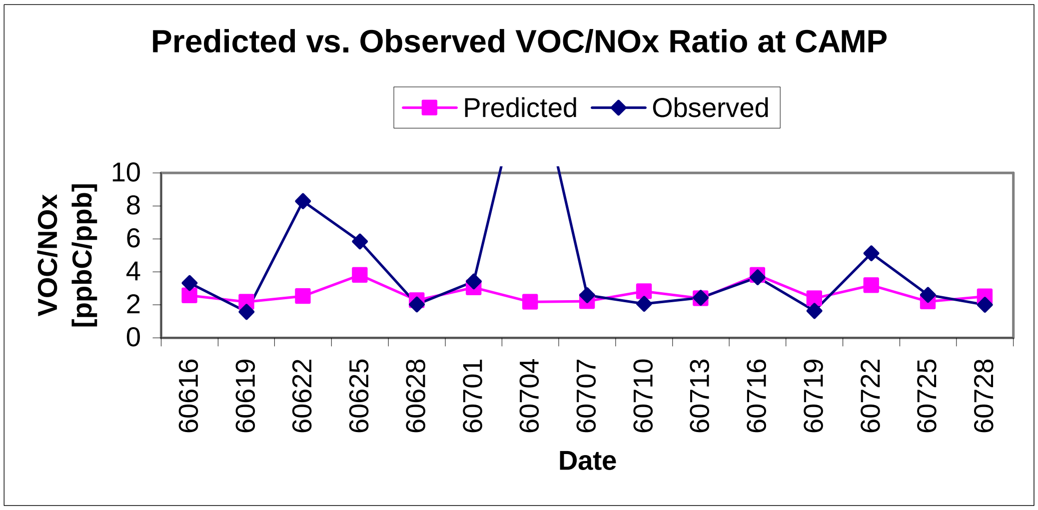
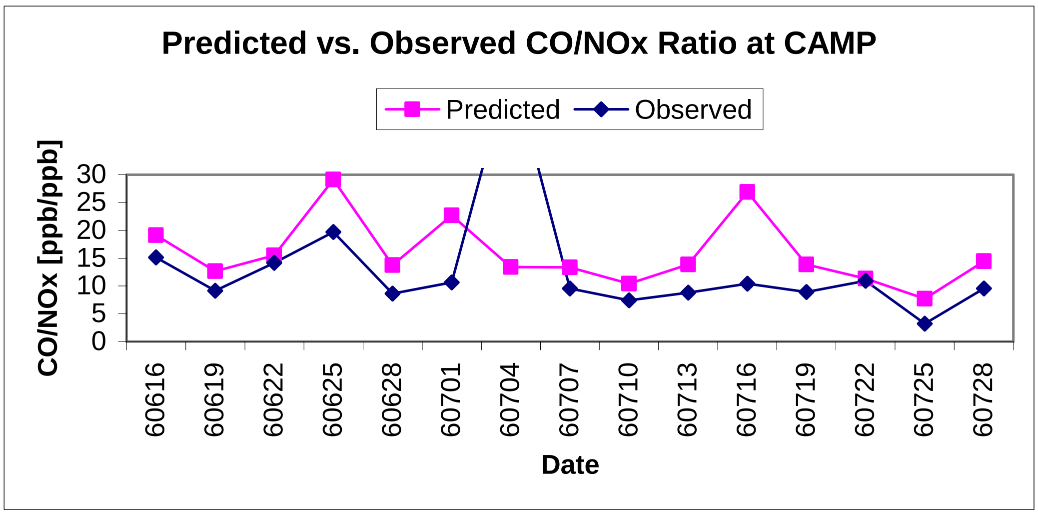


Figure 3-4a. Comparison of predicted and observed 3-hour average morning (5-8am MST) CB05-VOC, NOx and CO concentrations at the CAMP monitor for the CAMx Run 17 2006 base case simulation.





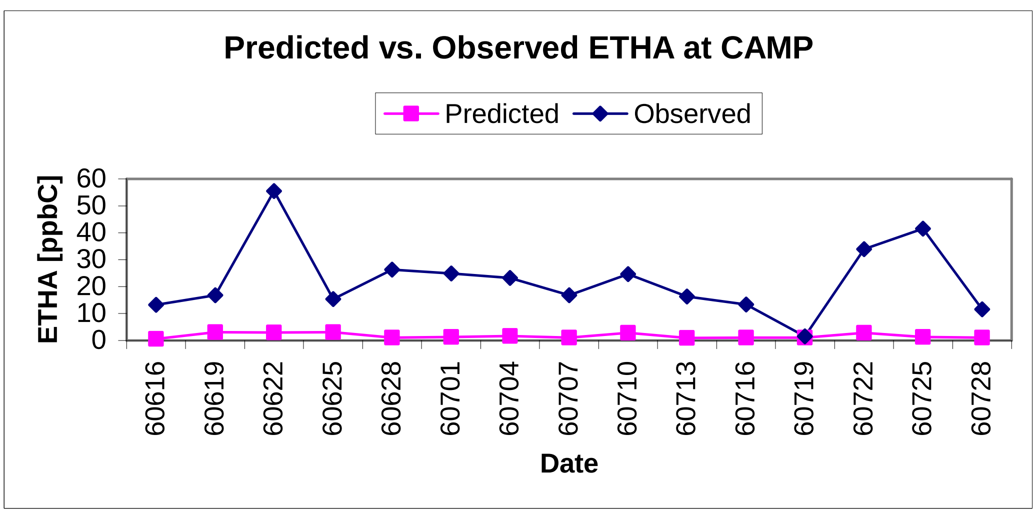


Figure 3-4b. Comparison of predicted and observed 3-hour average morning (5-8am MST) CB05-VOC/NOx and CO/NOx ratio and ethane (ETHA) concentrations at the CAMP monitor for the CAMx Run 17 2006 base case simulation.

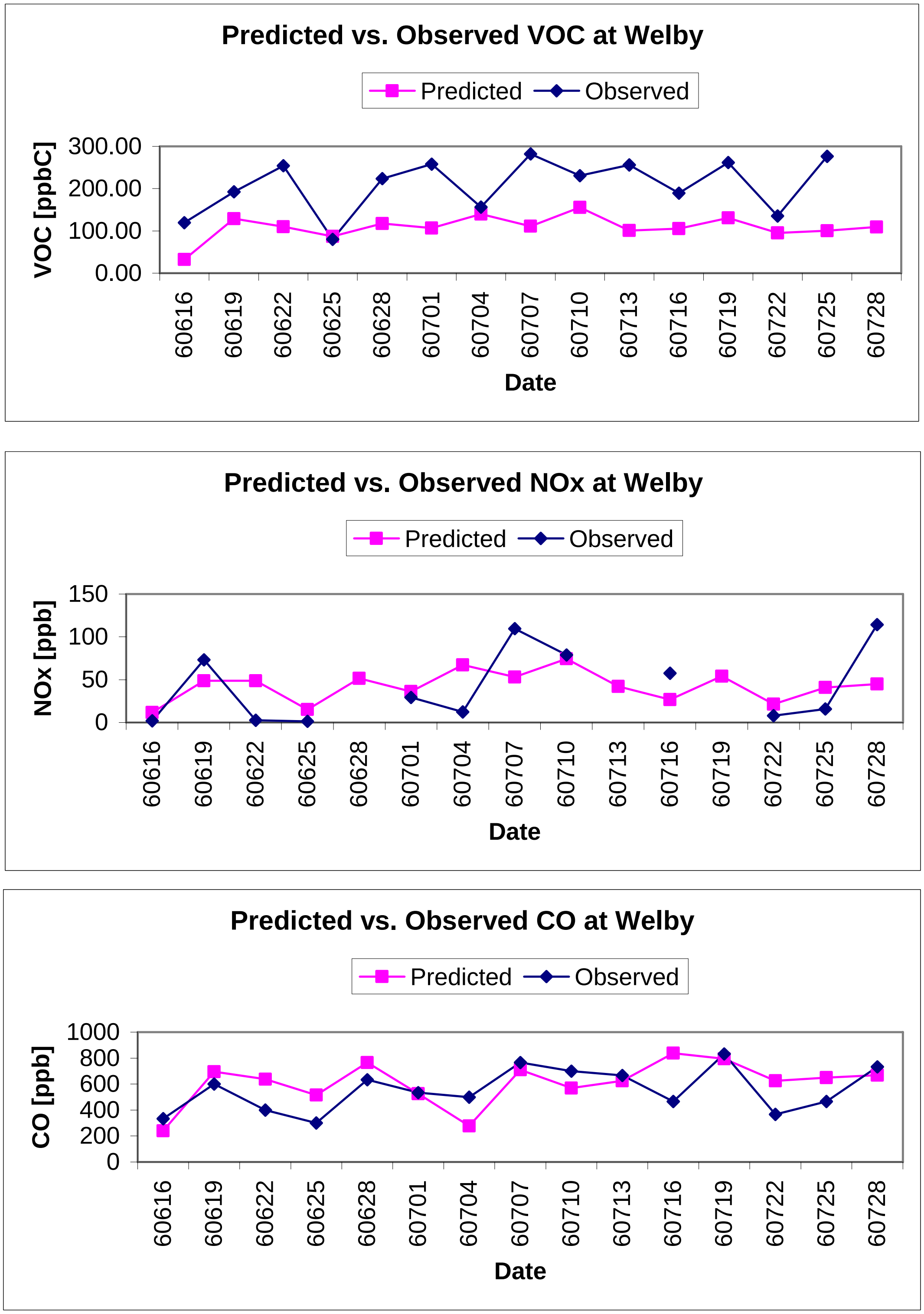


Figure 3-5a. Comparison of predicted and observed 3-hour average morning (5-8am MST) CB05-VOC, NOx and CO concentrations at the WELB monitor for the CAMx Run 17 2006 base case simulation.

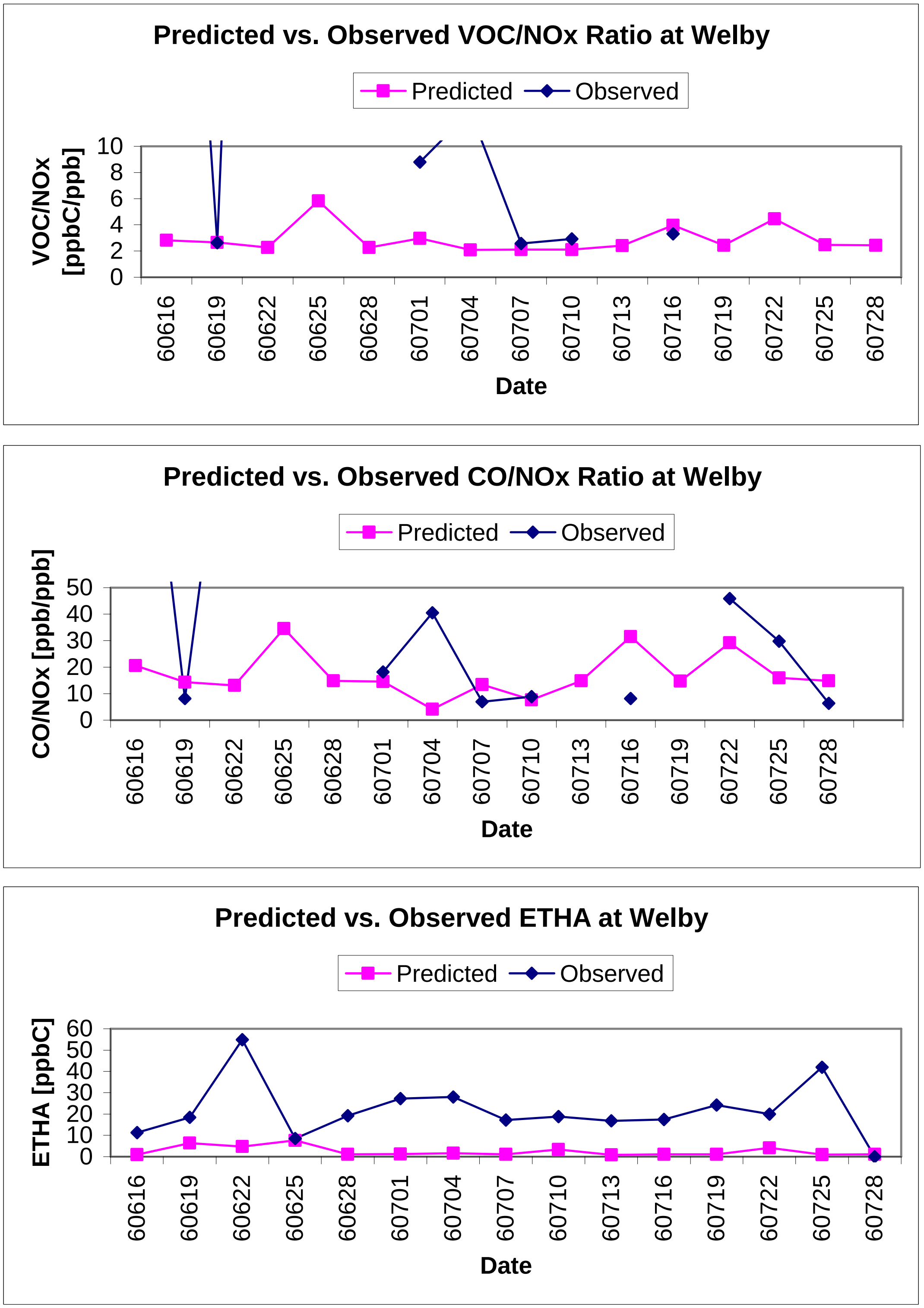


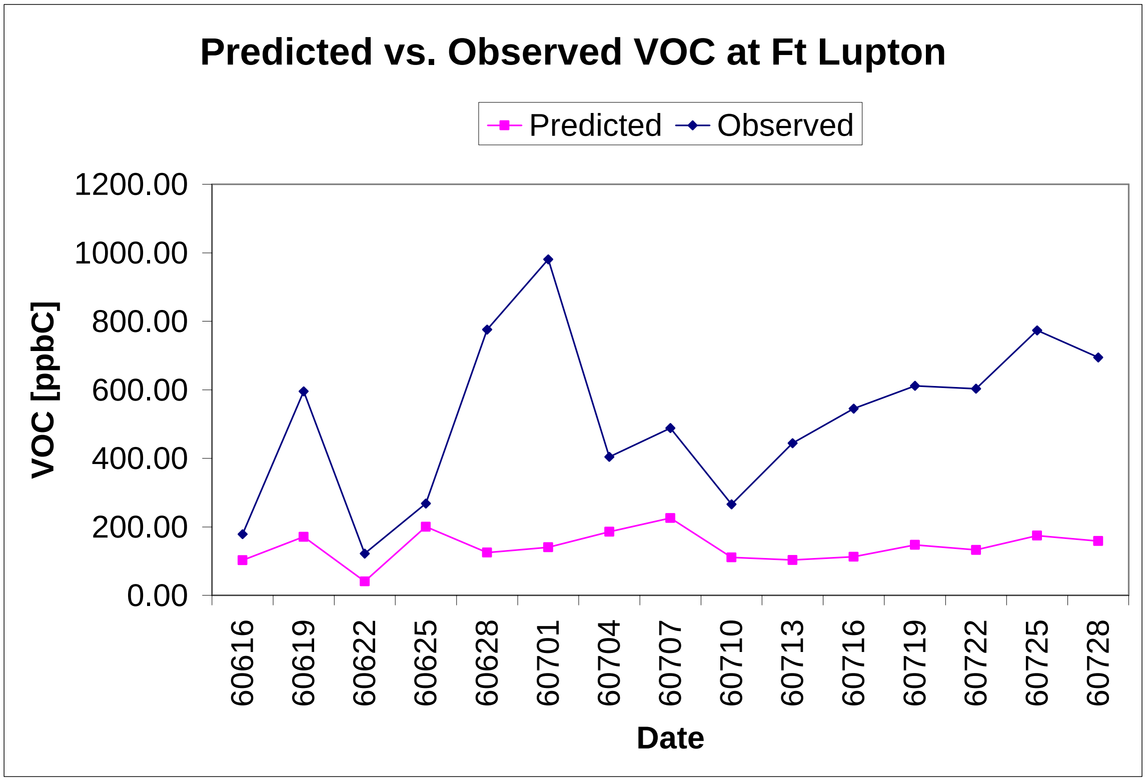
Figure 3-5b. Comparison of predicted and observed 3-hour average morning (5-8am MST) CB05-VOC/NOx and CO/NOx ratio and ethane (ETHA) concentrations at the Welby monitor for the CAMx Run 17 2006 base case simulation.

3.2.2.2 VOC Comparisons in Weld County

Unlike the two Denver VOC sampling sites, NOx and CO were not collected at the two Weld County sites so we can only make model-observed comparisons for total CB05-VOC and Ethane, which are shown in Figure 3-6. At Ft. Lupton the modeled VOC ranges from 40 to 226 ppbC, whereas the observed values range from 122 to 981 ppbC. Most modeled VOC values at Ft. Lupton are between 100-200 ppbC, whereas most observed values range from 250 to 700 ppbC. Similar results are seen at Platteville where the modeled VOC ranges from 50 to 200 ppbC, whereas the observed values range from 200 to 2,000 ppbC.

The model is also underpredicting the observed ethane concentrations at the two Weld County sites (Figure 3-7). At Ft. Lupton the observed ethane values range from 24 to 240 ppbC, with average values of around 150 ppbC. Whereas the model ethane predictions range from 6 to 43 ppb, with average values of approximately 25 ppbC that are over a 100 ppbC lower than observed on average. Even larger ethane underprediction bias is seen at Platteville with observed values of 35 to 600 ppbC and modeled values of 9 to 80 ppbC.

The model systematic underprediction of ethane in Denver and Weld County suggest that there are missing sources of natural gas in the inventory.



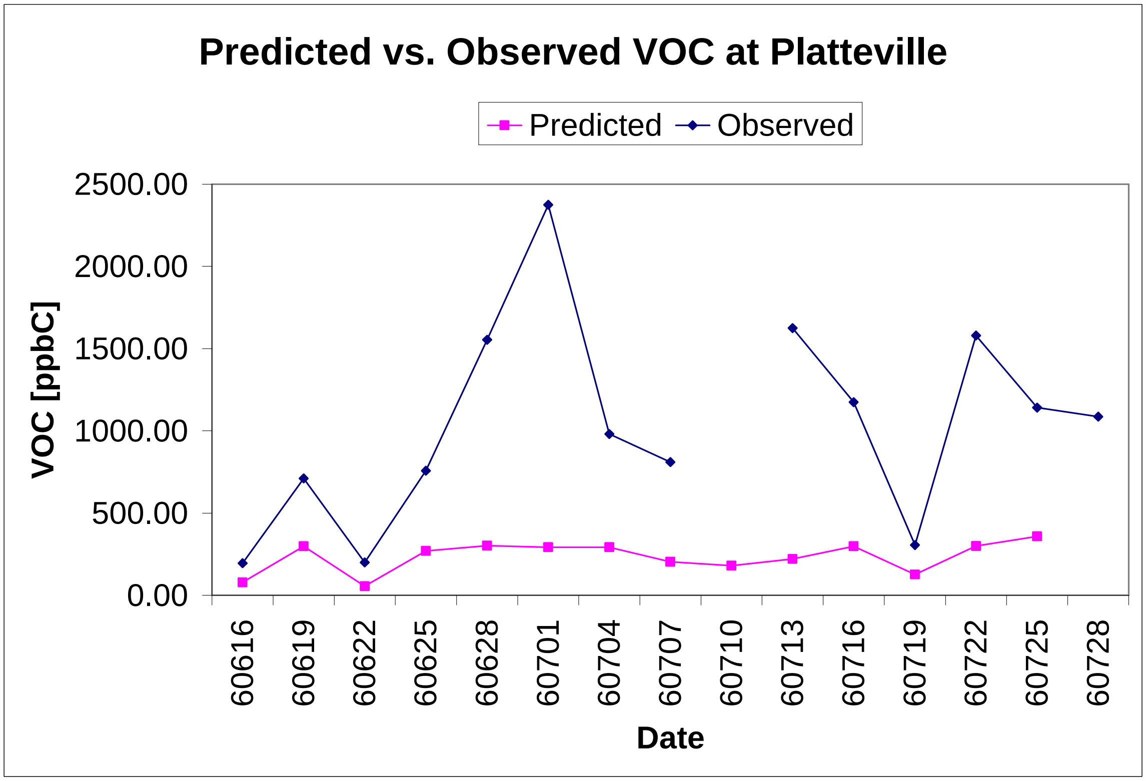
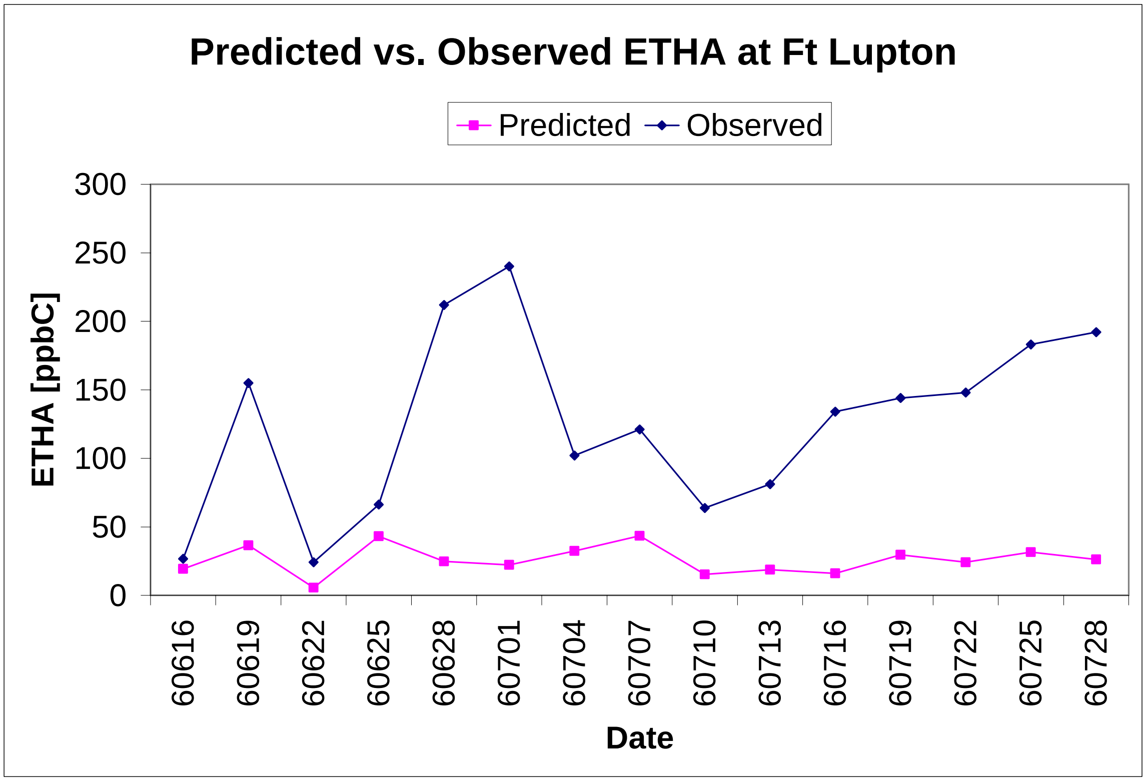


Figure 3-6. Comparison of the predicted and observed morning CB05-VOC concentrations at the Ft. Lupton and Platteville sites in Weld County.



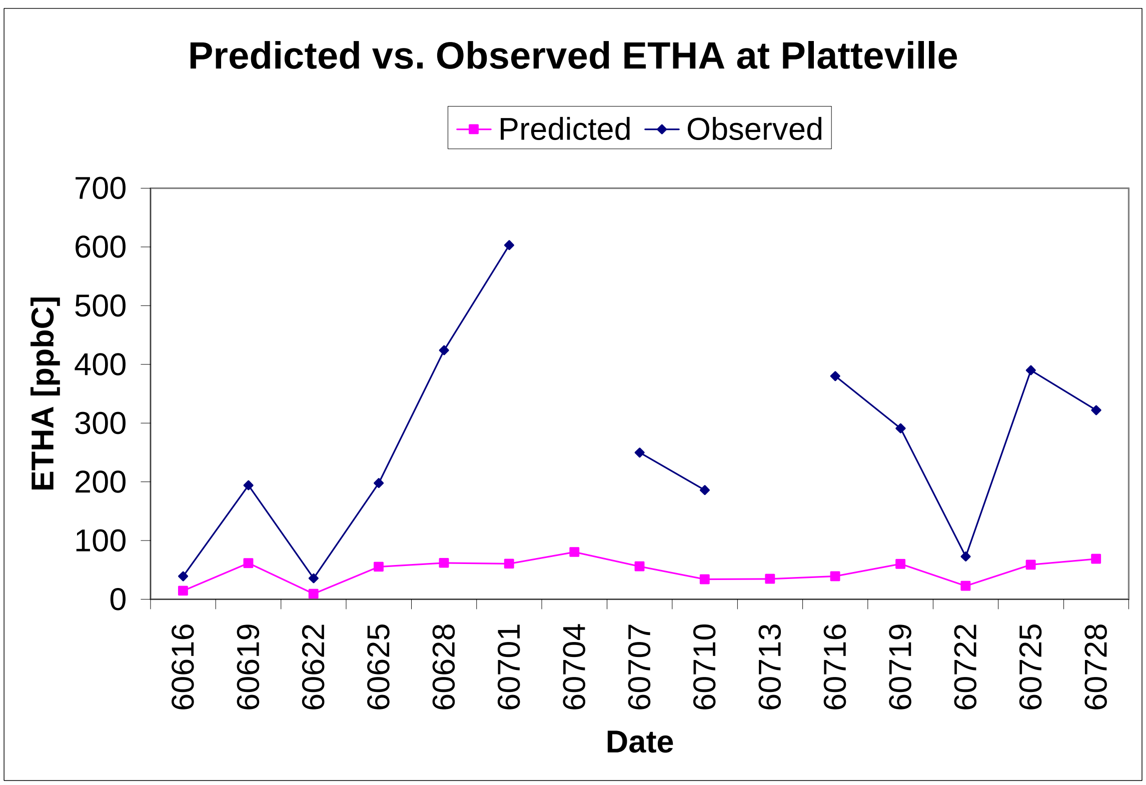


Figure 3-7. Comparison of the predicted and observed morning CB05-VOC concentrations at the Ft. Lupton and Platteville sites in Weld County.

3.2.3 Speciated VOC Comparisons

Figure 3-8 compares the speciated CB05 VOC concentrations for three days at the CAMP monitor. There is similarity in the speciated VOC model performance so just 3 days are reproduced. Paraffin (PAR) are reproduced well on June 19, but underestimated by 30-40 ppbC on July 13 and 28. Olefins (OLE) are underestimated by approximately a factor of two. The two aromatic species (TOL and XYL) are overestimated on June 19 but underestimated on the two July days. Formaldehyde (FORM) is underpredicted by approximately a factor of 2 on all three days. Acetaldehyde (ALD2) is greatly underestimated by the model with observed values of ~9 ppbC and modeled values a factor of ~6 lower at ~1.5 ppbC. Higher aldehydes are overestimated on June 19 and underestimated on the other two days. Ethene (ETH) is underestimated by 20-40%. ISOP and TERP, that are mainly biogenic VOC species, are almost nonexistent in the observed and modeled VOC concentrations at CAMP.

CB05 VOC species performance results at the Welby monitor (Figure 3-9) are similar to what was seen at CAMP. PAR is reproduced reasonable well on June 19, but underpredicted by 90 ppb on July 13 (samples for July 28 were missing). Formaldehyde is again underestimated by a factor of two, and acetaldehyde is underestimated by approximately a factor of 6. Ethane is underpredicted by a factor of 3 on June 19 and a factor of 20 on July 13.

The ETHA and PAR underestimation bias suggests missing natural gas emissions in the emissions inventory. This issue is discussed in more detail below when looking at the Weld County monitors. The underprediction of FORM is of concern since it is an important VOC species that initiates the radical cycle.

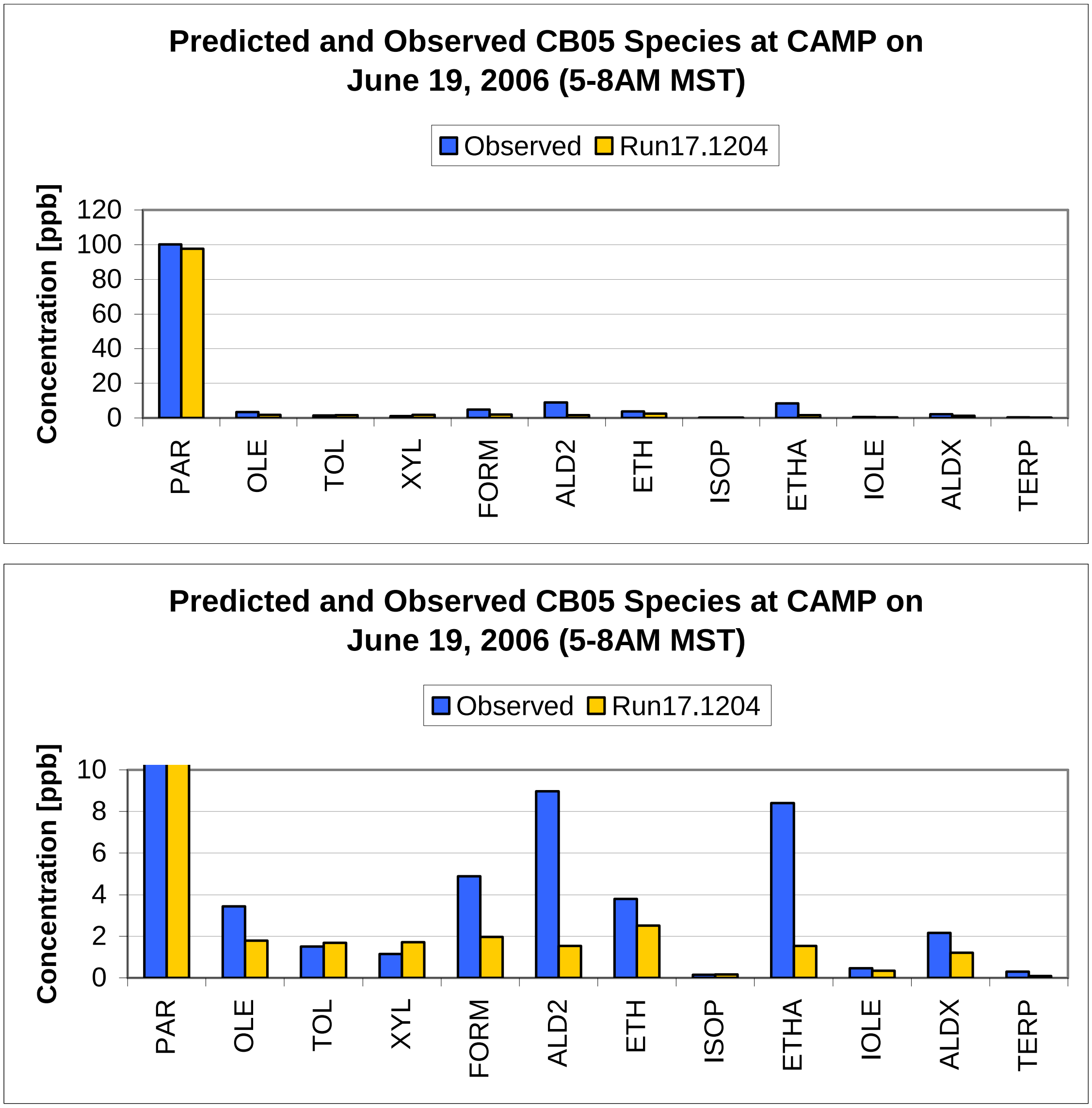


Figure 3-8a. Comparison of predicted and observed 5-8am MST CB05 VOC species at the CAMP monitor on June 19, 2006.

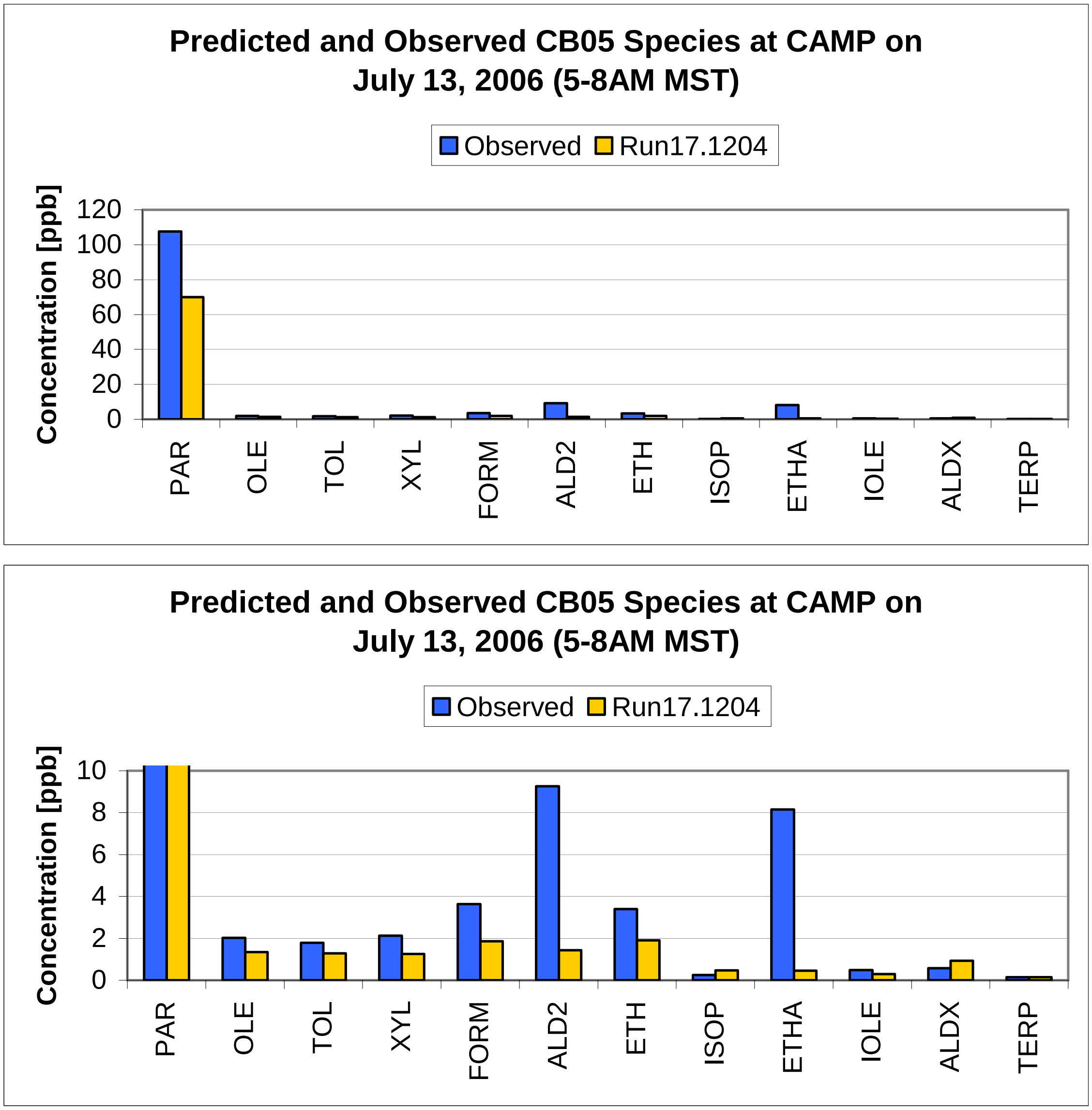


Figure 3-8b. Comparison of predicted and observed 5-8am MST CB05 VOC species at the CAMP monitor on July 13, 2006.

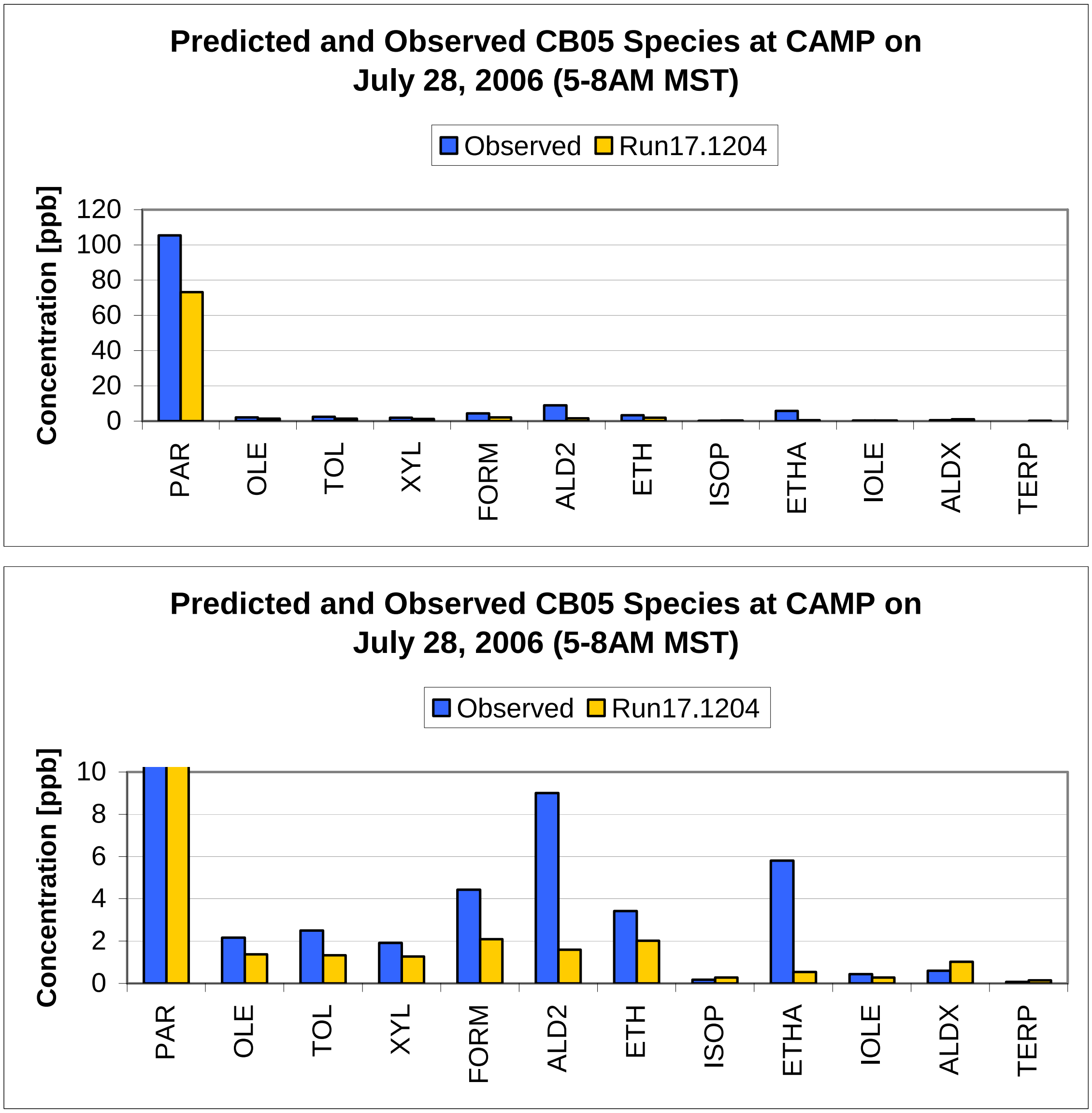


Figure 3-8c. Comparison of predicted and observed 5-8am MST CB05 VOC species at the CAMP monitor on July 28, 2006.

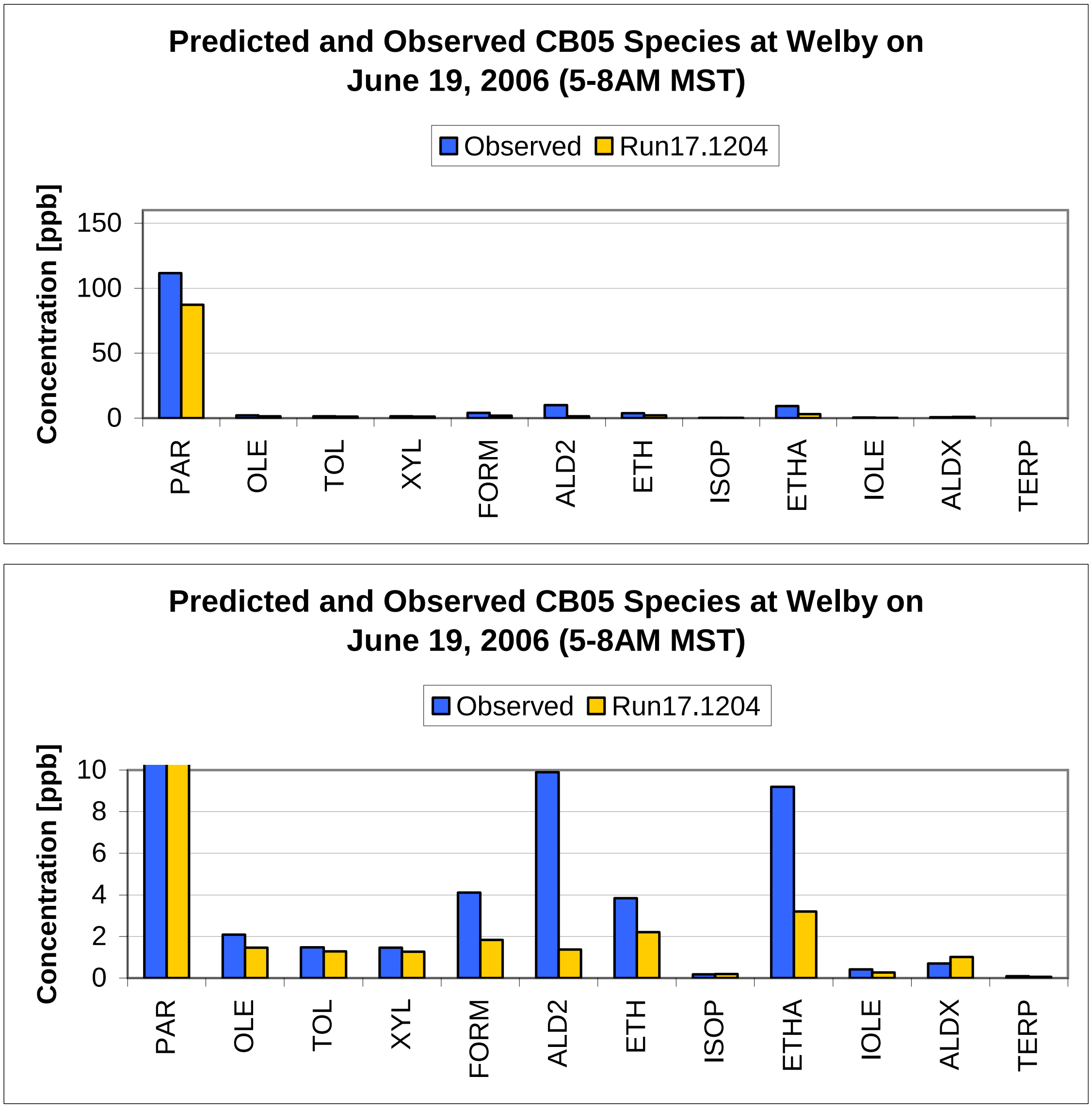
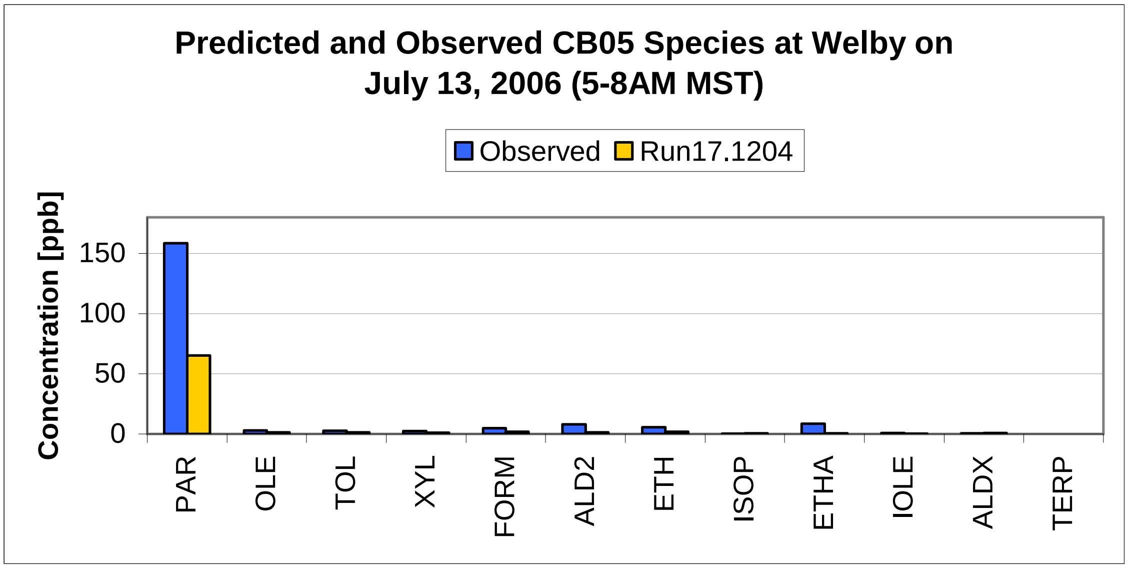


Figure 3-9a. Comparison of predicted and observed 5-8am MST CB05 VOC species at the Welby monitor on June 19, 2006.



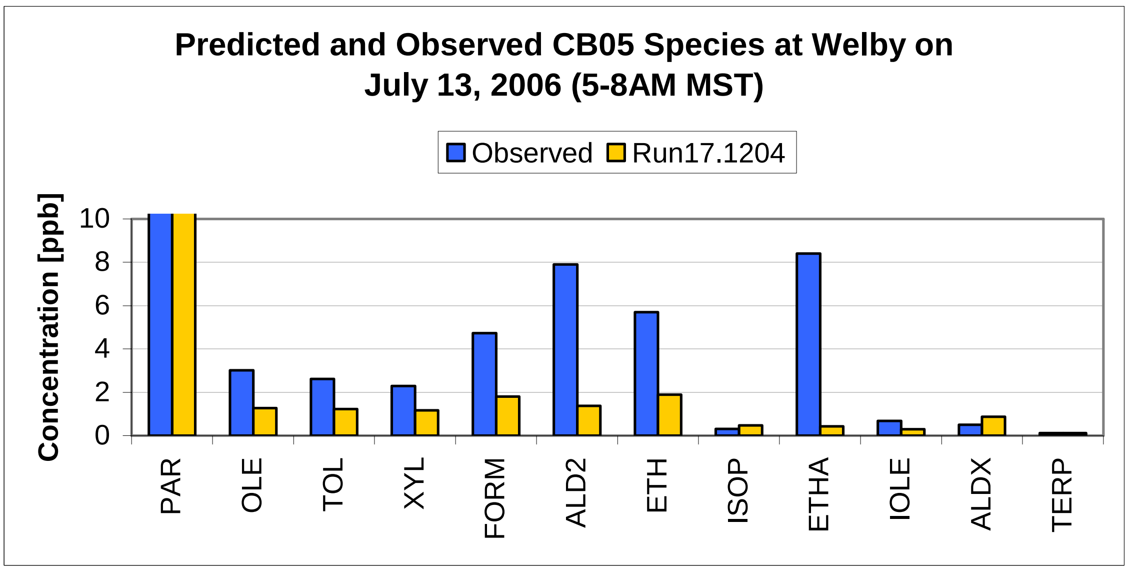


Figure 3-9b. Comparison of predicted and observed 5-8am MST CB05 VOC species at the Welby monitor on July 13, 2006.

VOC species at the two Weld County monitors are dominated by ethane (ETHA) and paraffin (PAR). Table 3-3 compares the predicted and observed PAR and ETHA concentrations at Ft. Lupton and Platteville and Figure 3-10 compares the other CB05 VOC species at Ft. Lupton and three days. The large underprediction of PAR and ETHA at these sites (typically -70% to -80%) indicate missing natural gas emissions in the inventory (Table 3-3). In addition to underestimating FORM and ALD2, as seen at the two Denver monitoring sites, the aromatic species are also underestimates at the Weld County sites, which suggest that gasoline combustion VOC emissions may be underestimated in the inventory as well.

Table 3-3. Comparison of predicted and observed morning paraffin (PAR) and ethane (ETHA) concentrations at the Weld County monitoring sites.

Site	Date	Observed (ppbC)	Predicted (ppbC)	Difference (ppbC)	Difference (%)
PAR					
Ft. Lupton	June 19	403	119	284	-70%
Ft. Lupton	July 13	321	67	254	-79%
Ft. Lupton	July 28	455	105	350	-77%
Platteville	June 19	484	224	260	-54%
Platteville	July 28	779	267	512	-66%
ETHA					
Ft. Lupton	June 19	88	18	70	-80%
Ft. Lupton	July 13	41	9	32	-77%
Ft. Lupton	July 28	96	13	83	-77%
Platteville	June 19	97	31	66	-68%
Platteville	July 28	161	34	127	-79%

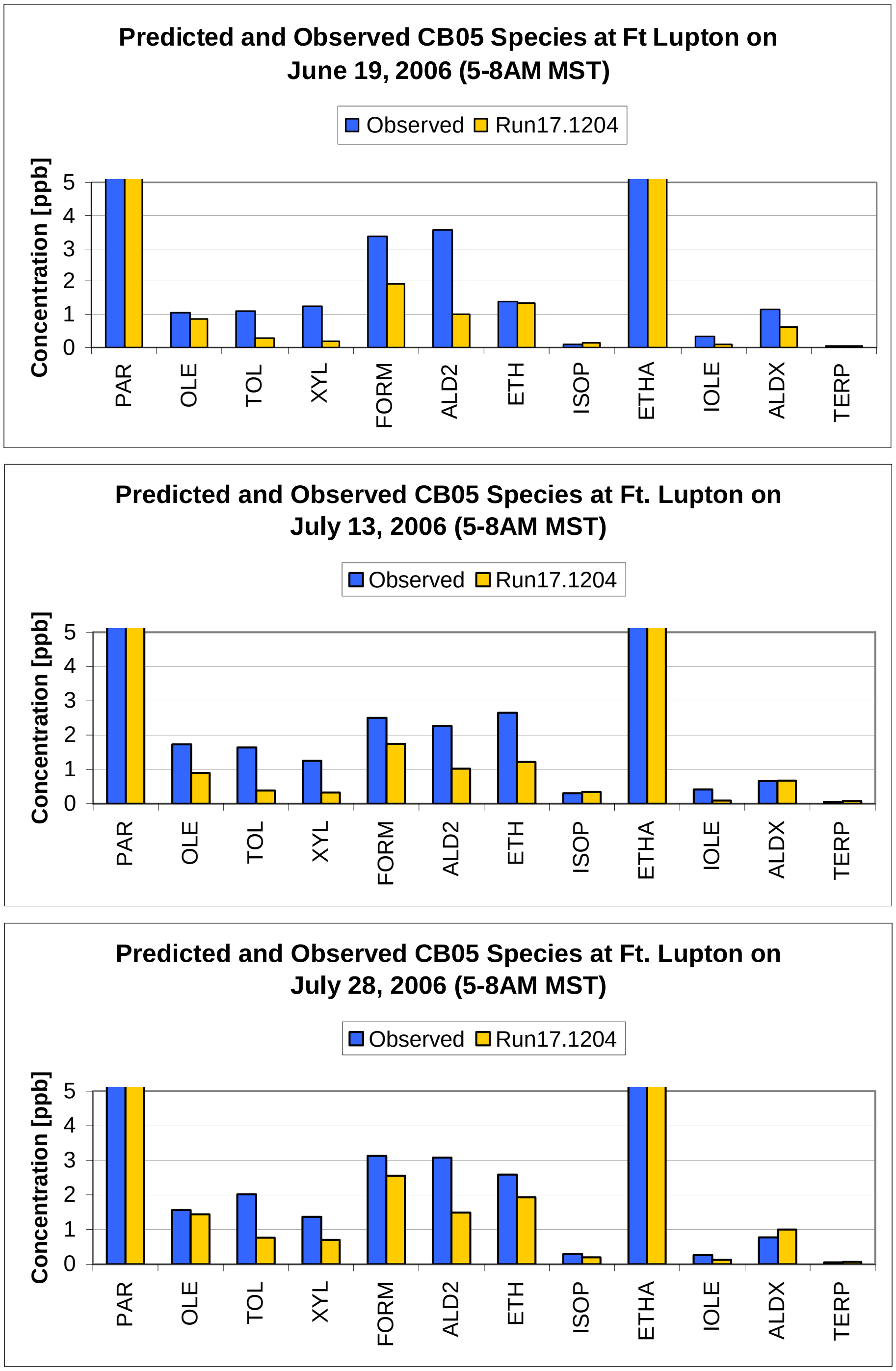


Figure 3-10. Comparison of predicted and observed CB05 VOC species at the Ft. Lupton monitoring site.

3.3 OZONE MODEL PERFORMANCE ALOFT

NOAA collected ozonesonde measurements launched at Boulder that overlapped with our modeling period for six days. An ozonesonde collects a vertical profile of ozone concentrations starting at the launch point (Boulder) and rising at a given rate that moves horizontally downwind by the prevailing winds. When matching the modeled vertical ozone profile with the ozonesonde data, we used the predicted ozone concentrations within the grid cell above the launch point of the ozonesonde. Thus, we did not match up the horizontal location or time of the ozonesonde with the modeling results. Although the ozonesonde measurements went up to 20-30 km, we only present the results for the lowest 10 km of the atmosphere as that is what is important for tropospheric ozone modeling.

One element of the Conceptual Model of high ozone events in the Denver areas is that on some days there may be a reservoir of ozone aloft that is entrained into the mixed layer as it rises during the day. Thus, it will be interesting to see whether elevated ozone exists aloft that could be entrained into the mixed layer.

Figure 3-11 compares the predicted and observed vertical ozone profiles at Boulder for the six days that ozonesonde measurements were available during the June-July 2006 modeling period. One general observation is that the model exhibits much less vertical variations in ozone concentrations than observed. This may be due in part by the fact that the model is just looking at vertical variations in ozone over the launch point, whereas the ozonesonde is measuring vertical, horizontal and temporal changes in ozone as the ozonesonde moves downwind.

On June 15th there is good agreement between the predicted and observed ozone in the lowest 2 km of the atmosphere (75-80 ppb). Between 2 km and 3 km AGL the observed ozone drops from 80 to 50 ppb, whereas the modeled values stay constant at 75-80 ppb. At ~5 km AGL the observed ozone rises from 50 to 90 ppb between 5 km and 6 km AGL and again matches the modeled value at 75-80 ppb between 6 km and 7 km. At 7 km the observed ozone rises to 250 ppb at 10 km AGL. This elevated ozone aloft is too high to be entrained in the mixing layer and is likely due to stratospheric ozone intrusion that is decoupled from the tropospheric ozone.

A comparison of the predicted and observed vertical ozone profiles for the morning of June 23 are given in Figure 3-11b. The model and observations agree on the reservoir of 75-80 ppb ozone above the morning inversion in the 1-2 km AGL height. However, above 2 km the observed values drop to a minimum of ~40 ppb at approximately 4 km AGL, whereas the modeled vertical ozone profile is constant at 75-80 ppb.

On June 29th the model estimates a nearly constant 65-75 ppb variation in ozone in the vertical from the surface to 10 km AGL (Figure 3-11c). The observed vertical profile is also relatively constant but has more variations from 55 ppb at the surface to 90 ppb at 10 km AGL.

On July 14, 2006 the model is predicting a constant ~70 ppb vertical ozone profile in the lowest 3 km of the atmosphere, whereas the observed values are 10-15 ppb higher (Figure 3-11d). Similarly, on July 21 the model (~55 ppb) is approximately 20 ppb lower than observed (~75 ppb) in the lowest 1 km of the atmosphere. Between 2 and 4 km AGL there is good agreement between the modeled and observed vertical profile with a steady increase of from 55 ppb to 70 ppb (model) and 80 ppb (observed). However, above ~4 km AGL the model exhibits increasing ozone with height, but the observed ozone drops ~50 ppb with the observed value at 10 km AGL (55 ppb) being about 30 ppb lower than the model (85 ppb).

On July 26 the modeled ozone is below the observed ozone throughout the vertical profile (Figure 3-11f). The modeled ozone ranges from ~55 ppb at the surface and increases to ~65 ppb at 10 km AGL, whereas the observed values range form about 60 ppb at the surface increasing to over 100 ppb at 5 km AGL and then down to 75 ppb at 10 km AGL.

Maximum afternoon mixing heights in the Denver area would be expected to be in the 2,000 to 5,000 m AGL range. There does not appear to be any evidence of a reservoir of elevated ozone aloft in the June ozonesonde measurements. However, the July ozonesonde measurements show elevated ozone aloft that is not captured by the model. Although these results are inconclusive, one potential explanation contributing to the underprediction of surface ozone concentrations at the high monitoring sites is the failure of the model to simulate the high ozone aloft that is entrained down to the surface as the mixing height rises.

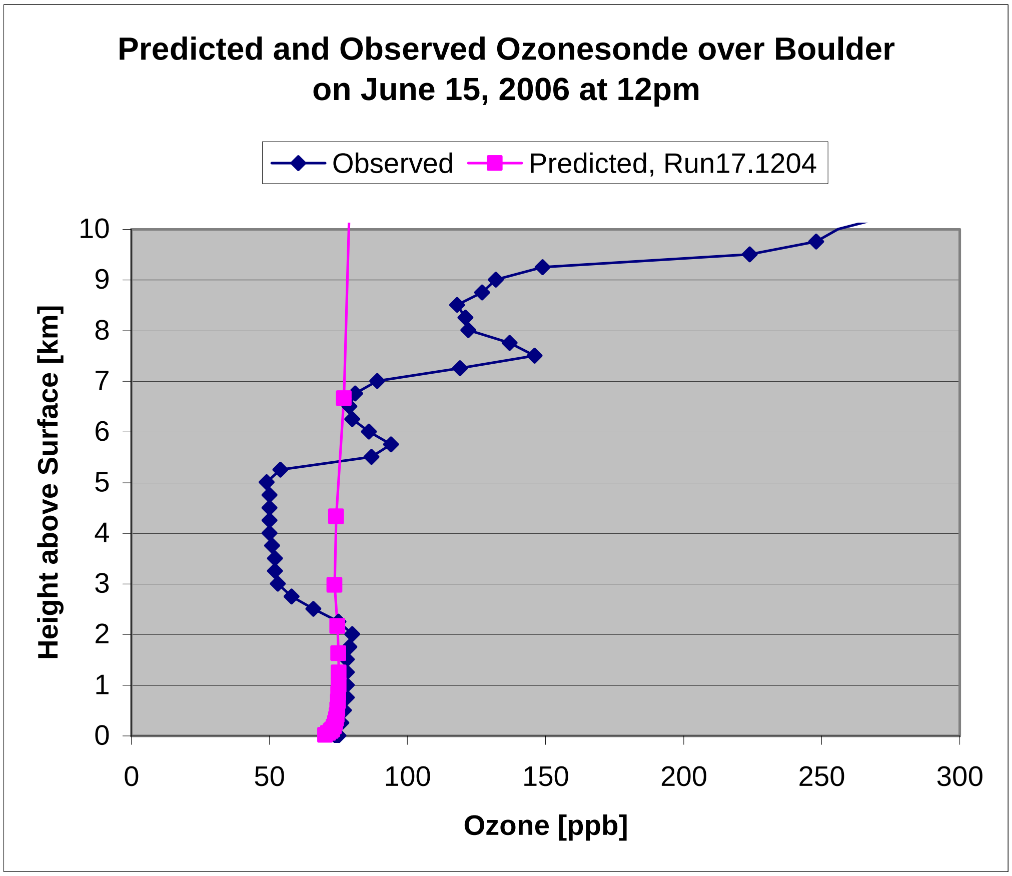


Figure 3-11a. Comparison of predicted and observed vertical distribution of ozone concentrations on June 15, 2006 for the CAMx Run 17 2006 base case simulation.

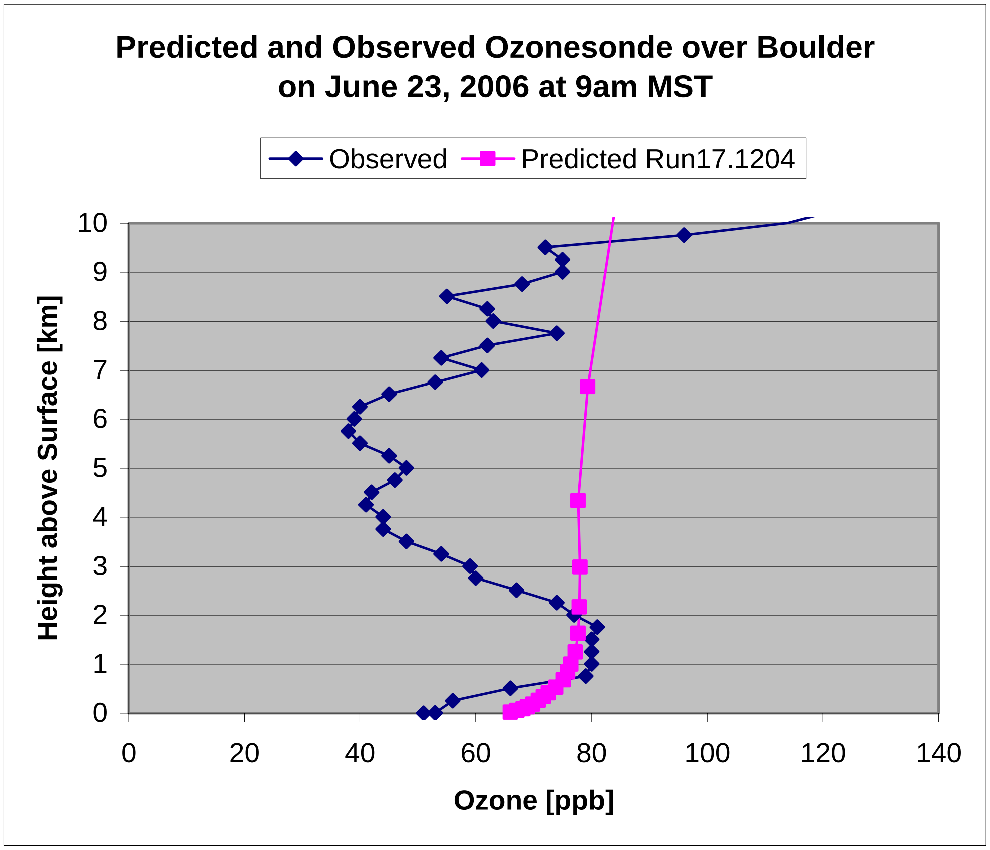


Figure 3-11b. Comparison of predicted and observed vertical distribution of ozone concentrations on June 23, 2006 for the CAMx Run 17 2006 base case simulation.

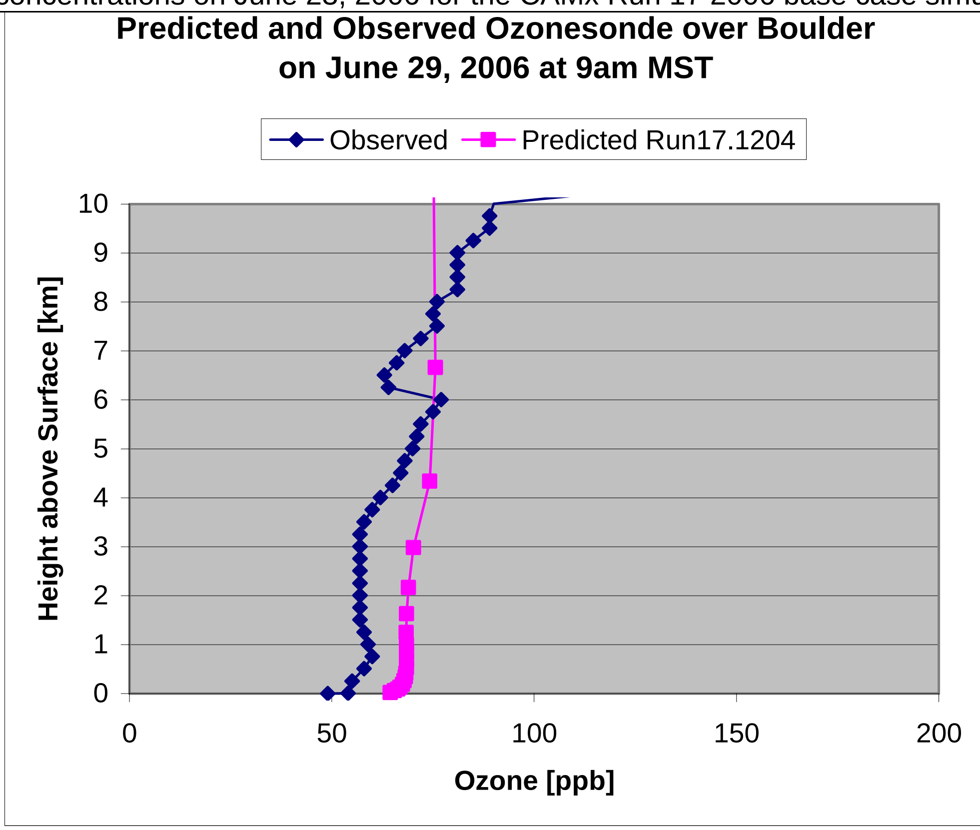


Figure 3-11c. Comparison of predicted and observed vertical distribution of ozone concentrations on June 29, 2006 for the CAMx Run 17 2006 base case simulation.

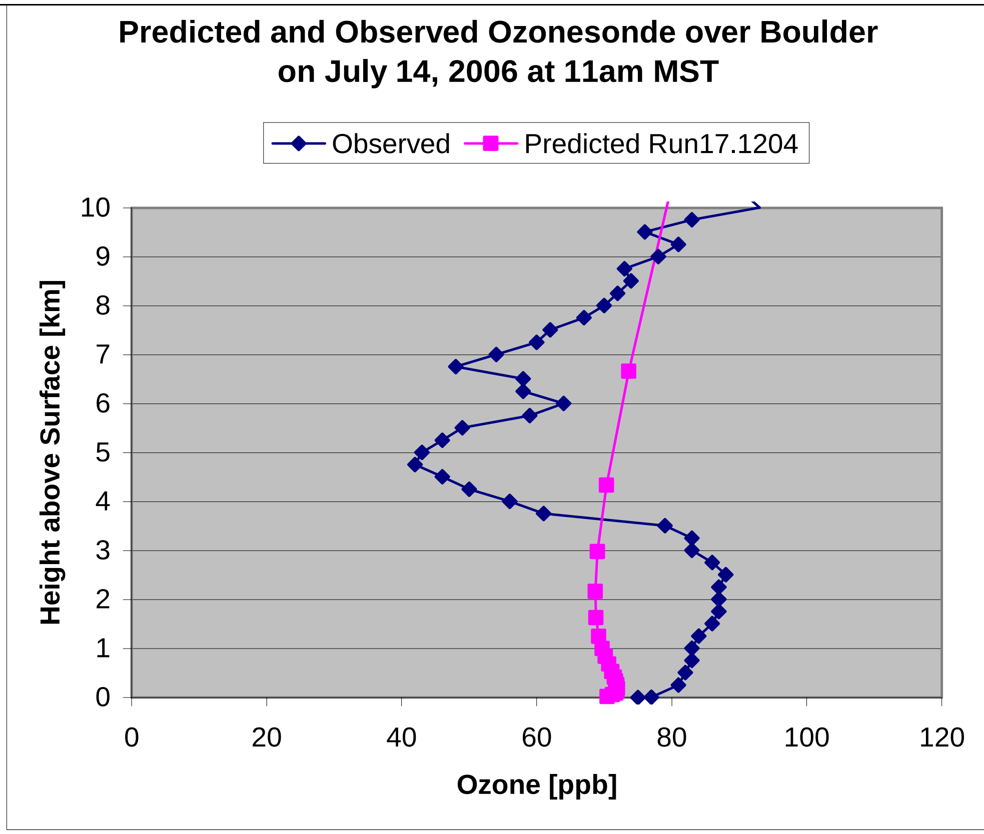


Figure 3-11d. Comparison of predicted and observed vertical distribution of ozone concentrations on July 14, 2006 for the CAMx Run 17 2006 base case simulation.

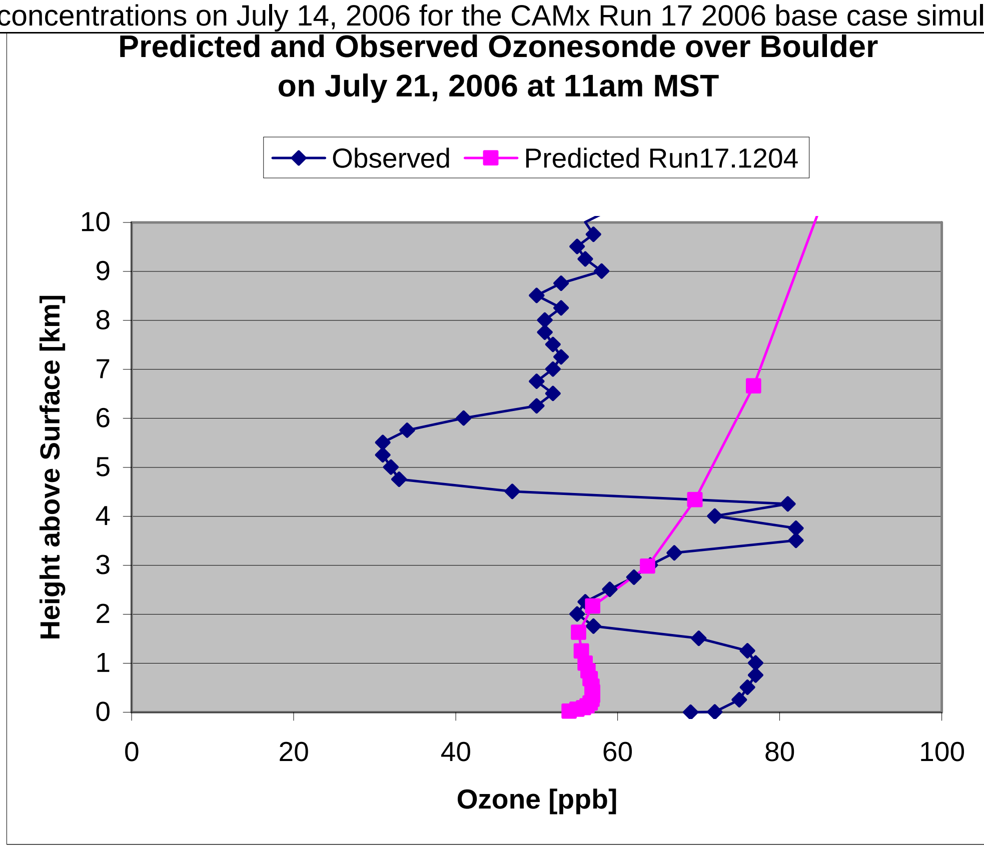


Figure 3-11e. Comparison of predicted and observed vertical distribution of ozone concentrations on July 21, 2006 for the CAMx Run 17 2006 base case simulation.

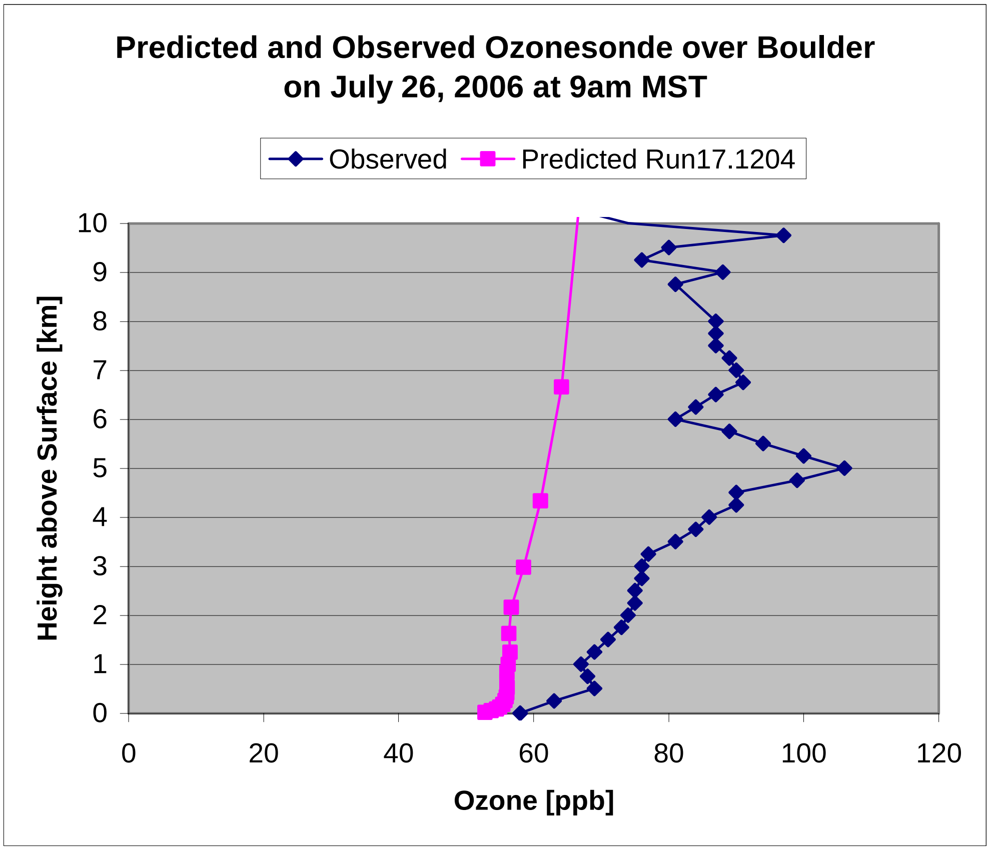


Figure 3-11f. Comparison of predicted and observed vertical distribution of ozone concentrations on July 26, 2006 for the CAMx Run 17 2006 base case simulation.

3.4 PM MODEL PERFORMANCE EVALUATION

In this section we compare the CAMx Run 17 2006 base case modeling results against particulate matter (PM) species and PM related species concentrations. However, the Denver June-July 2006 modeling database was set up for ozone modeling, not PM modeling. In fact, the CDPHE/APCD only provided 2006 base case emissions in Colorado for ozone precursor species (i.e., VOC, NOx and CO) and PM10 emissions for some categories . Thus, some of the PM emissions and PM related species are missing in Colorado. Where PM emissions data was available it was included, but given the time constraints of the study and the focus on ozone, no attempt was made to spend the extra resources and time to fill in the missing PM precursor emissions in Colorado.

Outside of Colorado the projected WRAP emissions inventory was used that includes PM precursors. However, these data were replaced with the CDPHE ozone precursor inventory in Colorado. For on-road mobile sources, the MOBILE6 emission factor model includes PM species with the SMOKE and CONCEPT emissions modeling so on-road mobile source emissions include PM precursors. For large stationary point sources we used CEM data that includes NOx and SO2 emissions. The MEGAN biogenic emissions model also includes PM precursor emissions. So the main source of missing PM emissions in Colorado is within the non-road mobile and area source categories. Given this, we would expect the model to underestimate PM concentrations. In particular, because most of the ammonia emissions are in the area source category, we would expect particulate nitrate (NO3) and ammonium (NH4) to be underestimated.

Total $PM_{2.5}$ mass measurements were collected at FRM and IMPROVE monitoring networks within the 12 km modeling domain. Figure 3-12 displays the predicted and observed scatter plots of 24-hour average $PM_{2.5}$ mass concentrations for the two networks and the June-July 2006 modeling period. Not surprising, given the missing PM precursor emissions in Colorado for some source categories, there is an underprediction tendency for total PM2.5 mass with fractional bias values of -90% to -100%.

Better performance is seen for SO4 concentrations, albeit with an underestimation tendency (Figure 3-13). The fractional bias for SO4 across the CASTNET, IMPROVE and STN networks in the 12 km domain are -74%, -58% and -64%, respectively. Although this underprediction bias is due in part to missing SO2 and SO4 emissions, it is also affected by too much wet deposition of SO4 as evident by the overprediction of wet deposited SO4 at the NADP sites. Note that the MM5 overstatement of the summer time convective rainfall in the Four Corners states is a common occurrence and much of the WRAP MM5 modeling effort was devoted to limiting the overstated summer rainfall. For the Denver MM5 modeling of the June-July 2006 period, we did not observe overstated convective rainfall in the Denver area. However, that does not mean MM5 did not overstate rainfall in other areas of the western U.S. that is likely causing the overstated of wet SO4 deposition across the NADP monitoring sites.

Particulate nitrate (NO3) is greatly underestimated by the model (Figure 3-14). A large part of this underprediction is due to missing ammonia emissions in Colorado; NO3 particles can not form unless there is a buffering species and ammonia is the most common buffering agent in the western U.S. Without ammonia, all of the oxidized NOx will stay as nitric acid (HNO3). In the top right panel of Figure 3-14 the modeled total nitrate (NO3+HNO3) is compared against the CASTNet measured total nitrate and a much better comparison is seen. Although there still is an underprediction bias in total nitrate, it is much lower than for NO3 and comparable to the other species.

Figure 3-15 displays the model performance for organic carbon (OC) and elemental carbon (EC) across the IMPROVE and STN monitoring networks. Note that the OC and EC measurements are more uncertain than the other PM species. Also note that although the monitors measure OC, the model predicts organic carbon matter (OCM) that includes other elements besides carbon. For the OC model evaluation the observed OC was multiplied by 1.4 for comparison with the modeled OC in Figure 3-15.

As expected, both EC and OC are underestimated due to missing emissions, with the underestimation comparable to the other species. The exception is EC at the STN network that exhibits fairly reasonable fractional bias (-29%). This is likely because the EC emissions were included in the on-road mobile source emissions and the urban-oriented STN sites are likely dominated by on-road mobile sources.

Because of the deficient PM precursor inventory, the PM evaluation is inconclusive. As expected the model is underpredicting, and the underprediction appears to be consistent across the PM species. Given this, we elected not to expend any effort evaluating the model using the NPS ROMANS study database until better PM precursor emissions can be developed.

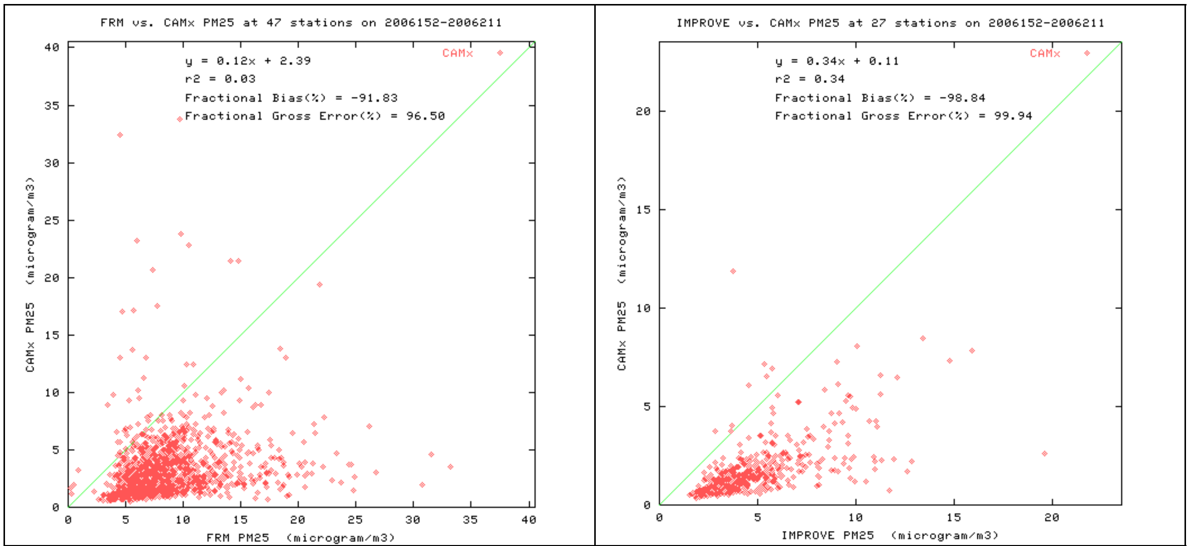


Figure 3-12. Comparison of predicted and observed total $PM_{2.5}$ mass model performance at FRM (left) and IMPROVE (right) sites in the 12 km modeling domain.

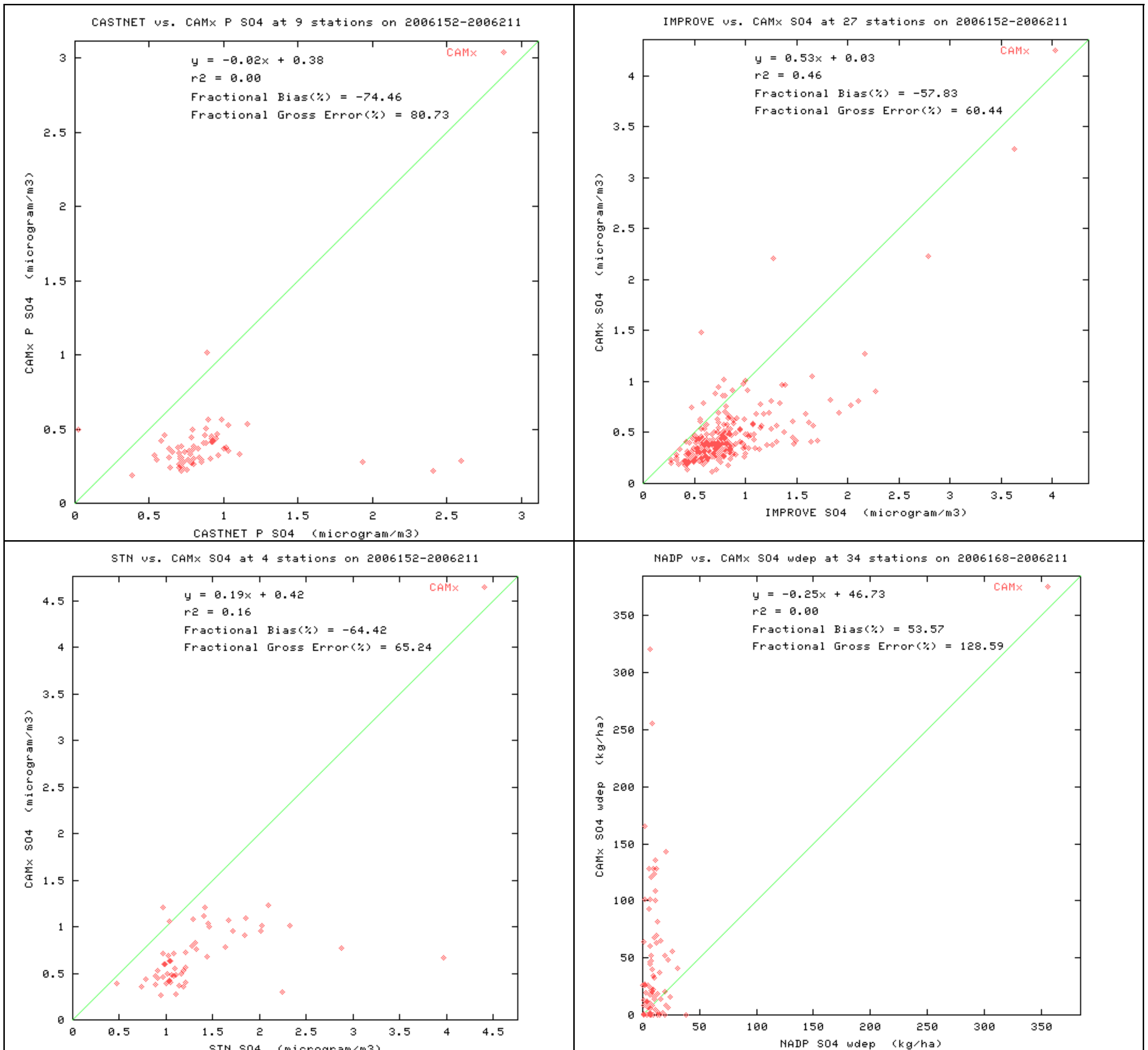


Figure 3-13. Comparison of predicted and observed total sulfate (SO4) model performance at CASTNET (top left), IMPROVE (top right), STN (bottom left) and NADP (bottom right) monitoring sites in the 12 km modeling domain.

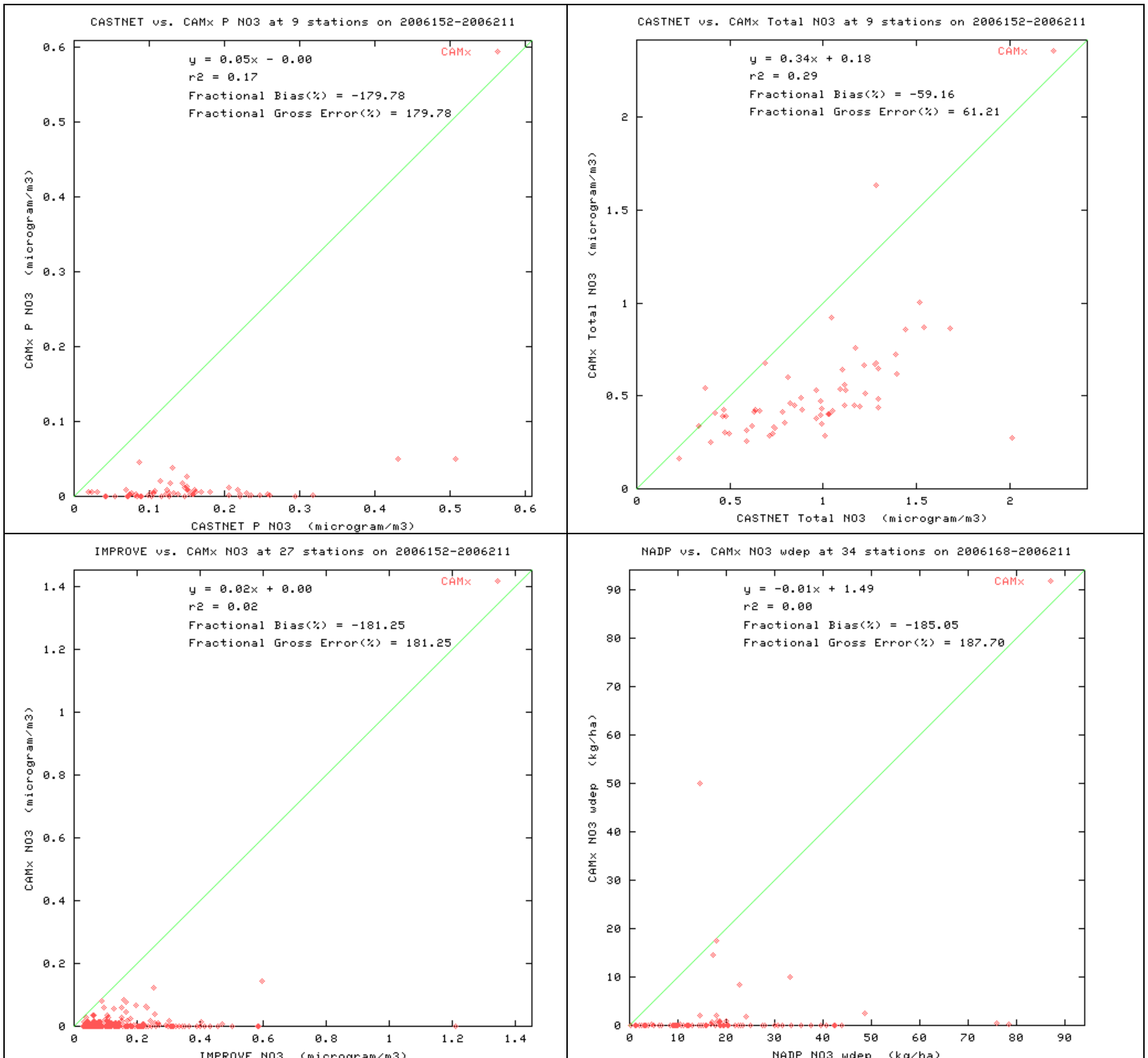


Figure 3-14. Comparison of predicted and observed total nitrate (NO3) model performance at CASTNET (top left), CASTNET for total NO3 (NO3+HNO3) (top right), IMPROVE (bottom left) and NADP (bottom right) monitoring sites in the 12 km modeling domain.

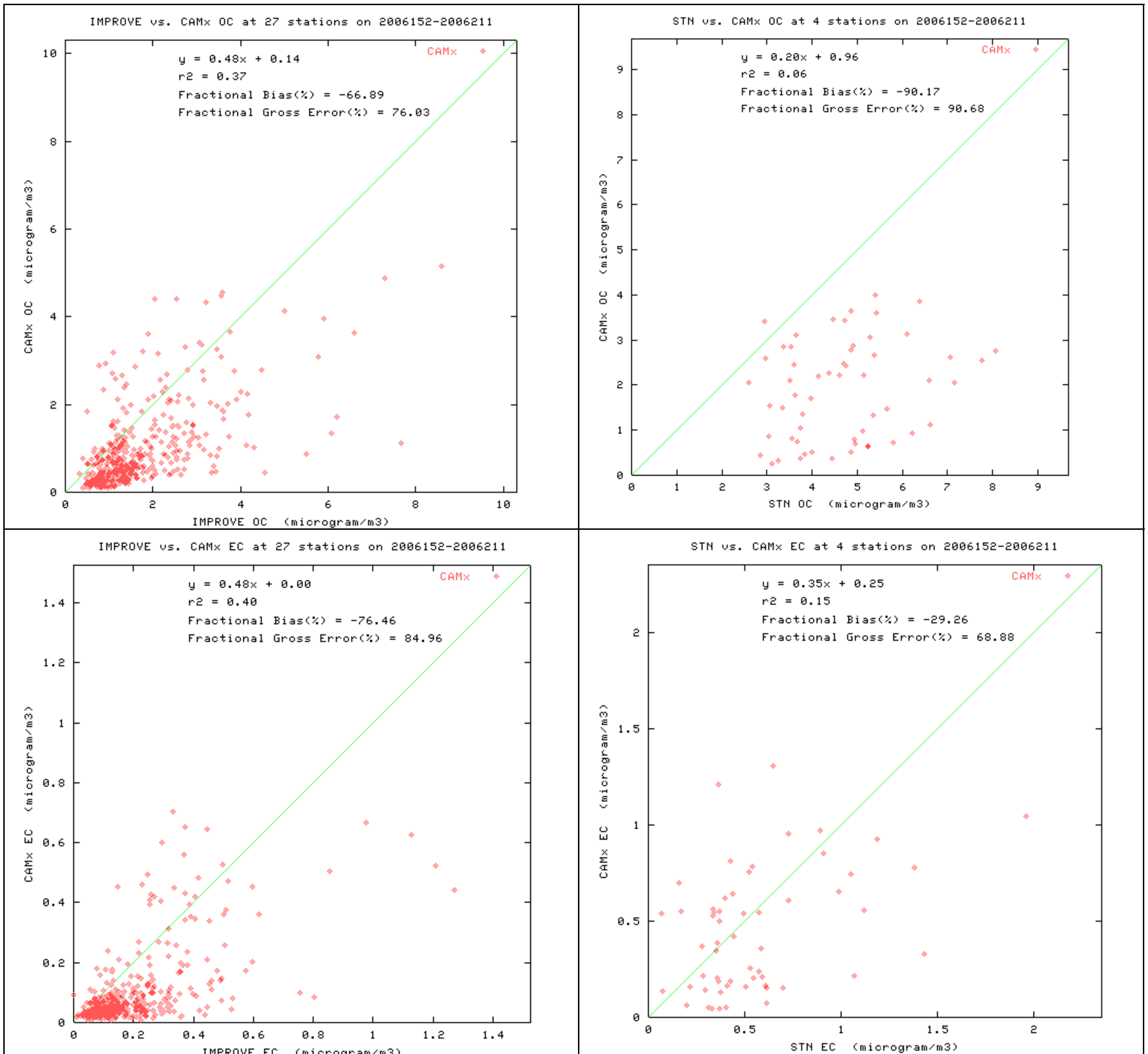


Figure 3-15. Comparison of predicted and observed Organic Carbon (OC; top) and Elemental Carbon (EC; bottom) model performance at IMPROVE (left) and STN (right) monitoring sites in the 12 km modeling domain.

3.5 DIAGNOSTIC MODEL PERFORMANCE CONCLUSIONS

The diagnostic model performance evaluation provides additional support that the Denver June-July 2006 modeling database is working sufficiently well for projecting future year changes in ozone concentrations in response to changes in emissions. It has also identified areas of further analysis and refinement can be achieved to obtain a better photochemical modeling database.

The mostly good agreement between the predicted and observed VOC/NOx ratios at the metropolitan Denver sites suggests that we are characterizing the on-road mobile sources well and capturing the correct chemical regimes in Denver. However, the comparisons for ethane and paraffin at the Denver sites, and especially the Weld County sites, suggest that natural gas emission sources are likely understated. In addition, the VOC speciation is an area that should be reviewed in the future with the model generally underestimating carbonyls (e.g., formaldehyde).

The ozone aloft performance evaluation was inconclusive due to only having six comparisons available. But the results do lend credence to the hypotheses that the model is not predicting as high ozone aloft that is brought to the ground through vertical mixing. The PM evaluation was also inconclusive due to missing PM precursor emissions in the database, which is also an area for future improvements.

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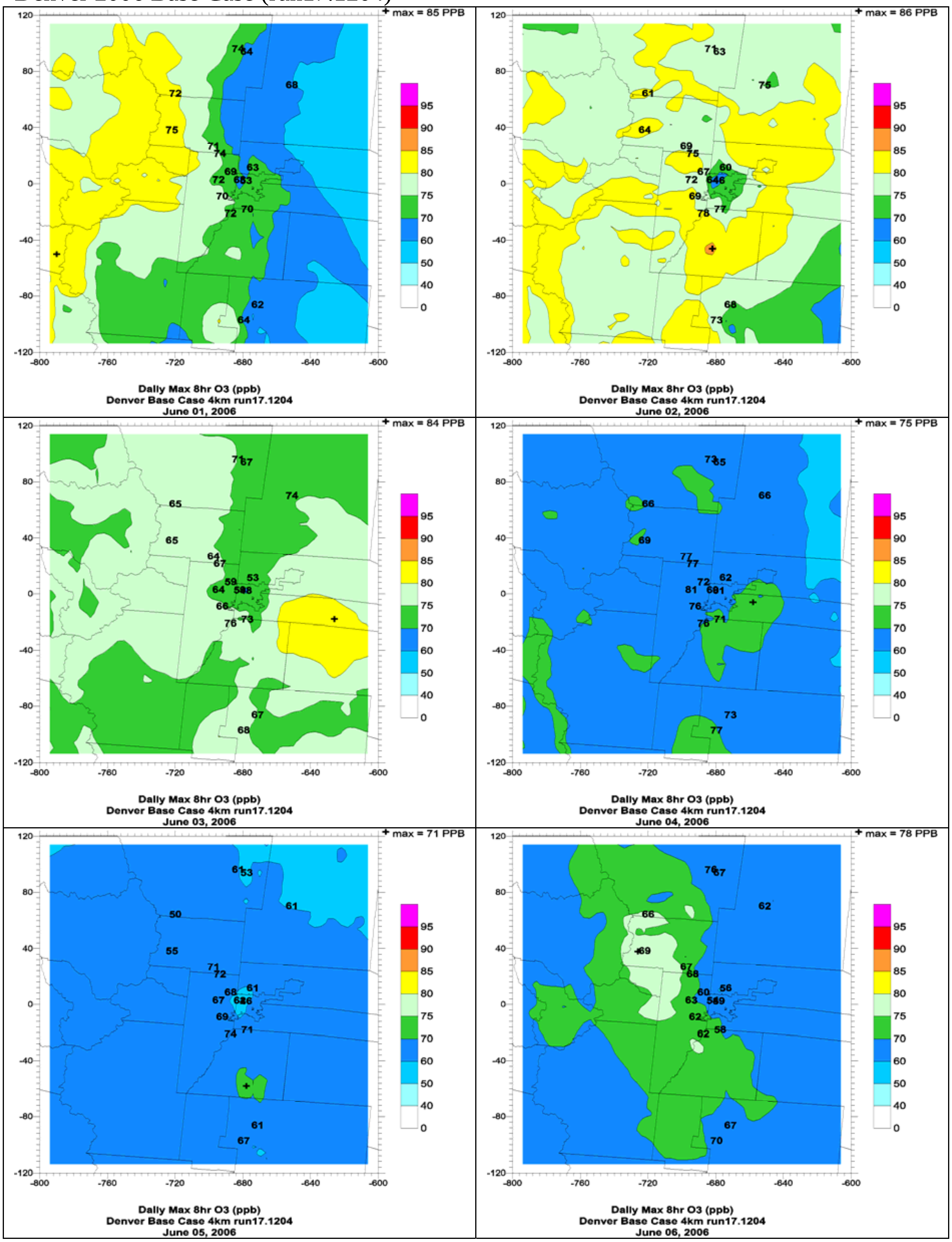
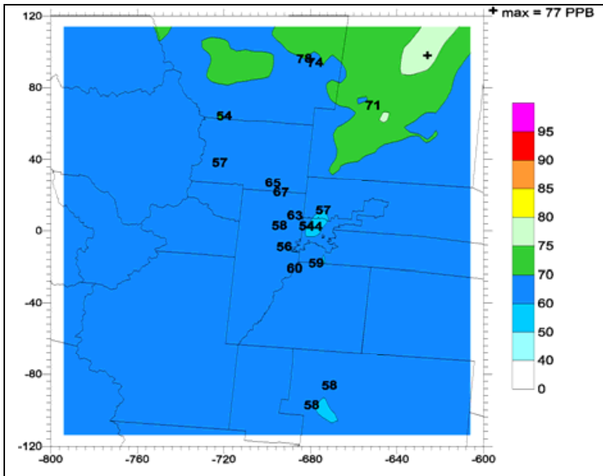
APPENDIX A

Comparison of Predicted and Observed Spatial Distributions of the Daily Maximum 8-Hour Ozone Concentrations in the Denver Area during June-July 2006 for the Final CAMx 2006 Base Case (Run 17) Simulation

Denver 2006 Base Case (run17.1204)





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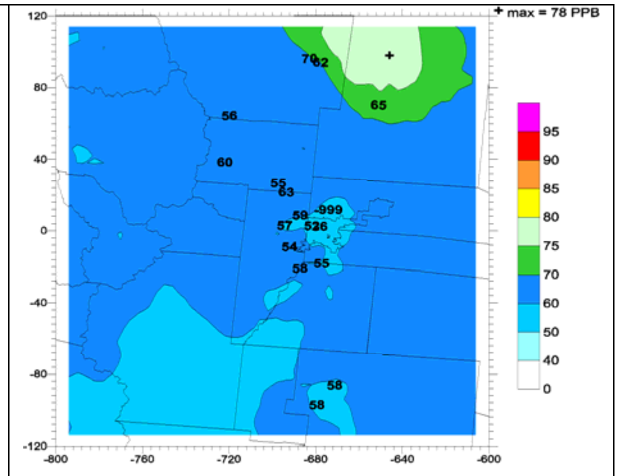

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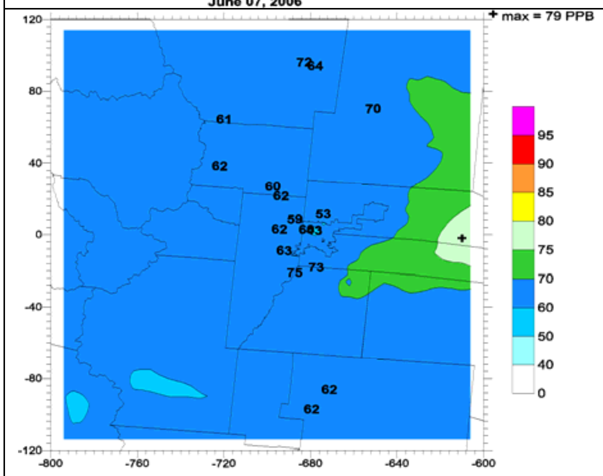

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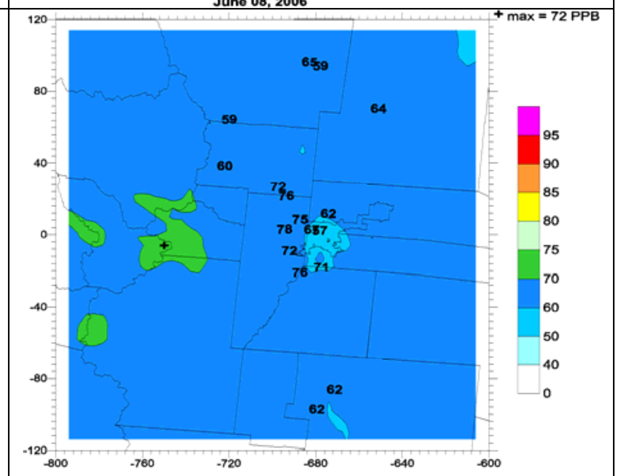

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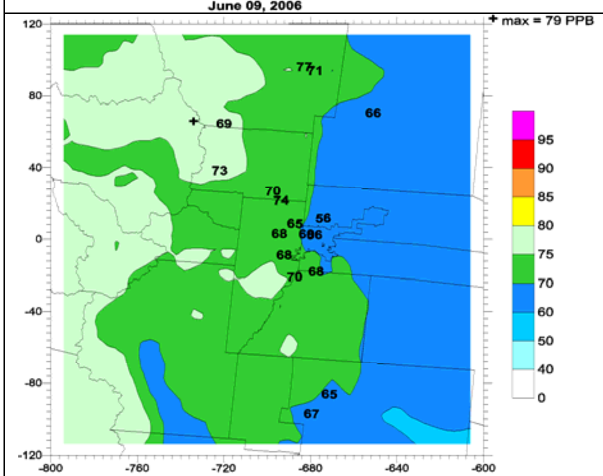

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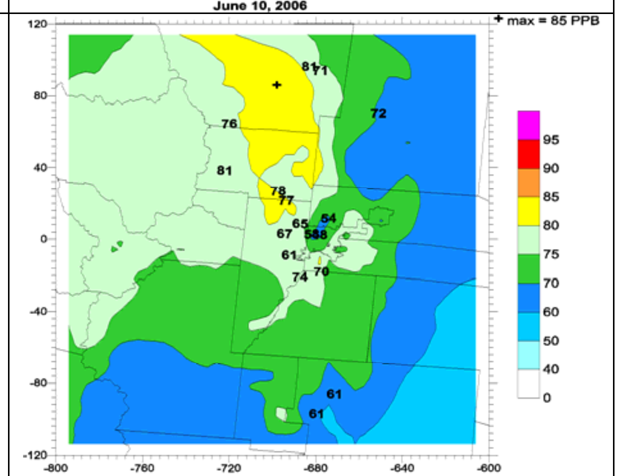

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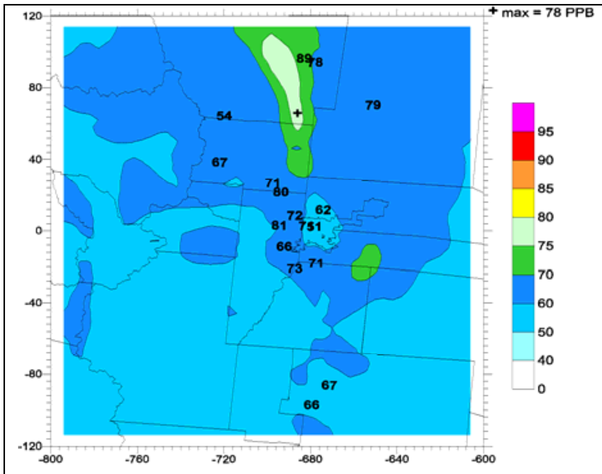

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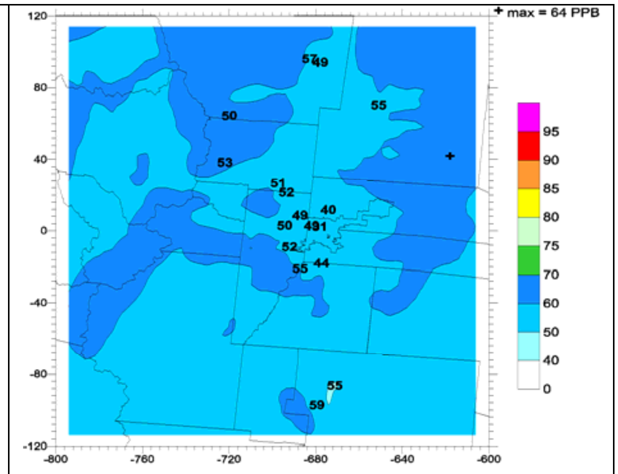

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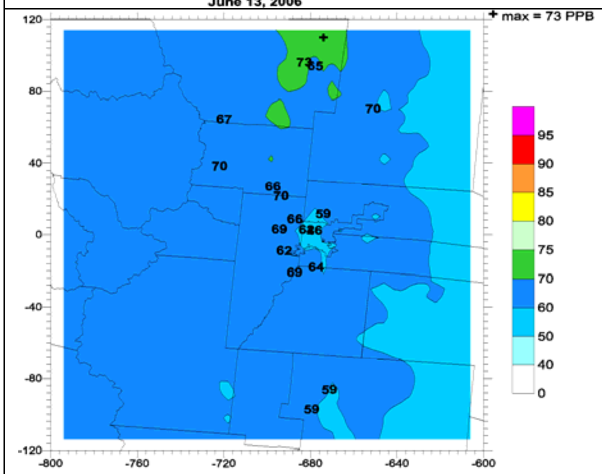

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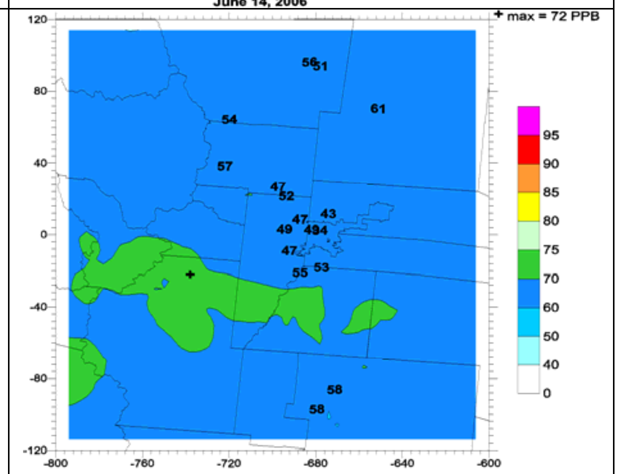

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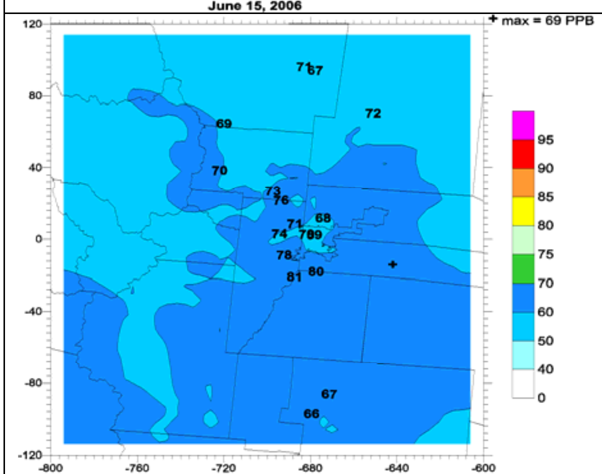

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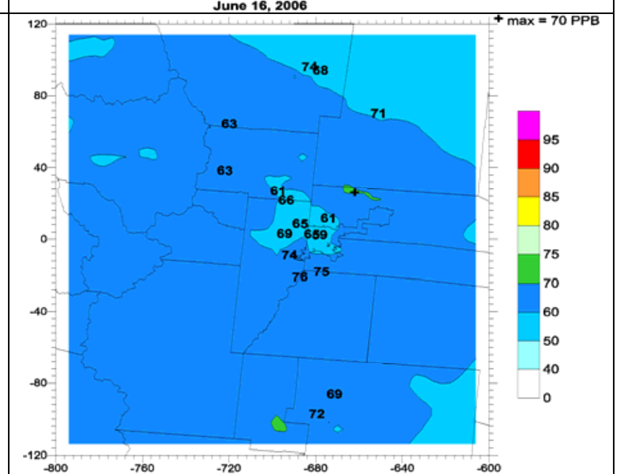

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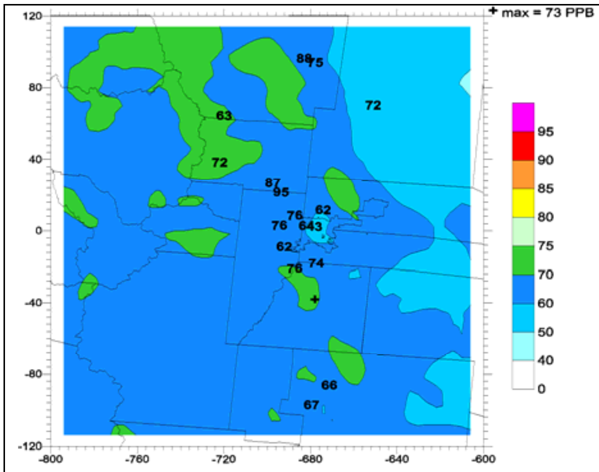

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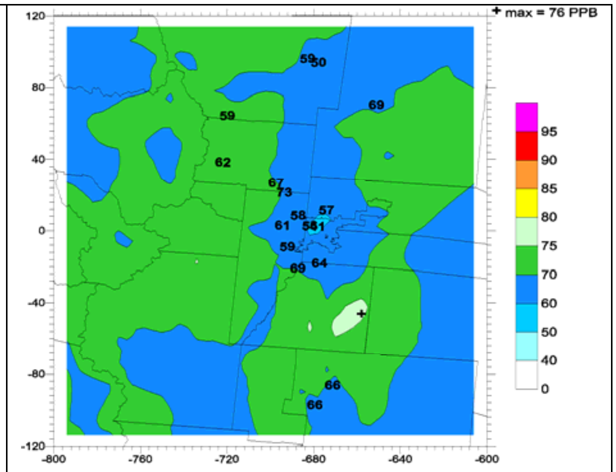

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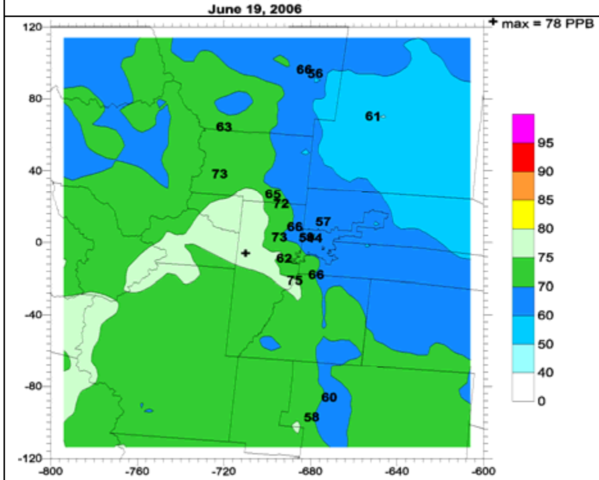

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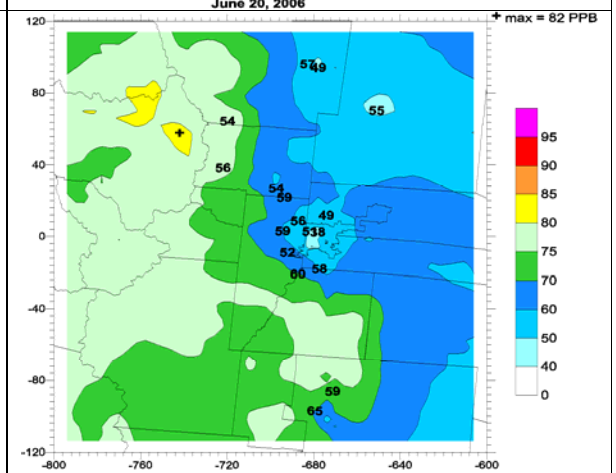

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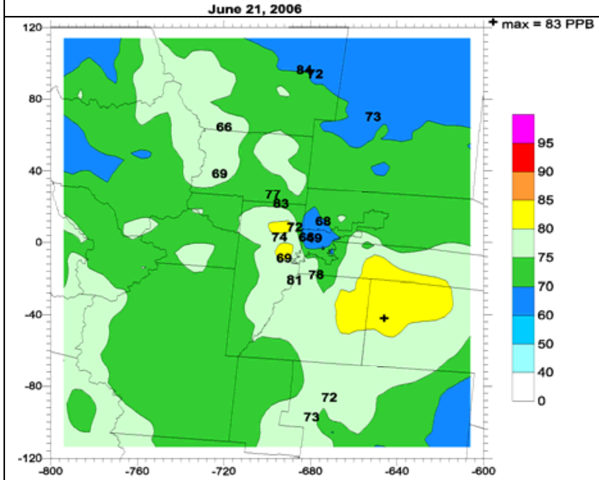

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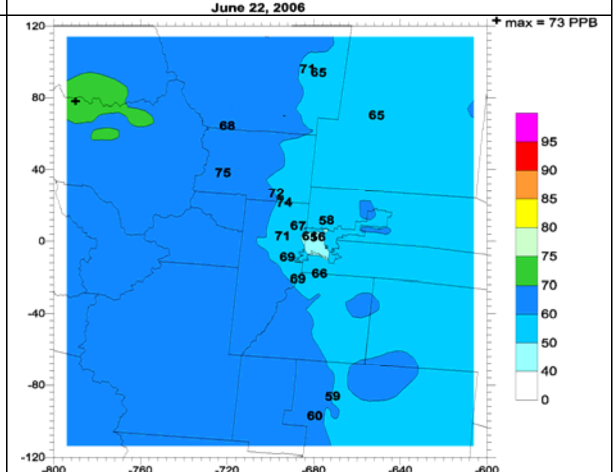

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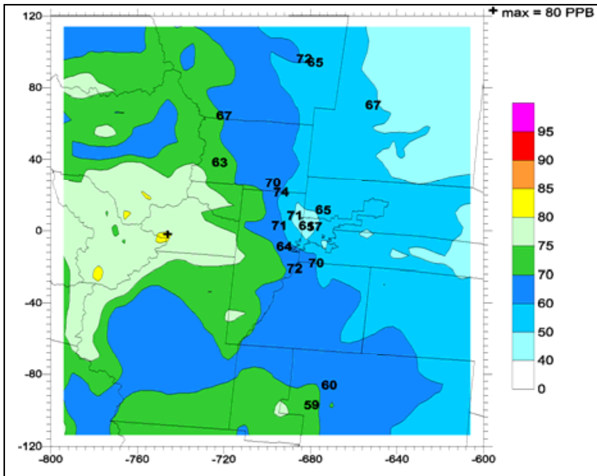

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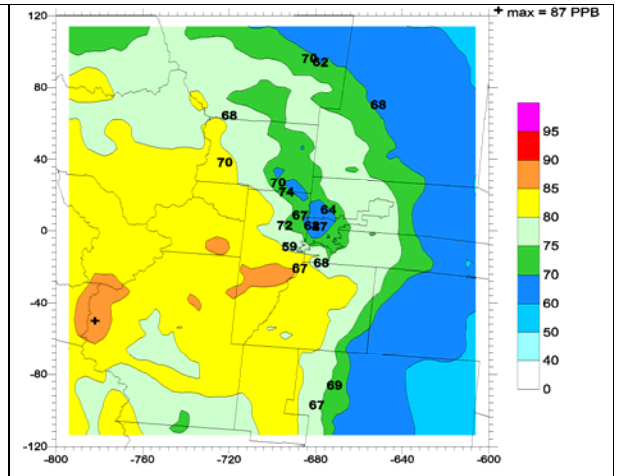

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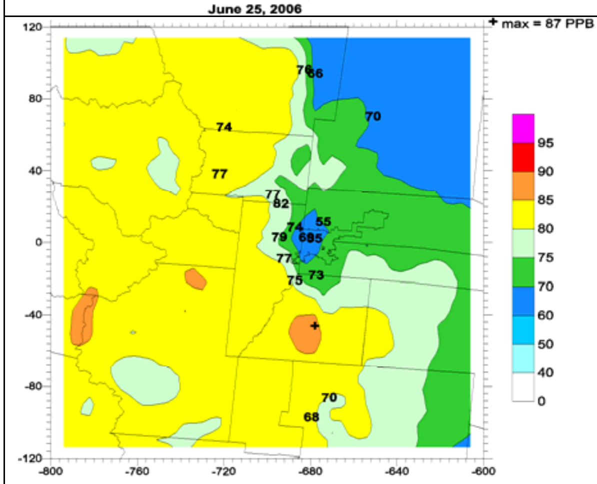

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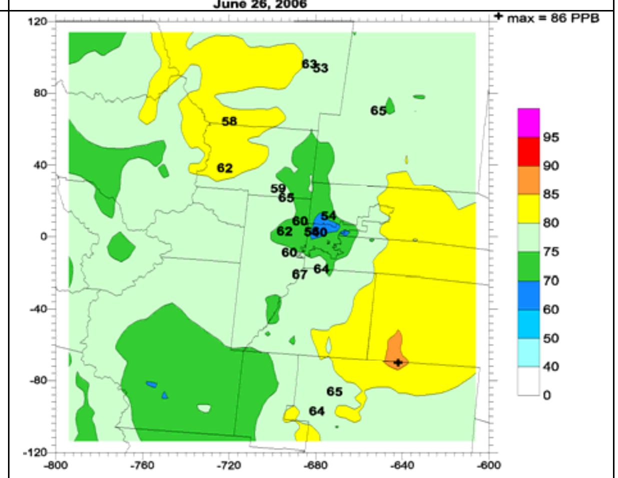

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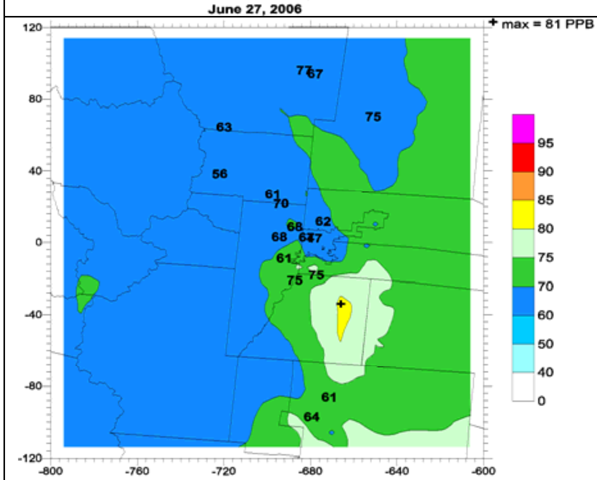

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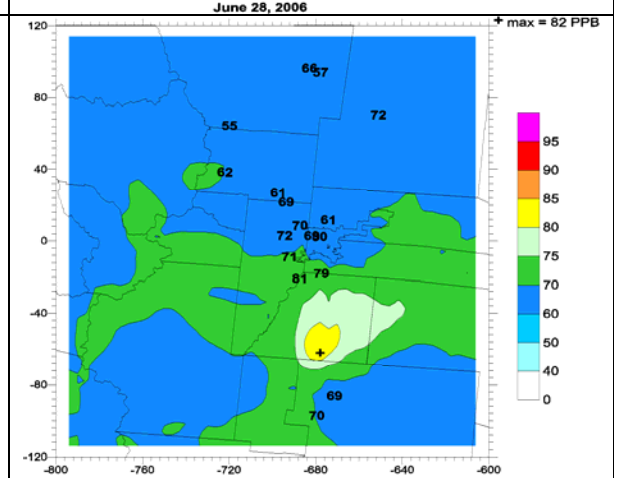

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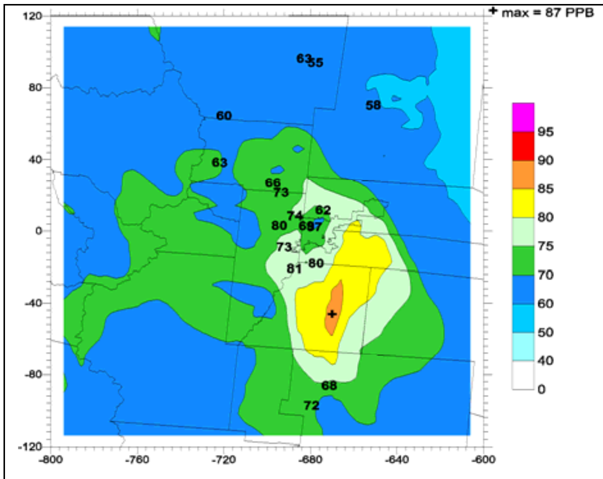

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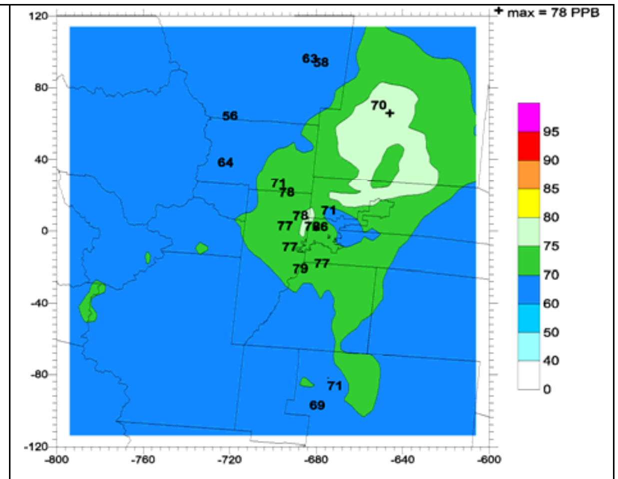

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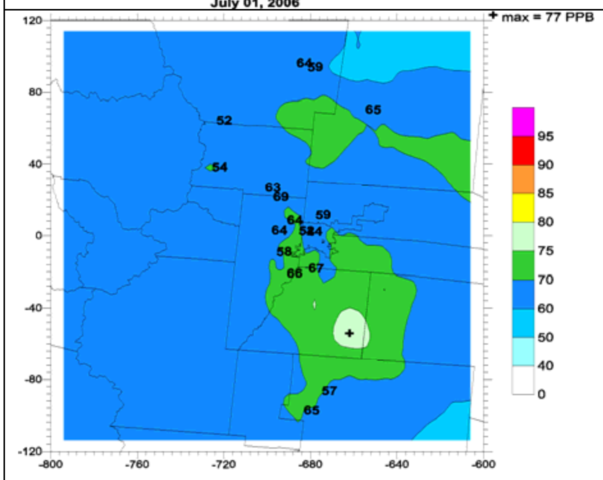

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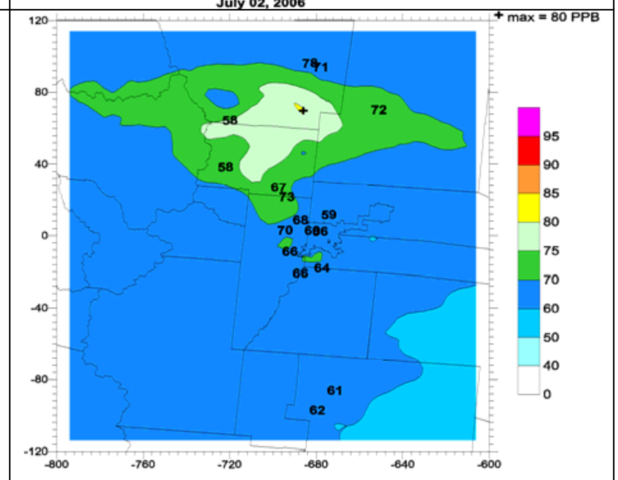

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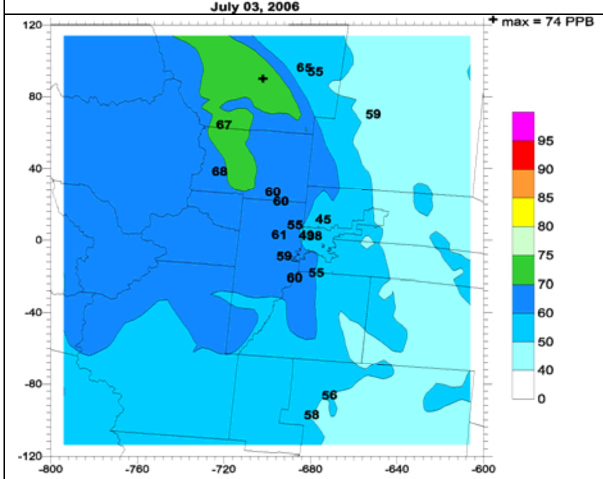

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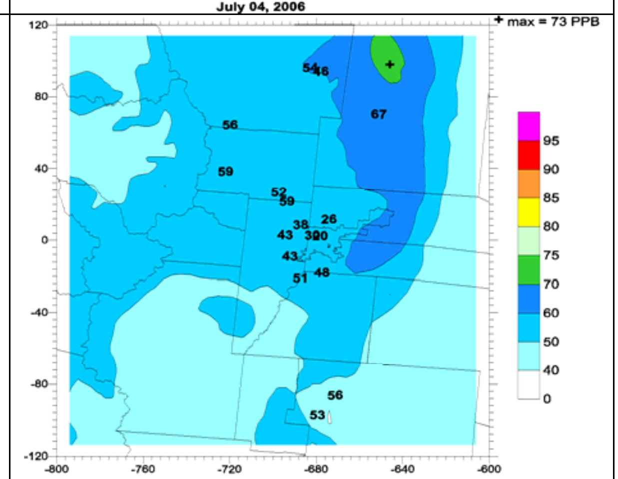

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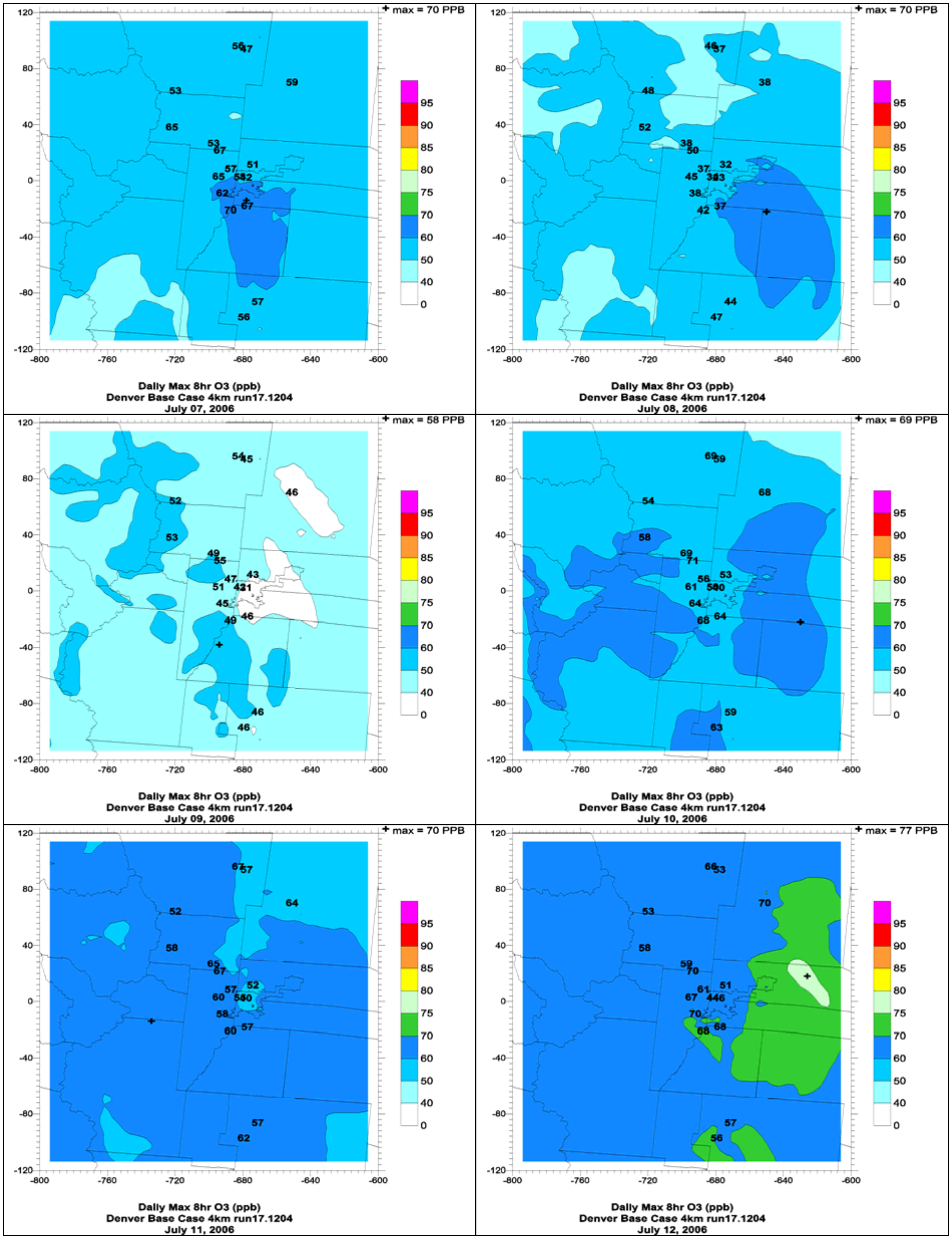
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Daily Max 8hr O3 (ppb)
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+ max = 70 PPB
Daily Max 8hr O3 (ppb)
Denver Base Case 4km run17.1204
July 08, 2006
+ max = 58 PPB
Daily Max 8hr O3 (ppb)
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Daily Max 8hr O3 (ppb)
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+ max = 70 PPB
Daily Max 8hr O3 (ppb)
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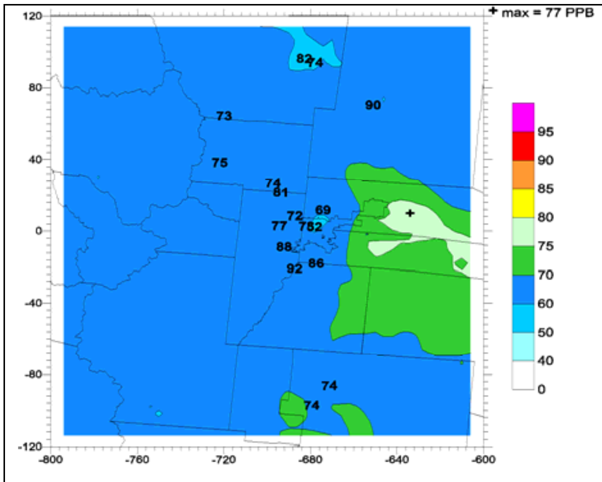

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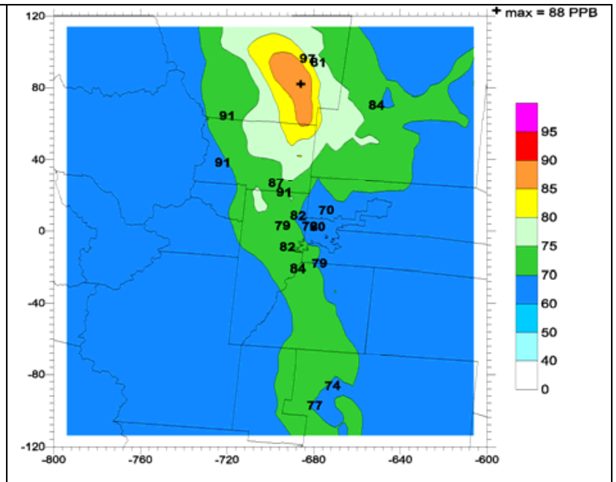

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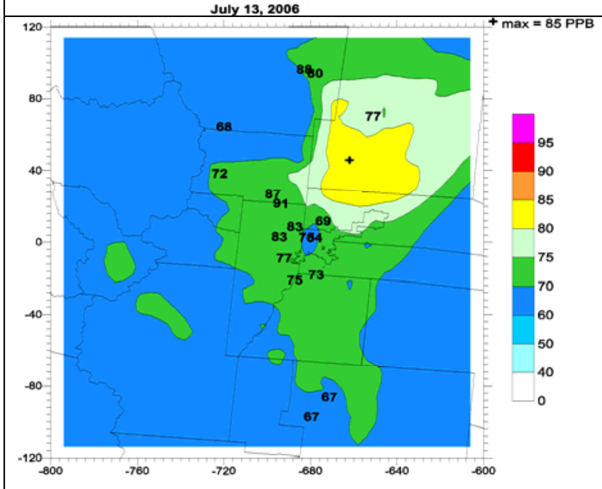

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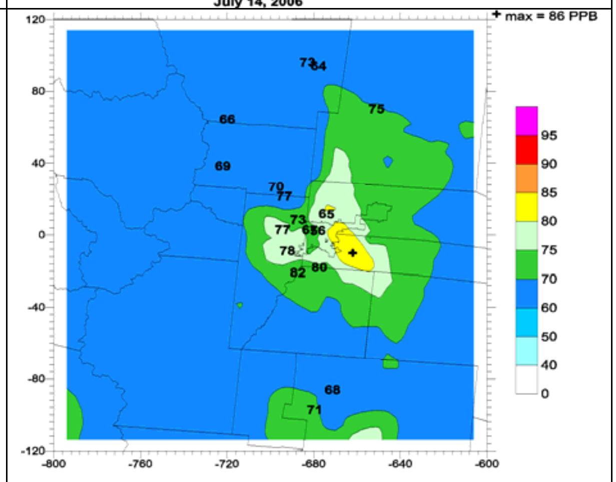

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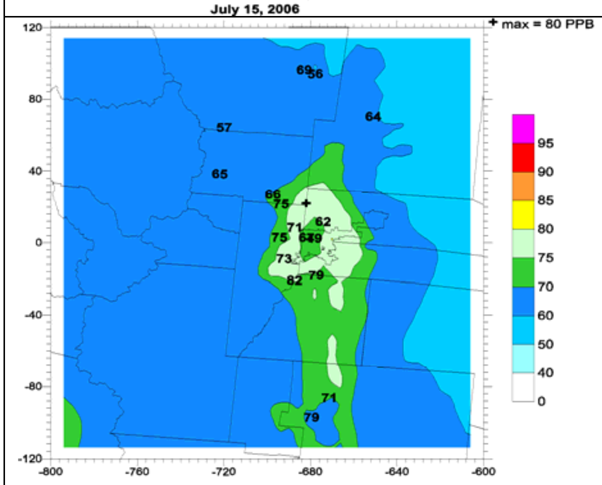

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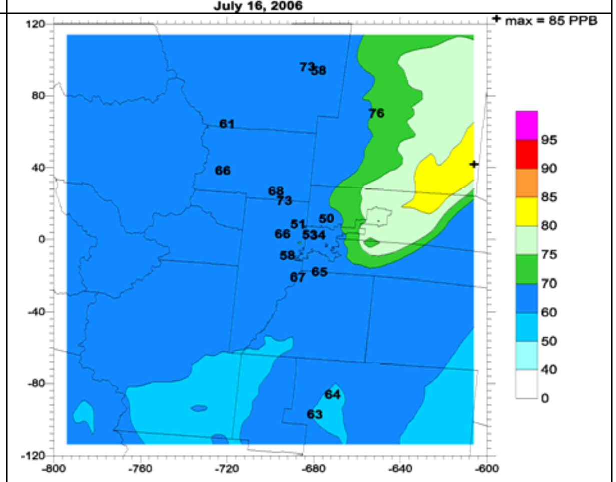

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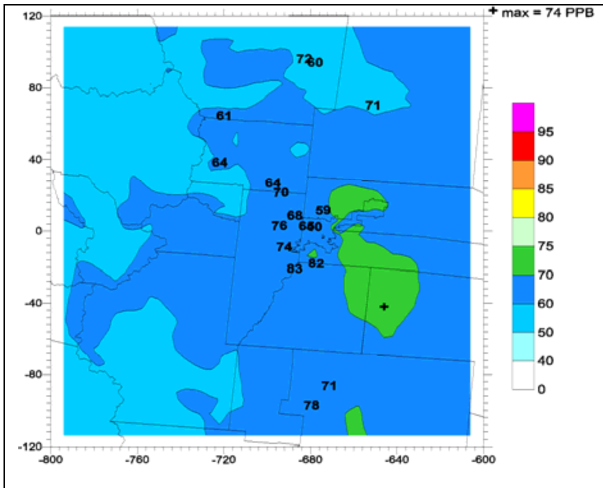

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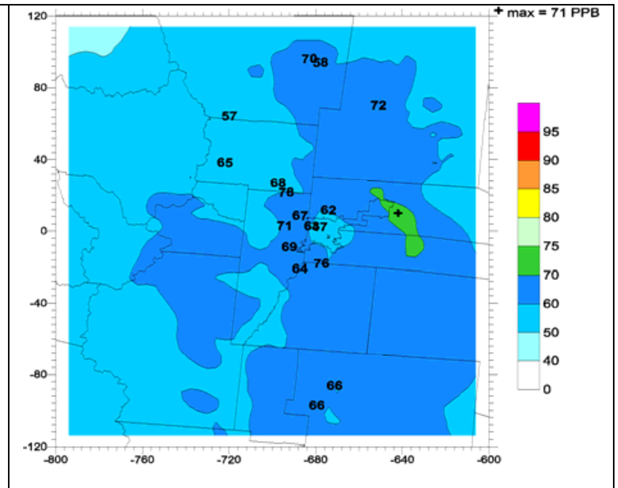

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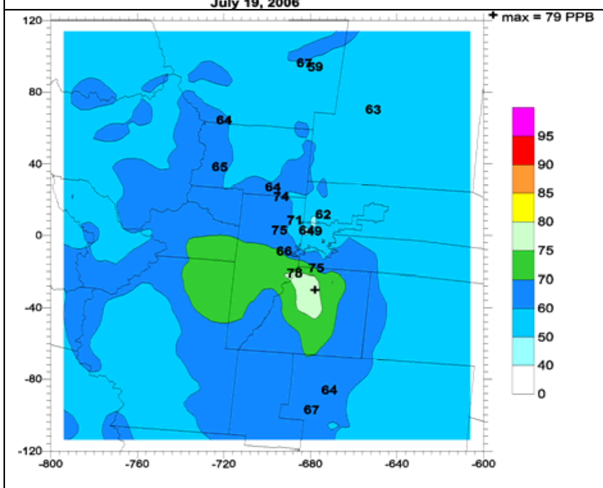

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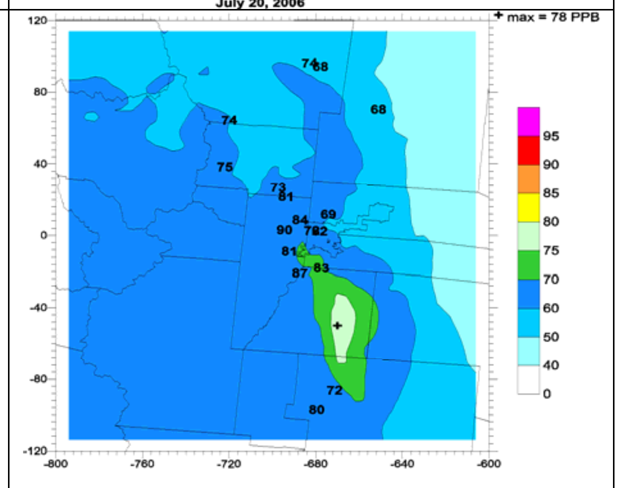

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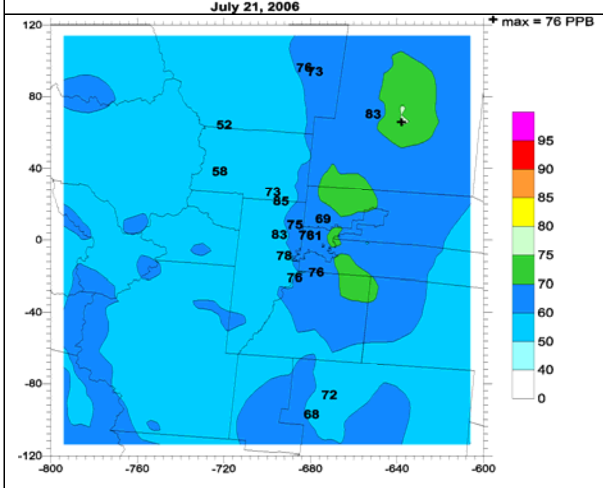

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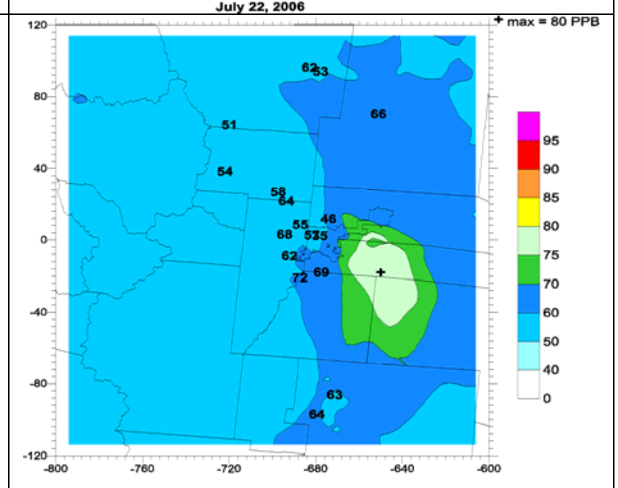

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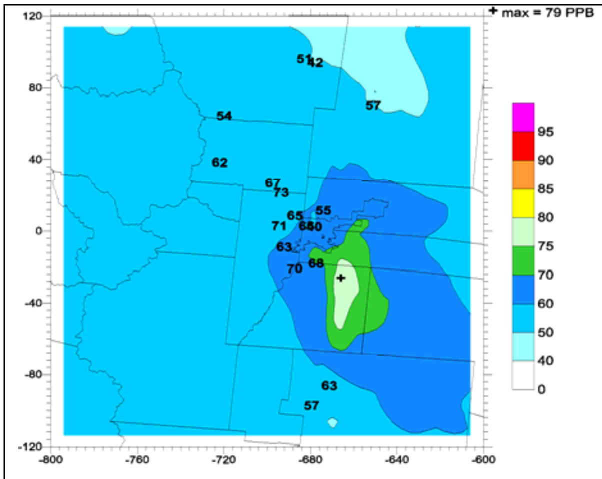

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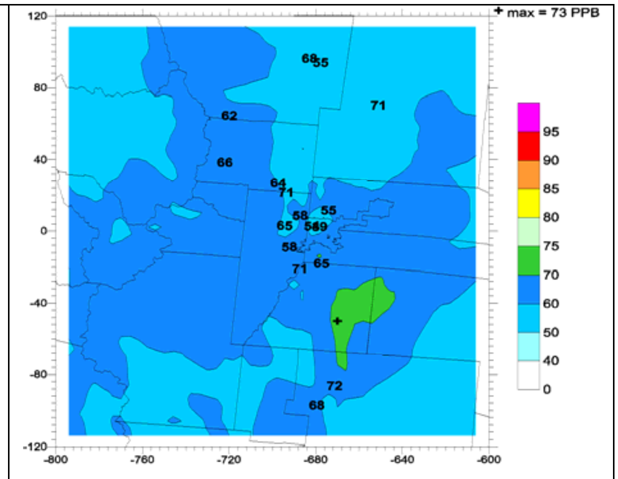

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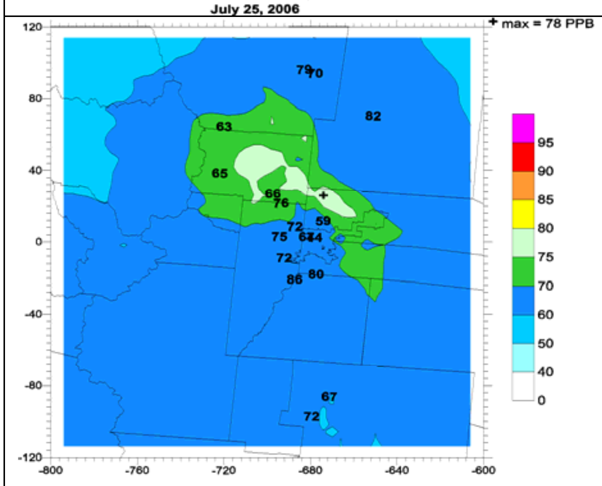
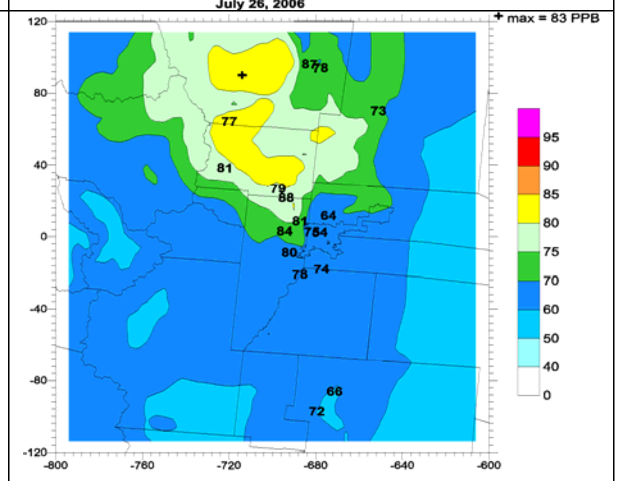
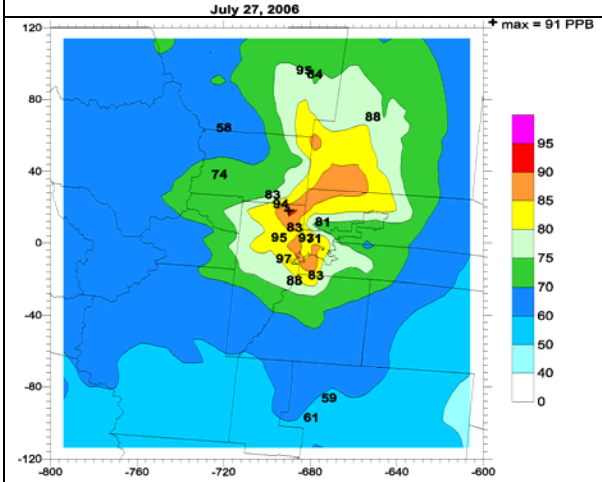
Denver Base Case 4km run17.1204
July 26, 2006



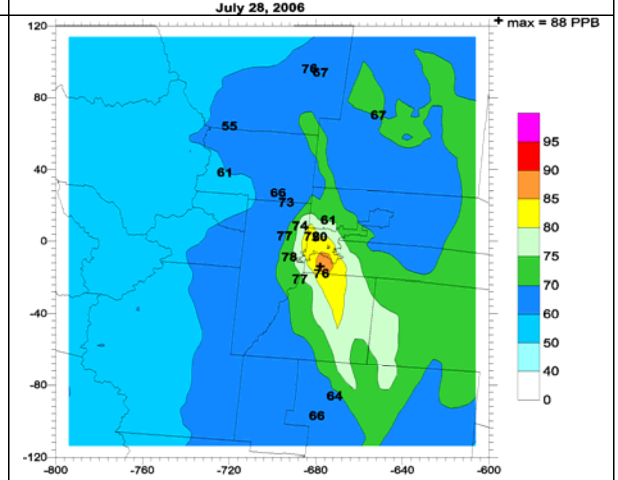
Daily Max 8hr O3 (ppb)
Denver Base Case 4km run17.1204
July 27, 2006



Daily Max 8hr O3 (ppb)
Denver Base Case 4km run17.1204
July 28, 2006



Daily Max 8hr O3 (ppb)
Denver Base Case 4km run17.1204
July 29, 2006



Daily Max 8hr O3 (ppb)
Denver Base Case 4km run17.1204
July 30, 2006